Scalable Inference of Symbolic Adversarial Examples

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We present a novel method for generating symbolic adversarial examples: input regions guaranteed to only contain adversarial examples for the given neural network. These regions can generate real-world adversarial examples as they summarize trillions of adversarial examples.

We theoretically show that computing optimal symbolic adversarial examples is computationally expensive. We present a method for approximating optimal examples in a scalable manner. Our method first selectively uses adversarial attacks to generate a candidate region and then prunes this region with hyperplanes that fit points obtained via specialized sampling. It iterates until arriving at a symbolic adversarial example for which it can prove, via state-of-the-art convex relaxation techniques, that the region only contains adversarial examples. Our experimental results demonstrate that our method is practically effective: it only needs a few thousand attacks to infer symbolic summaries guaranteed to contain $\approx 10^{258}$ adversarial examples.

Additional Key Words and Phrases: Adversarial Examples, Verification, Machine Learning, Abstract Interpretation, Neural Networks

1 INTRODUCTION

Deep neural networks were recently shown to be vulnerable to adversarial attacks: small input perturbations causing the network to misclassify (Szegedy et al. 2013). This has caused an increased interest in designing powerful attacks (Andriushchenko et al. 2019; Athalye et al. 2018; Carlini and Wagner 2017; Croce and Hein 2019; Dong et al. 2018; Goodfellow et al. 2015; Gowal et al. 2019; Madry et al. 2018; Tramèr et al. 2020; Wang et al. 2019; Xiao et al. 2018; Zheng et al. 2019) for generating adversarial examples. However, the practical relevance of these examples remains unclear. This is because these models assume that the examples can be directly supplied to the neural networks. It can happen that these examples when reconstructed in the real-world and observed through a camera are no longer adversarial.

To have any practical utility, adversarial examples need to be robust (Athalye et al. 2018), meaning they should be invariant to changes in the environment such as variations in lighting conditions, or noise in camera perception. Robust examples are therefore more likely to be reproducible in real-world conditions than non-robust ones. One way of demonstrating robustness is by creating large continuous regions containing only adversarial examples. Quantifying the number of examples in the continuous region provides a measure of the degree of robustness of the generated examples.

Continuous regions have other applications beyond robustness: for explaining the source of adversarial examples, e.g., whether certain pixels in an image contribute more to the examples (Ilyas et al. 2019), for runtime monitoring of adversarial examples (Grosse et al. 2017; Liu et al. 2020; Lu et al. 2017), or for training more robust models (Madry et al. 2018). Ideally, we would like to obtain a symbolic summary capturing a set of adversarial examples. The existing approaches for generating adversarial examples are inherently not suitable for generating such summaries. This is because they provide only a single concrete adversarial example as output. Running these attacks
Fig. 1. Symbolic adversarial example for an MNIST convolutional network with 6 layers and 48K neurons. All images in our region are classified as 3 by the network instead of 5.

Our method is non-trivial: we first collect several isolated adversarial examples using existing attacks and then extrapolate them to obtain a large convex region, possibly containing spurious adversarial examples. We then generate samples containing both correctly-classified points and
adversarial examples based on Frank-Wolfe optimization (Frank and Wolfe 1956) and linear programming. We then remove spurious adversarial examples from our extrapolated region by cutting it with linear classifiers learned from the sampled points. The cutting is applied iteratively until we can certify that the region contains only the adversarial examples.

Main Contributions. Our key contributions are:

• The concept of a symbolic adversarial example – a convex region containing a large set of concrete adversarial examples that can be used for creating real-world examples.
• A novel scalable method for generating symbolic adversarial examples, combining specialized sampling, hyperplane cutting, shrinking of spurious regions and state-of-the-art neural network certification techniques.
• A complete end-to-end implementation of our method and a thorough experimental evaluation demonstrating that it can generate symbolic examples containing $10^{265}$ concrete adversarial examples on a CIFAR10 convolutional network, within 5 minutes on average.

2 HARDNESS OF GENERATING SYMBOLIC ADVERSARIAL EXAMPLES

Neural networks are often applied to high-dimensional input domains, such as images and audio, which are particularly vulnerable to adversarial examples, as demonstrated by Gilmer et al. (2018); Khoury and Hadfield-Menell (2018). Therefore, it is crucial that algorithms for creating symbolic adversarial regions scale to high-dimensional inputs. In this work, we focus on a family of algorithms that compute symbolic regions via a greedy approach. Our experimental observations in Section 7 confirm that such algorithms are more scalable and precise than other known alternatives (Gopinath et al. 2019; Zhang et al. 2018) that generate regions by enumerating all paths in the network which are exponential in the number of neurons for ReLU based networks considered in our work. Combining these regions for producing a single convex symbolic region again has exponential complexity in the number of input dimensions. In this section, we provide a theoretical analysis of the complexity of greedily generating optimal (in terms of volume) polyhedral symbolic adversarial examples. Our analysis shows that this has exponential complexity in the number of input dimensions.

Let $C$ be the set of all binary classifiers with continuous decision boundaries that assign labels from $\{-1, 1\}$ to a connected subspace $I$ of $\mathbb{R}^d$. Note that all neural networks with continuous activation functions are in $C$. Let $f \in C$ be a ground-truth binary classifier which we want to approximate using a learning algorithm. The algorithm creates an approximation $c \in C$ of $f$ based on a finite dataset of training samples $\mathcal{D} = \{(x_i, f(x_i))\}_{i=1,...,m}$. Here, the $x_i$’s are drawn from an unknown input probability distribution $P$ on $I$. To simplify analysis, we assume that the approximate classifier $c$ correctly classifies all the points in $\mathcal{D}$. 

Fig. 2. An example neural network decision boundary in the 2D setting (in blue). The green subregion represents a polyhedral underapproximation $P \subseteq \mathcal{A}_c$. 

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We call the region $\mathcal{A}_c = \{ x \in I \mid c(x) \neq f(x) \}$ the adversarial region of $c$. We note that $\mathcal{A}_c$ does not contain any points from $D$. $\mathcal{A}_c$ is usually a disjoint union of connected regions (instead of being a single connected region). Figure 2 shows $\mathcal{A}_c$ (in blue) for a ReLU based neural network. The green region in the figure represents a polyhedral approximation $\mathcal{P} \subseteq \mathcal{A}_c$. Since $\mathcal{P}$ is a polyhedron, it must be contained entirely within one of the connected subregions of $\mathcal{A}_c$. Note that the algorithms developed in this paper can be applied to generate multiple regions $\mathcal{P}$ for each subregion of $\mathcal{A}_c$. However, this is generally computationally prohibitive for neural networks, where many such regions exist. To simplify notation, we use $\mathcal{A}_c$ to refer to the connected subregion containing $\mathcal{P}$ for the remainder of this section.

Our algorithms create $\mathcal{P}$ iteratively by cutting volume away from $I$ until $\mathcal{P} \subseteq \mathcal{A}_c$. i.e., we generate a sequence of polyhedra $\{\mathcal{P}_i\}_{i=0,\ldots,m}$ where $\mathcal{P}_0 = I$ and $\mathcal{P} = \mathcal{P}_m \subseteq \mathcal{A}_c$. Each polyhedron in the sequence is created from the previous one by intersecting it with an additional half-space constraint $h_i : a_i x + b_i \leq 0$ with parameters $a_i \in \mathbb{R}^d, b_i \in \mathbb{R}$. The linear classifier $h_i$ is estimated from a separate dataset $D_i$, sampled using the input distribution $P$ and evaluated using $f$. In order to fit the linear classifiers $h_i$ we require each dataset $D_i$ to contain both positive samples ($x$ such that $f(x) \neq c(x)$) and negative samples ($x$ such that $f(x) = c(x)$).

A positive sample $x$ is correctly classified by $h_i$ if $a_i x + b_i \leq 0$ — that is, $h_i$ keeps it in $\mathcal{P}_i$, and incorrectly classified otherwise. Similarly, a negative sample $x$ is correctly classified by $h_i$ if $a_i x + b_i \geq 0$ — that is, $h_i$ removes it from $\mathcal{P}_i$, and incorrectly classified otherwise. To simplify notations, we assume that samples $x$, for which $a_i x + b_i = 0$ can be regarded as both correctly classified and missclassified. We use the volume ratio $\frac{\text{vol}(\mathcal{P})}{\text{vol}(\mathcal{A}_c)}$ to quantify the effectiveness of our algorithms.

For the remainder of this section, we focus on analyzing the aforementioned family of algorithms under a simplified setting to intuitively demonstrate the inherent hardness of computing symbolic adversarial examples and thereby motivating the need for the methods developed in this paper. We will show that our problem is hard even in this simplified setting; in the more general setting, our problem may be even harder.

We choose a setting where we have an analytic characterization of the decision boundary learned by the model and thus an explicit formula for $\text{vol}(\mathcal{A}_c)$. We choose $\mathcal{A}_c$ to be a $d$-dimensional hyperbox $[0, \sigma]^d$ for some $\sigma \in (0, 1)$ with $d$ decision boundaries. The $i$th decision boundary of our chosen $\mathcal{A}_c$ is $a^\text{best}_i \cdot x + b^\text{best}_i = 0$ with $a^\text{best}_i = e_i$ and $b^\text{best}_i = -\sigma$ for all input dimensions $i \in \{1, \ldots, d\}$, where $e_i$ is the $i$th unit vector. We further assume that $I = [0, 1]^d$ and that points in $D_i$ used for learning $h_i$ are sampled from the uniform distribution on $I$.

We require that for each hyperplane $h_i$, the fraction of volume removed from $\mathcal{A}_c$ by $h_i$ is not more than a chosen $v \in [0, 1]$, i.e., we have $\frac{\text{vol}(h_i \cap \mathcal{A}_c)}{\text{vol}(\mathcal{A}_c)} \geq v$. To ensure this, we enforce that for $i \in \{1, \ldots, m\}$, the classifier associated with $h_i$ picks its slope parameters $a_i$ close to $a^\text{best}_i$ for some input dimension $k(i) \in \{1, \ldots, d\}$. We quantify the distance between $a_i$ and $a^\text{best}_i$ in terms of the cosine similarity $ω_i = \frac{(a_i, a^\text{best}_i)}{||a_i|| \cdot ||a^\text{best}_i||}$. To enforce the closeness, we assume the existence of a chosen lower bound $ω_{\text{min}} \in (0, 1]$ such that $ω_i \geq ω_{\text{min}}$ for all $i \in \{1, \ldots, m\}$. A possible geometric interpretation of these assumptions is that all classifiers are given imprecise information on $a^\text{best}_i$ — the true slopes of the decision boundaries of $\mathcal{A}_c$, in terms of a maximal error angle $α = \arccos(ω_{\text{min}})$ between them and $e_i$, but no information about the biases $b^\text{best}_i$. This is demonstrated in the 2D setting in Figure 3(a).

We formally define the maximal width cut in the $k(i)$th dimension of $\mathcal{A}_c$ by a half-space constraint $h_i$, as the solution of the optimization problem $\max_{x \in \mathcal{A}_c} σ - x[k(i)]$, such that $x$ is missclassified by
with green pluses and red minuses, respectively. In (a), the angle \( \delta \) to this end, we introduce separate error terms \( a \) and quantify how the uncertainty in \( a \) and \( b \) affects the volume cut from \( \mathcal{A}_c \) by the classifier \( h_i \). To this end, we introduce separate error terms \( \delta_i \) and \( \epsilon_i \) for the maximal width cut in the \( \kappa(i)^{th} \) dimension by deviations in \( a_i \) and \( b_i \) from the optimal \( a_{\kappa(i)}^{\text{best}} \) and \( b_{\kappa(i)}^{\text{best}} \), respectively.

To find the worst-case width \( \delta_i \), we search for pairs of points \( (p_1, p_2) \), such that \( p_1, p_2 \in \mathcal{A}_c \) and the property that \( p_2 \) is correctly classified and \( p_1 \) is not. Intuitively, as \( p_1[\kappa(i)] \) approaches 0 and \( p_2[\kappa(i)] \) approaches \( \sigma \), the slope \( a_i \) goes further and further away from the optimal \( e_i \). Since, the cosine similarity between these vectors is lower-bounded, there exists \( p_1^{\text{min}} \) and \( p_2^{\text{max}} \) such that \( p_2^{\text{max}}[\kappa(i)] - p_1^{\text{min}}[\kappa(i)] \) is maximal. One can look at this difference as the maximum width allowed to be additionally cut in the \( \kappa(i)^{th} \) dimension, given that we have ensured some \( p_2^{\text{max}} \) close to the decision boundary is correctly classified. Following this intuition, we formally define:

\[
\delta_i = \max_{p_1, p_2 \in \mathcal{A}_c, \ a_i \in \mathbb{R}^d, \ b_i \in \mathbb{R}} \quad p_2[\kappa(i)] - p_1[\kappa(i)] \\
\text{subject to} \\
a_i \cdot p_1 + b_i \geq 0, \\
a_i \cdot p_2 + b_i \leq 0, \\
\omega_i \geq \omega_{\text{min}}.
\]

The next lemma shows that the optimization problem defined by Equation 1 is independent of \( b_i \), as required by our intuitive definition of \( \delta_i \), and provides its analytical solution:

**Lemma 2.1.** For all \( i \in \{1, \ldots, m\} \), \( \delta_i \) is given by the formula

\[
\delta_i = \sigma \frac{\sqrt{(d-1)(1-\omega_{\text{min}}^2)}}{\omega_{\text{min}}}
\]

and therefore independent of \( b_i \).

**Proof.** Let \((p_1^{\text{min}}, p_2^{\text{max}}, a_i^{\text{max}}, b_i^{\text{max}})\) be an assignment of values to \( p_1 \), \( p_2 \), \( a_i \) and \( b_i \), respectively, that together maximize \( \delta_i \). Then, the assignment \((p_1^{\text{min}} + c \cdot e_{\kappa(i)}, p_2^{\text{max}} + c \cdot e_{\kappa(i)}, a_i^{\text{max}}, b_i^{\text{max}} - c \cdot a_i^{\text{min}}[\kappa(i)])\)
also maximizes $\delta_i$ for all $c \in \mathbb{R}$ — that is, the problem is translation invariant in the $\kappa(i)\text{th}$ dimension. Additionally, the hyperplane $a_i \cdot x + b_i = 0$ passes through the points $p_1^\min$ and $p_2^\max$ that maximize $\delta_i$, since otherwise one can choose smaller $p_1[\kappa(i)]$ and bigger $p_2[\kappa(i)]$ until they do, while also improving the objective. Therefore, we can reformulate Equation 1 in the equivalent form:

$$
\begin{align*}
\delta_i &= \maximize_{p_1, p_2 \in A_c, \ a_i \in \mathbb{R}^d} \ p_2[\kappa(i)] - p_1[\kappa(i)] \\
\text{subject to} \quad a_i \cdot (p_2 - p_1) &= 0, \\
&\quad a_i[\kappa(i)] \geq \omega_{\min}, \\
&\quad \|a_i\|_2 = 1,
\end{align*}
$$

(2)

where the last two constraints come from the definition of $\omega_{\min}$. We can rewrite $a_i \cdot (p_2 - p_1) = 0$ as

$$
p_2[\kappa(i)] - p_1[\kappa(i)] = \frac{\sum_{j \in \{1, \ldots, d\}\setminus\{\kappa(i)\}} a_i[j] \cdot (p_1[j] - p_2[j])}{a_i[\kappa(i)]}.
$$

Since $p_1, p_2 \in A_c$, we know $p_1[j] - p_2[j] \leq \sigma$ for all input dimensions $j \in \{1, \ldots, d\} \setminus \{\kappa(i)\}$. The bound is tight and can be achieved for $p_1[j] = \sigma$ and $p_2[j] = 0$, for all input dimensions $j \in \{1, \ldots, d\} \setminus \{\kappa(i)\}$ independently. Setting $S = \sum_{j \in \{1, \ldots, d\}\setminus\{\kappa(i)\}} a_i[j]$, we can rewrite Equation 2 as follows:

$$
\delta_i = \maximize_{a_i \in \mathbb{R}^d} \frac{S \cdot \sigma}{a_i[\kappa(i)]} \\
\text{subject to} \quad a_i[\kappa(i)] \geq \omega_{\min}, \\
&\quad \|a_i\|_2 = 1
$$

(3)

One can use Lagrangian multipliers to demonstrate that under the conditions in Equation 3, $S$ is maximized when $a_i[\kappa(i)] = \omega_{\min}$ and all other dimension of $a_i$ are equal to $\sqrt{1 - \sigma^2 / d - 1}$. Therefore, $\delta_i$ is also maximized under the same conditions and it is given by the formula given in Lemma 2.1. □

Lemma 2.1 demonstrates that $\delta_i$ is independent of $i$. For the rest of this section, we refer to its value as simply $\delta$ to simplify the notation.

Let $\epsilon_i$ be the worst-case width cut from the $\kappa(i)\text{th}$ dimension of $A_c$, for the simple case when $a_i$ is optimal ($\omega_{\min} = 1$). Since $h_i$ correctly classifies all samples in $D_i$, $\epsilon_i$ is given by:

$$
\epsilon_i = \maximize_{p \in D_i} \quad \sigma - p[\kappa(i)] \\
\text{subject to} \quad p \in A_c.
$$

(4)

Next, we show that the worst-case width cut, in the general case $\omega_{\min} \leq 1$, is given by the sum of $\delta$ and $\epsilon_i$.

**Lemma 2.2.** The worst-case width cut from the $\kappa(i)\text{th}$ dimension of $A_c$ by the classifier $h_i$ is given by the sum of $\delta$ and $\epsilon_i$.

**Proof.** Due to the translational invariance property, Equation 1’s solution remains the same if we additionally require $p_2[\kappa(i)] = \sigma - \epsilon_i$. From Equation 1, we know $p_1[\kappa(i)] \geq p_2[\kappa(i)] - \delta_i$. Therefore, $p_1[\kappa(i)] \geq \sigma - \delta_i - \epsilon_i$. In other words, the minimal width that cannot be removed from the $\kappa(i)\text{th}$ dimension of $A_c$, provided $p$ is correctly classified is $\sigma - \delta_i - \epsilon_i$. Therefore, the worst-case width that can be cut is at most $\delta_i + \epsilon_i$. This bound is tight, as the equality is achieved for the case, where $p$ has all of its coordinates except the $\kappa(i)\text{th}$ equal to 0. □
Next, we introduce Lemma 2.3, which quantifies the expected number of samples needed in $D_i$ to guarantee $\frac{\text{vol}(h_i \cap A_c)}{\text{vol}(A_c)} \geq v$ for a chosen $v \in [0, \frac{\sigma - \delta}{\sigma}]$. Note that $v$ cannot be more than $\frac{\sigma - \delta}{\sigma}$, as we cannot guarantee to preserve more than $\sigma - \delta$ of the width in the $\kappa(i)$th dimension under any $\varepsilon_i \in [0, \sigma]$ owing to the uncertainty in the estimation of slopes $a_i$.

**Lemma 2.3.** For $v \in [0, \frac{\sigma - \delta}{\sigma}]$ and $i \in \{1, \ldots, m\}$, the expected number of samples $n_s = \mathbb{E}[|D_i|]$ until $\frac{\text{vol}(h_i \cap A_c)}{\text{vol}(A_c)} \geq v$ holds is $n_s = \frac{1}{\sigma^d(1 - \frac{2}{n} - v)}$ in the worst case.

**Proof.** We look at the probability of a point $p$ to be contained $D_i$, such that $p[\kappa(i)] \geq \sigma - \varepsilon$ for a given $\varepsilon \in [0, \sigma]$. When such point exists, we know $\varepsilon_i \leq \varepsilon$. That is, for a given $\varepsilon \in [0, \sigma]$, we are interested in the probability of sampling a point in the hyperrectangle $\prod_{i=1}^d \{s_i, \sigma\}$ with $s_i = 0$ for all dimensions $i \in \{1, \ldots, d\} \setminus \{\kappa(i)\}$ and $s_\kappa(i) = \sigma - \varepsilon$. Since we sample $D_i$ from the uniform distribution on $I$, the probability is given by the ratio of the volumes of $I$ and the hyperrectangle, which has volume $\sigma^d - \varepsilon$. Therefore, the probability of sampling $p$ is $\sigma^d - \varepsilon$ and the expected number of samples $n_s$ to get such point $p$, which is a geometrically distributed random variable, is $\frac{1}{\sigma^d - \varepsilon}$.

From Lemma 2.2, we know that $\frac{\text{vol}(h_i \cap A_c)}{\text{vol}(A_c)} \geq \frac{\sigma - \varepsilon - \delta}{\sigma} \geq \frac{\sigma - \varepsilon - \delta}{\sigma}$, since at least $\sigma - \varepsilon - \delta$ portion of the width of the $\kappa(i)$th dimension of $A_c$ cannot be removed by $h_i$. Therefore, if we choose $\varepsilon = \sigma - \delta - \varepsilon \delta$, we can guarantee $\frac{\text{vol}(h_i \cap A_c)}{\text{vol}(A_c)} \geq v$. Plugging our choice of $\varepsilon$ we conclude that $n_s = \frac{1}{\sigma^d(1 - \frac{2}{n} - v)}$ is the worst-case expected number of points we need to sample to obtain $h_i$, such that $\frac{\text{vol}(h_i \cap A_c)}{\text{vol}(A_c)} \geq v$ holds.

Next, we generalize this result to the full region $P$:

**Theorem 2.4.** For all $V \in [0, \left(\frac{\sigma - \delta}{\sigma}\right)^m]$ the expected number of samples $n_s = \mathbb{E}[|D_i|]$, such that $\frac{\text{vol}(P)}{\text{vol}(A_c)} \geq V$ holds is at most $n_s = \frac{1}{\sigma^d(1 - \frac{2}{n} - V^n)}$.

**Proof.** Applying Lemma 2.3 with $v = V \frac{1}{n}$ for all half-space constraints in $P$ and multiplying the individual volume bounds together we obtain the required result.

In the next theorem, we consider the even simpler setting of $\omega_{\text{min}} = 1$ — that is the setting in which our binary classifiers only considers axis-aligned half-space constraints. We also assume the datasets $D_i$ are collected uniformly at random from $P_i$. We demonstrate that ensuring that $P$’s volume shrinks by certain amount becomes more difficult as $P$ approaches $A_c$:

**Definition 2.5.** For all $i \in \{0, \ldots, m\}$ corresponding to the polyhedra sequence $P_i$, and all input dimensions $k \in \{1, \ldots, d\}$, we call $u^k_{\pi_i} = \max_{x \in P_i}[\kappa(k)]$ the upper bound of dimension $k$ in $P_i$.

**Theorem 2.6.** For all $i \in \{0, \ldots, m - 1\}$ corresponding to the polyhedra sequence $P_i$, for which $u^k_{\pi_i} > \sigma$ and for all $v \in (0, 1]$, the expected number of samples $n_s = \mathbb{E}[|D_{i+1}|]$ needed to create $h_{i+1}$ such that $\frac{u^{(i+1) - \sigma}}{u^k_{\pi_i} - \sigma} \leq v$ holds is $n_s = \frac{u^{(i+1) - \sigma}}{(u^k_{\pi_i} - \sigma) \cdot v}$. Here, the quantity $\frac{u^{(i+1) - \sigma}}{u^k_{\pi_i} - \sigma}$ quantifies the shrinking in the $\kappa(i + 1)$th dimension in step $i + 1$.

**Proof.** We show a depiction of our proof of Theorem 2.6 in the 2D setting in Figure 3(b). We consider $\kappa(i+1)$th dimension of $A_c$ (the horizontal dimension in Figure 3(b)). Similarly to Lemma 2.3, we quantify the probability that there exists a negative sample $p \in D_b$ such that its $\kappa(i + 1)$th
dimension has a coordinate in $[\sigma, (u_i^{k(i+1)} - \sigma) \cdot v + \sigma]$. Figure 3(b) depicts the region of possible locations for $p$ as an orange rectangle. We know that if such point $p$ exists, due to the assumption $h_{i+1}$ correctly classifies all samples the condition $\frac{u_i^{k(i+1)} - \sigma}{u_i^{k(i+1)} - \sigma} \leq v$ holds. Since $D_{i+1}$ is uniformly sampled from $P_I$ the probability of sampling such $p$ is given by the ratio of the volumes of the orange region and $P_I$. This probability is $\frac{u_i^{k(i+1)} - \sigma \cdot v}{u_i^{k(i+1)} - \sigma \cdot v}$. The number of samples need for $p$ to exist is geometrically distributed and its expectation is given by $n_s = \frac{u_i^{k(i+1)}}{(u_i^{k(i+1)} - \sigma) \cdot v} < \infty$. □

3 PRACTICAL IMPLICATIONS OF OUR THEORETICAL RESULTS

We next discuss the impact of our theoretical results in the previous section on the design of our algorithms. Theorem 2.4 demonstrates that despite our simplifying assumptions it is computationally expensive to create $P$ for high values of $d$ or $V$. It can also be seen that small inaccuracies in the estimated half-space constraint slopes can lead to big portions of the volume being cut. In particular, we see that the quantity $(\frac{\sigma - \delta}{\sigma})^n$ acts like an upper bound on the volume of $A_c$ that can be guaranteed to be kept. For example with $d = m = 10$, and a slope difference of only up to $4^\circ$, the upper bound on the volume guaranteed to be kept is $V \approx 0.9$. For $d = m = 100$ and the same upper bound on the volume, the maximum slope difference allowed is only $\approx 0.12^\circ$. Last but not least, we see that the algorithm is particularly sensitive to $V$ especially in high dimensions – e.g. for $d = m = 100$, $\sigma = 0.8$, $\frac{\sigma - \delta}{\sigma} = 1$ increasing $V$ from 0.9 to 0.95 doubles the number of samples required at each iteration from $\approx 4.7 \times 10^{12}$ to $\approx 9.6 \times 10^{12}$. We further note that the above results assume that there is an exact procedure to determine whether a given region is adversarial. Exact verifiers for neural networks do not scale on the sizes of networks considered in our experiments, therefore we actually use inexact verifiers in our algorithms for scalability which can make the problem even harder. Overall, for the general case encountered in our experiments, where $A_c$ can be an arbitrary connected shape and inexact verifiers are used, the complexity of sampling would be at least as hard as our results.

Since computing optimal regions is computationally expensive, we use heuristics to preserve as much of $A_c$ as possible in our algorithms presented in Section 6. In Theorem 2.4, $n_s$ is inversely proportional to the quantity $\sigma^d$ which suggests that the effort of constructing a precise $P$ is less when the volume of $A_c$ is close to that of $I$. Therefore, we start with an input region $I$ such that the ratio $\frac{\text{vol}(A_c)}{\text{vol}(I)}$ is not too low by estimating tight bounding boxes around $A_c$ before initiating the half-space generation portion of our algorithm (Section 6.1). As per Theorem 2.4, the amount of incorrectly removed volume grows with the angle between the hyperplane $h_i$ and the decision boundary, our sampling procedure in Section 6.4 employs heuristics so this angle is small.

From Theorem 2.6 for a constant $v$ it follows that $\lim_{u_i^{k(i+1)} \to \sigma} n_s = \infty$. Therefore, with each new half-space it becomes harder and harder for a general sampling algorithm to progress. Another way to look at Theorem 2.6 is that for a constant number of samples $n_s$ the guaranteed volume removed from $P_I$ goes to 0 as $i \to \infty$. This theoretical prediction is consistent with what we observe in practice, where our algorithm sometimes will take a lot of iterations to converge. In Section 6.6, we propose a shrinking procedure to deal with this issue.

4 BACKGROUND

We now discuss necessary methods which we leverage in the remainder of the paper. In this paper, we focus on ReLU based neural networks. We note that our concepts can also be extended to networks with other activations such as sigmoid and tanh. We consider neural networks with $l$
layers $f_i$ of the form $f_i(x) = \max(0, A_i \cdot x + b_i)$ for $i \in \{1, \ldots, l - 1\}$ and $f_l(x) = A_l \cdot x + b_l$. The neural network $f$ is the composition of those layers: $f = f_l \circ \cdots \circ f_0$. If we denote by $z_{i,j}^r$, the input to the $j$-th ReLU activation in layer $i$ and by $z_{i,j}^a$ the corresponding ReLU output, we can represent the neural network as the system of constraints

$$
z_{i,j}^a = [b_i]_j + \sum_{k=1}^{n_{i-1}} [A_i]_{j,k} \cdot z_{i-1,k}^r,
$$

$$
z_{i,j}^r = \max(0, z_{i,j}^a).
$$

Here, $z_{0,j}^r$ describes the $j$-th input activation. We call the two types of constraints affine and ReLU constraints, respectively. Let $n_0$ be the number of inputs to the network, if our inputs $z_{0,j}^r$ are points of a polyhedron $P \subseteq \mathbb{R}^n_0$, an adversarial class $y_t$ has the highest score on all inputs in $P$ if $\min(z_{l,y_t}^a - z_{l,y_t}^a) > 0$ for all $y \in \{1, \ldots, n_l\} \setminus \{y_t\}$ with respect to all constraints. Note that $\{1, \ldots, n_l\} \setminus \{y_t\}$ includes the true class $y_t$. Our goal in this paper will be to find the polyhedron $P$ for which this is true.

**Linear approximations of ReLU.** As reasoning about neural network constraints directly is often intractable, given bounds $l_{i,j} \leq z_{i,j}^a \leq u_{i,j}$, the triangle approximation (Ehlers 2017) relaxes the ReLU constraints such that all involved inequalities are linear:

$$
z_{i,j}^r \geq z_{i,j}^a, \quad z_{i,j}^r \geq 0,
$$

$$
z_{i,j}^r \leq \lambda_{i,j} \cdot z_{i,j}^a + \mu_{i,j}.
$$

Figure 4 (a) visualizes the triangle approximation. Here, $\lambda_{i,j} = u_{i,j}/(u_{i,j} - l_{i,j})$ and $\mu_{i,j} = -l_{i,j} \cdot u_{i,j}/(u_{i,j} - l_{i,j})$ are selected such that this set of constraints describes the convex hull of the constraints obtained from the two branches of ReLU $\{l_{i,j} \leq z_{i,j}^a \leq u_{i,j}, z_{i,j}^a \geq 0, z_{i,j}^r = z_{i,j}^a\}$ and $\{l_{i,j} \leq z_{i,j}^a \leq u_{i,j}, z_{i,j}^a \leq 0, z_{i,j}^r = 0\}$, in the $(z_{i,j}^a, z_{i,j}^r)$-plane. We can obtain bounds $l_{i,j}$ and $u_{i,j}$ by optimizing each component of $z_{i,j}^a$ according to the previously determined constraints for layers 0, $\ldots$, $l$. 

Fig. 4. Convex approximations for the ReLU function: (a) shows the triangle approximation (Ehlers 2017) with the minimum area in the input-output plane, (b) and (c) show the two convex approximations used in DeepPoly (Singh et al. 2019). In the figure, $\lambda_{i,j} = u_{i,j}/(u_{i,j} - l_{i,j})$ and $\mu_{i,j} = -l_{i,j} \cdot u_{i,j}/(u_{i,j} - l_{i,j})$. 

We now provide an overview of our approach for generating symbolic adversarial regions. The work of Singh et al. (2019) for verification. For the rest of the paper, we refer to either abstract or concrete value of $\min\{z^a_{l,y}, z^s_{l,y}\}$ for each hyperplane. The process stops when the candidate region bounded by these hyperplanes separating the two categories. Multiple hyperplanes uses alongside the initial adversarial examples to fit a hyperplane (dashed black line in Figure 5(b)), separating the two categories. Multiple hyperplanes $h_1$ are fitted by collecting new counterexamples for each hyperplane. The process stops when the candidate region bounded by these hyperplanes.

**LP objective.** If we replace the original ReLU constraints by their triangle approximation, the value of $\min\{z^a_{l,y}, z^s_{l,y}\}$ can at most decrease. Therefore, if it is still larger than 0 even with the relaxed constraints, we know that this is also true with the original constraints. The DeepPoly approximation (Singh et al. 2019) further relaxes the triangle approximation by keeping only one of the lower bounds on each variable $z^a_{l,y}$. It picks either $z^a_{l,y} \geq z^s_{l,y}$ or $z^a_{l,y} \geq 0$, whichever minimizes the area of the resulting triangle in the $(z^a_{l,y}, z^s_{l,y})$-plane. Figure 4(b) and (c) show the two convex relaxations used in DeepPoly. Both the triangle approximation and the DeepPoly approximation lead to linear constraints that can be used as part of linear programming (LP) problems.

We call $O(P) = \min\{z^a_{l,y}, z^s_{l,y}\}$ where $y \in \{1, \ldots, n_l\} \setminus \{y_l\}$ computed with respect to the polyhedron $P$ defining the set of inputs, affine network constraints and the linear relaxations of the ReLU as the LP objective.

**Frank-Wolfe optimization.** In addition to LP, our approach also relies on the Frank-Wolfe optimization algorithm (Frank and Wolfe 1956). The algorithm finds a series $x_1, \ldots, x_k$ of approximations to the solution of an optimization problem $\min_{x \in \mathcal{D}} f(x)$ for compact convex $\mathcal{D}$. Here $f$ is a convex, differentiable real-valued function. The approximations are related by $x_{i+1} = x_i + \gamma_i \cdot (s_i - x_i)$. Let us consider the candidate region $P_i$ generated after the $i^{th}$ iteration of our algorithm. Concrete counterexamples are points $x \in P_i$ for which the expression $f(x_i)_{y} - [f(x)]_y$ evaluates to a negative number for some class $y \in \{1, \ldots, n_l\} \setminus \{y_l\}$. In the case of binary classification, these are just examples that are classified correctly.

Exact verifiers (Katz et al. 2017; Tjeng et al. 2019) for verifying whether the region computed by our algorithm contains only adversarial examples do not scale for the network sizes considered in our experiments. Therefore we use inexact verifiers for scalability, which have false positives meaning they may fail to verify the region $P_i$ as adversarial even though it is adversarial. Abstract counterexamples are points in $P_i$ that are either concrete counterexamples or those that prevent us from verifying (using our inexact verifier) that the entire $P_i$ contains only adversarial examples. Formally, abstract counterexamples are points in $P_i$ for which minimizing the expression $z^a_{l,y} - z^s_{l,y}$ for some class $y \in \{1, \ldots, n_l\} \setminus \{y_l\}$ with respect to $P_i$ evaluates to a negative number using our inexact verifier. In this paper, we use either the triangle based LP verifier (Ehlers 2017) or DeepPoly (Singh et al. 2019) for verification. For the rest of the paper, we refer to either abstract or concrete counterexamples just as counterexamples.

Our algorithm first collects adversarial examples and computes an initial box region around them (dashed blue square in Figure 5(a)). Next, the algorithm collects counterexamples, which it uses alongside the initial adversarial examples to fit a hyperplane (dashed black line in Figure 5(b)), separating the two categories. Multiple hyperplanes $h_1$ are fitted by collecting new counterexamples for each hyperplane. The process stops when the candidate region bounded by these hyperplanes.
is either proven, via standard neural network verification techniques, to contain only adversarial examples, or alternatively, a predetermined maximal number of hyperplanes is reached. In the latter case, the region is further shrunk until it is proven to contain only adversarial examples. Figure 5(c) depicts the shrinking process by which the violet-shaded polygon is shrunk to obtain the red-shaded polygon.

5.1 Computing an Initial Region
The computation of the initial box region $P_0$ is based on collecting adversarial examples. In principle, any algorithm that produces adversarial examples can be used. We use both the Frank-Wolfe optimization algorithm outlined in Section 4, as well as standard PGD attacks (Madry et al. 2018). Having obtained these samples, we fit a box around them. We do so by finding the minimum and maximum of each input space coordinate for adversarial examples in the set, as shown by the dashed blue box in Figure 5(a).

5.2 Hyperplane Fitting
To generate the hyperplanes $h_i$ that bound our symbolic adversarial region, we rely on fitting a linear classifier on a dataset $D_i$ consisting of adversarial examples and counterexamples. To compose the dataset, we use the adversarial examples obtained during the computation of the initial box region and add to them counterexamples sampled individually for each hyperplane.

We consider the $i^{th}$ iteration of our algorithm. To sample counterexamples, we first use an optimization procedure to find the worst-case counterexample $x^* \in P_{i-1}$: a concrete counterexample for which $[f(x^*)]_{y_i} - [f(x')]_{(1, \ldots, n_l) \setminus \{y_i\}}$ is the smallest, or an abstract counterexample for which $z^*_t - z^*_{t, (1, \ldots, n_l) \setminus \{y_i\}}$ is minimized by the LP verifier. We obtain concrete worst-case counterexamples using the Frank-Wolfe optimization algorithm and abstract counterexamples by simply solving the LP involved in the verification process. In Figure 5(b) we represent the worst-case counterexample using a green circle.

Heuristic for generating samples. Next, our algorithm finds the point $x^+$ within our current input region $P_{i-1}$ that is furthest away from $x^*$. In Figure 5(b) that point is represented by a red circle. Connecting those two points results in a vector that we use as a sampling direction. We take equally-spaced points on this sampling direction, each of which we use as a center of a Gaussian with a covariance matrix of type $\rho^2 I$. In Figure 5(b) those points are represented as blue circles. Each $\rho$ is determined separately using a binary search so that a large portion of samples obtained from
the Gaussian are both within the input region, are counterexamples and ρ is as large as possible. Finally, we use the counterexamples obtained from the Gaussians, alongside the original set of adversarial examples, as a classification dataset. We use a linear classifier to optimally separate the two, similar to Garg et al. (2014).

Intuitively, our sampling approximates the following idealized counterexample sampling procedure to reduce the angle between \( h_1 \) and the true decision boundary, which in turn, reduces the amount of incorrectly removed volume (Theorem 2.4): 1) Choose a vertex \( x^* \) of \( \mathcal{P}_{t-1} \) with worst verification objective, 2) choose sampling direction passing through \( x^* \) and the center of \( \mathcal{P}_{t-1} \) and 3) for each point on the direction segment contained in \( \mathcal{P}_{t-1} \), create samples, as close as possible, to the nearest decision boundary of the neural network.

Since computing the center of \( \mathcal{P}_{t-1} \) is computationally expensive, instead of the direction pointing to the center of \( \mathcal{P}_{t-1} \), in our procedure we choose the direction with associated maximal L1 length segment contained in \( \mathcal{P}_{t-1} \). We use binary search on the ρ of the Gaussians as a way to sample points close to the nearest neural network decision boundary.

### 5.3 Fast Counterexample Evaluation

![Diagram of a ReLU based fully-connected network with four layers](image)

Fig. 6. Fast counterexample evaluation on a ReLU based fully-connected network with four layers. The values \( \hat{g}_i \) approximate the worst-case neuron values of the candidate \((0.5, -0.5)\). The values \( g^* \) correspond to the worst possible abstract counterexample \((1, -1)\).

Determining a single hyperplane cut takes at least the time required to detect whether samples coming from the Gaussians are counterexamples. To check whether a candidate sample is a concrete counterexample, we simply evaluate the neural network on that candidate. However, to check whether a candidate sample is an abstract counterexample, we have to solve the neural network’s verification LP. Depending on the size of the neural network, this can be quite slow. To avoid this issue, we soundly approximate the LP solution based on the information gathered while solving the same LP for the worst-case abstract counterexample \( x^* \).

Figure 6 demonstrates our approach. The figure depicts the LP encoding of a ReLU based fully-connected neural network that uses the triangle approximation for ReLU activations. The network has four layers — an input layer, two hidden layers, and an output layer. In this example, we are trying to verify that the box region \((z_1, z_2) \in [-1, 1]^2\) is adversarial. The correct class is \(z_{11}\) and the
adversarial class is \( z_{12} \). Therefore, when to check whether a candidate is an abstract counterexample, the LP solver needs to check whether the objective \( z_{12} - z_{11} \) can attain negative values. Figure 6 demonstrates how the candidate \( x = (0.5, -0.5) \) is proved to be an abstract counterexample based on the worst-case counterexample \( x^* = (1, -1) \), obtained by exactly minimizing the LP objective with respect to the input variables \( z_1 \) and \( z_2 \).

In Figure 6, we have denoted with \( g^*_i \) the values the LP solver has assigned to the individual neurons in order to obtain the optimal \( x^* \). At each ReLU node, Figure 6 depicts the inequalities generated by the triangle approximation (shown in Figure 4 (a)) for this node. Observe that, given a ReLU input value, the triangle approximation simply gives three bounds on the corresponding ReLU output value — two lower bounds and one upper bound. For example, given \( g^*_5 = -1 \), the lower bounds of \( z_{10} \) are 0 and \( -1 \) and the upper bound is 0.5. Also observe that the values assigned by the optimizer to the ReLU neurons in Figure 6 always happen to be one of those three bounds. Empirically, we have observed this is often the case when optimizing LPs created using the triangle approximation in our experiments, however there is no theoretical guarantee.

Based on this assumption, we compute, in a feedforward fashion, an approximation to the neuron values of the candidate \( x \) that minimize the LP objective \( z_{12} - z_{11} \). We denote these neuron values with \( \hat{g}_i \). We start by computing \( \hat{g}_3 \) and \( \hat{g}_4 \). Since \( z_3 = z_1 + z_2 \), we compute \( \hat{g}_3 = \hat{g}_1 + \hat{g}_2 = 0 \) and similarly \( \hat{g}_4 = 1 \). Next, we need to compute \( \hat{g}_5 \) and \( \hat{g}_6 \). As discussed, given \( \hat{g}_3 \) and \( \hat{g}_4 \), the triangle approximation forces \( \hat{g}_5 \in [0, 1] \) and \( \hat{g}_6 \in [1, 1.5] \). We have \( g^*_6 = 2 \), which is given by the lower boundary \( z_6 \geq z_4 \). In order to choose the value of \( \hat{g}_6 \) in \([1, 1.5] \), which minimizes the LP objective, we carry over the choice taken by the LP optimizer for the worst-case abstract adversarial example to the candidate \( x \) and, therefore, we assign \( \hat{g}_6 = \hat{g}_4 = 1 \). Similarly, \( \hat{g}_3 = 1 \) is given by the neuron’s upper boundary. Note that we have no guarantees that \( \hat{g}_6 = 1 \) will be an optimal assignment for the LP when evaluated on \( x \). However, we know that if we choose this value, the value of the objective obtained this way will be an upper bound on the optimal (i.e., minimal) objective value for the candidate. We continue this process and compute the values for \( \hat{g}_{11} = 4 \) and \( \hat{g}_{12} = 1 \).

Finally, we calculate the approximate objective \( \hat{g}_{12} - \hat{g}_{11} = -3 \). Because the approximate objective is negative, we are guaranteed that the optimal objective for \( x \) is also negative and thus the candidate is an abstract counterexample. It is worth pointing out that the optimal objective is \(-3.5 \), which is close to the value \(-3 \) obtained by our approximation. We also point out that in the rare cases when \( g^*_i \) is not assigned a boundary value, we can choose a value for \( \hat{g}_i \) as a linear interpolation between the larger of the two lower bounds and the upper bound, using an interpolation coefficient derived from \( g^*_i \) and its respective bounds. This does not change the essential properties of our approximation.

### 5.4 Shrinking the Candidate Region

As shown in Theorem 2.6, the amount of volume removed decreases with every iteration which can slow down convergence. Therefore if, after generating the specified maximum number of hyperplanes, we still fail to verify the candidate region, we perform a final shrinking on it so to accelerate convergence towards obtaining a symbolic adversarial example. In particular, we choose a center — the component-wise median of the adversarial examples (a green circle in Figure 5(c)) — and shrink the input region towards it. This is done by modifying the hyperplanes the algorithm has already fit, including those describing the original input box. If the original hyperplanes are represented by the set of linear inequalities \( Wx \leq c \), the shrinking algorithm seeks to choose a new set of biases \( c' \leq c \). The algorithm chooses the components of \( c' \) in terms of a parameter \( \theta \in [0, 1] \), that linearly interpolates the hyperplanes between their original state and the state in which they go through the center of shrinking. A binary search on \( \theta \) is used to obtain the final
set of hyperplanes, where the change is minimal. Figure 5(c) shows a generated region before and after shrinking and illustrates how positions of different hyperplanes change.

The chosen shrinking method preserves the shape of the region, as the hyperplanes’ slopes do not change, but it shrinks it in volume. The volume is interpolated between 0, when $\theta = 0$ and the region is a single point — the center, and the original volume when $\theta = 1$. The choice of the center of shrinking is important, as it dictates the rate of change of the bias of the individual hyperplanes — that is, how fast we cut additional volume in that direction. The choice of the median is dictated by our desire to keep as many points of the original dataset of adversarial examples as possible in the shrunk volume.

6 OUR FRAMEWORK

In this section, we present our method in more formal terms. Throughout the section we assume a given ReLU-activated feedforward neural network $f: \mathbb{R}^{n_0} \rightarrow \mathbb{R}^{n_l}$ with $l - 1$ layers of the form $f_i(x) = \max(0, A_i x + b_i)$ and a final layer $f_l(x) = A_l x + b_l$, where $f_i: \mathbb{R}^{n_{i-1}} \rightarrow \mathbb{R}^{n_i}$, $A_i \in \mathbb{R}^{n_i \times n_{i-1}}$, $b_i \in \mathbb{R}^{n_i}$ for $i \in \{1, \ldots, l\}$. We also assume a given input image $x_0 \in \mathbb{R}^{n_0}$ to attack, classified correctly by the network to label $y_0$, an L-infinity ball of radius $\epsilon$ around $x_0$ in which attacks are to be searched, as well as a target adversarial label $y_t$. Finally, our framework assumes an adversarial attack algorithm $a(x_0, y_t, \epsilon, s)$ that computes an adversarial attack contained in the $\epsilon$-L-infinity ball around $x_0$ for any given target class $y_t$ and random seed $s$. Our method is shown in Algorithm 1.

We define a candidate adversarial region for $x_0$ to be any input region $\mathcal{P}$ which is entirely contained in the specified $\epsilon$-ball and can be described by a set of $m$ linear inequalities $Wx_0 \leq c$, with $x_0 \in \mathbb{R}^{n_0}$, $W \in \mathbb{R}^{m \times n_0}$ and $c \in \mathbb{R}^{n_0}$. Our algorithm first collects adversarial samples from $\sigma$ to construct the initial set of positive samples $\mathcal{D}^+_0$ of size $s_\epsilon$ (Line 19-23), which are then used to obtain an initial region $\mathcal{P}_0$ (Line 24). For a user-specified $t_{\text{max}} \in \mathbb{Z}$, representing the maximum number of half-space constraints we can use, we iteratively create candidate adversarial regions $\mathcal{P}_0 \supset \mathcal{P}_1 \supset \ldots \supset \mathcal{P}_{t_{\text{max}}}$. If a candidate region $\mathcal{P}_t$ with $0 \leq t \leq t_{\text{max}}$ is found that verifiably contains only adversarial examples, the algorithm returns $\mathcal{P}_t$ as the output. We use the function VerifyRegion defined in Section 6.3 for this check.

Otherwise, we employ a heuristic to obtain a smaller verified region to

At every step $t$, the algorithm constructs the dataset of positive examples $\mathcal{D}^+_t$ for iteration $t$ by simply removing samples from $\mathcal{D}^+_0$ that are not part of polyhedron $\mathcal{P}_{t-1}$ computed at the previous step (Line 31). Next, the algorithm chooses a method $m_t$ — either Frank-Wolfe (FW) or LP, via the function ChooseMethod shown in Algorithm 2. The algorithm uses $m_t$ for refining $\mathcal{P}_{t-1}$ using GenerateRegion function also shown in Algorithm 1. The function collects a dataset of negative samples $\mathcal{D}^-_t$ of size $s_\epsilon$ (Line 2-4) based on the worst-case adversarial example $x^*_t$ computed at Line 2, the point $x^*_t$ that is furthest away from it, in terms of L1 distance, computed at Line 3, and the Gaussian sampling procedure to reduce the amount of incorrectly removed volume as per Theorem 2.4 described in Section 6.4 (Line 4). $\mathcal{D}^-_t$ is combined with negative samples from older iterations stored in $\mathcal{H}_{t-1}$ to produce the negative sample dataset $\mathcal{H}_t$ (Line 5). Finally, we use $\mathcal{D}^+_t$ and $\mathcal{H}_t$, to fit a binary linear classifier $h_t$ (Line 6). $h_t$ is then added to the set of linear inequalities of $\mathcal{P}_{t-1}$ to form the next polyhedron in the sequence $\mathcal{P}_t$. We next check if $\mathcal{P}_t$ contains only the adversarial examples (Line 34). If yes, then the algorithm terminates otherwise it moves to the next iteration. By Theorem 2.6, it can happen that the volume removed by each linear classifier decreases with each iteration and is not sufficient to obtain a verified region within the specified number of maximum iterations. Therefore, after the maximum number of iterations $t_{\text{max}}$ are reached and $\mathcal{P}_t$ is still not proven to be adversarial then it is shrunk using the ShrinkRegion function defined in Section 6.6 (Line 39).
Algorithm 1 Symbolic adversarial example generation

1: function GENERATE_REGION(m_t, \( \mathcal{P}_{t-1} \), s_\ldots, \( \mathcal{D}^+_t \))
2: \( x^*_t = \text{FIND_WORST_COUNTER_EXAMPLE}(\mathcal{P}_{t-1}, m_t) \)
3: \( x^*_t = \max_{x \in \mathcal{P}_{t-1}} \{ ||x^*_t - x||_1 \} \)
4: \( \mathcal{D}^+_t = \text{GAUSSIAN_SAMPLE}(x^*_t, x^*_t, s_\ldots) \)
5: \( \mathcal{H}_t = \text{UPDATE_HISTORY}(\mathcal{D}^+_t, \mathcal{H}_{t-1}) \)
6: \( h_t = \text{LIN CLASSIFIER}(\mathcal{H}_t, \mathcal{D}^+_t) \)
7: \( \mathcal{P}_t = h_t \cap \mathcal{P}_{t-1} \)
8: return \( \mathcal{P}_t \)
9: end function

10: function COMPUTE_SYM_ADEx(f, \( x_0 \), \( y_t \), \( \epsilon \), s_\ldots, p, \( \alpha \))
11: Parameters:
12: \( f \) : the neural network, \( x_0 \) : the input point for which we create the region
13: \( y_t \) : the target class of the attack, \( \epsilon \) : the radius of the \( L_{\infty} \) ball
14: \( s_\ldots \) : number of attacks used to create original region
15: \( s_\ldots \) : number of negative samples used to create each individual hyperplane
16: \( p \) : number of iterations between change of method
17: \( \alpha \) : an adversarial attack algorithm
18:▷ compute the initial region \( \mathcal{P}_0 \)
19: for \( i \in \{1, 2, \ldots, s_\ldots \} \) do
20: \( D^+_i[1] = \alpha(x_0, y_t, \epsilon, s_i) \)
21: end for
22: \( \mathcal{P}_0 = \text{GET_INIT_REGION}(D^+_i) \)
23: if \( \text{VERIFY_REGION}(\mathcal{P}_0) \) then
24: return \( \mathcal{P}_0 \)
25: end if
26: \( m_0 = \text{CHOOSE_RANDOM}(FW, LP), \mathcal{H}_0 = \emptyset \)
27:▷ At each step \( t \), compute the new dataset \( \mathcal{D}_t \) and \( \mathcal{P}_t \)
28: for \( t \in \{1, 2, \ldots, t_{\text{max}} \} \) do
29: \( D^+_t = \text{FILTER}(D^+_0, \mathcal{P}_{t-1}) \)
30: \( m_t = \text{CHOOSE_METHOD}(t, m_{t-1}, \mathcal{P}_{t-1}, \mathcal{D}^+_t, p, s_\ldots) \)
31: \( \mathcal{P}_t = \text{GENERATE_REGION}(m_t, \mathcal{P}_{t-1}, s_\ldots, \mathcal{D}^+_t) \)
32: if \( \text{VERIFY_REGION}(\mathcal{P}_t) \) then
33: return \( \mathcal{P}_t \)
34: end if
35: end for
36:▷ Shrink \( \mathcal{P}_t \) if it cannot be proved to be adversarial
37: \( \mathcal{P}^* = \text{SHRINK_REGION}(\mathcal{P}_t) \)
38: return \( \mathcal{P}^* \)
39: end function

6.1 Computing an Initial Candidate Region
Before the first iteration of our framework, we collect a dataset \( \mathcal{D}_0^+ \) by invoking the algorithm \( \alpha \) a predetermined number of times with different seeds \( s_i \). Using \( \mathcal{D}_0^+ \) we instantiate a candidate region \( \mathcal{P}_0 \) by creating a set of interval constraints \( \{ \min_{a \in \mathcal{D}_0^+} a_j \leq z_{0,j} \leq \max_{b \in \mathcal{D}_0^+} b_j \} \) for each \( j \in \{1, \ldots, n_0\} \). We also initialize \( m_0 \) randomly to be either FW or LP and \( \mathcal{H}_0 = \emptyset \).
We denote the workings of the method (Line 31). We represent the constraint \( w^t \cdot z_0 \leq c^t \) for some weights \( w^t \) and \( c^t \), to obtain \( \mathcal{P}_t = h_t \cap \mathcal{P}_{t-1} \). To compute \( h_t \), two datasets are created — a counterexample dataset \( \mathcal{D}_t^- \) and an adversarial example dataset \( \mathcal{D}_t^+ \). \( \mathcal{D}_t^- \) is simply obtained by removing samples from \( \mathcal{D}_t^+ \) that are not part of \( \mathcal{P}_{t-1} \) by calling the Filter method (Line 31). \( \mathcal{D}_t^- \) is collected separately for each \( \mathcal{P}_t \) by the method described in Section 6.4.

The counterexamples collected in \( \mathcal{D}_t^- \) can either be obtained via FW or LP. We use the heuristic Choose Method function to periodically update the method for obtaining counterexamples with a user-supplied period \( p \). Its implementation is shown in Algorithm 2. It first computes the LP objective \( o \) over \( \mathcal{P}_{t-1} \). The computation of this LP objective is described in Section 6.3. The value of the LP objective over the candidate polyhedra obtained using Frank-Wolfe and LP as well as the runtime for obtaining them are recorded. We measure the improvement in LP objective by subtracting the obtained objectives separately from \( o \). The method with the higher ratio between the improvement and runtime is then chosen.

For high dimensional input spaces, we empirically observe that sometimes the difference in the LP objective between two consecutive candidate regions \( \mathcal{P}_{t-1} \) and \( \mathcal{P}_t \) gets small as \( t \) grows large. We conjecture that this is due to a lack of diversity in the examples contained within \( \mathcal{D}_t^- \). To alleviate the issue for high dimensional input spaces, we implement a counterexample history set \( H_t \) containing all the counterexamples in \( \mathcal{D}_{t-n}^-, \ldots, \mathcal{D}_t^- \) for a given history size \( n \). In our experiments, we use \( n = 5 \). The parameters \( w^t, c^t \) are then fitted to the dataset \( \mathcal{H}_t, \mathcal{D}_t^+ \). In our experiments, we use logistic regression for obtaining \( h_t \), as we found it to perform better for high dimensional data than other alternatives such as support vector machines.

### 6.3 Verifying Candidate Regions

We now define the workings of the Verify Region used in Algorithm 1. For each \( t \in \{0, \ldots, t_{\text{max}}\} \), we construct the triangle convex relaxation \( T_t \) of \( f \) for the input region \( \mathcal{P}_t \). We represent the triangle relaxation \( T_t \) in terms of the tuple \( (I, A, R, T^I, T^A, T^R) \), where \( I \) is a set of input LP variables, \( A \) is a set of affine LP variables, \( R \) a set of ReLU LP variables and \( T^I, T^A \) and \( T^R \) are sets of constraints that define the values that variables in \( I, A \) and \( R \) can take. We denote the \( j^{th} \) variable in \( I \) with \( z_{0,j} \). We denote the \( j^{th} \) affine LP variable on layer \( i \) with \( z_{i,j}^a \). We denote the \( j^{th} \) ReLU LP variable on...
layer $i$ with $z_{i,j}^r$. We denote with $T^A_{i,j}$ the set of constraints governing the value of $z_{i,j}^a$. Similarly we define $T^R_{i,j}$ and $T^L_{i,j}$. Equation 5 describes how these sets are computed with respect to $\mathcal{P}_t$:

$$T^A_{i,j}(\mathcal{P}_t) = \{z_{i,j}^a = [b_1]_j + \sum_{k=1}^{n_{i+1}} [A_i]_{j,k} \cdot z_{i-1,k}^r\}$$

$$T^R_{i,j}(\mathcal{P}_t) = \begin{cases} 
\{z_{i,j}^r = z_{i,j}^a\}, & \text{if } \min_{z_0 \in \mathcal{P}_t} (z_{i,j}^a) \geq 0 \\
\{z_{i,j}^r = 0\}, & \text{if } \max_{z_0 \in \mathcal{P}_t} (z_{i,j}^a) \leq 0 \\
\{z_{i,j}^r \geq 0\}, & \text{otherwise} \\
\{z_{i,j}^r \geq z_{i,j}^a\}, & \text{if } z_{i,j}^r \geq z_{i,j}^a \\
\{z_{i,j}^r \leq \lambda_{i,j} \cdot z_{i,j}^a + \mu_{i,j}\}, & \text{otherwise}
\end{cases}$$

(5)

$$T^L_{i,j}(\mathcal{P}_t) = \mathcal{P}_t$$

We define $T^A(\mathcal{P}_t)$ as the union of the $T^A_{i,j}(\mathcal{P}_t)$ for all $i$ and $j$. Analogously, we also define $T^L(\mathcal{P}_t)$ and $T^R(\mathcal{P}_t)$. At the end of each iteration, we use $T(\mathcal{P}_t)$ in conjunction with an off-the-shelf LP solver to compute the LP objective for $\mathcal{P}_t$:

$$O(\mathcal{P}_t) = \min_{x \in \mathcal{P}_t} (z_{l,y}^a - z_{l,(1,\ldots,n_l) \setminus \{y_l\}}^a)$$

(6)

If $O(\mathcal{P}_t) \geq 0$ for some $0 \leq t \leq t_{\max}$, then we have proved that $\mathcal{P}_t$ is a symbolic adversarial example and therefore we terminate our algorithm.

**Optimization for computational gains.** Naive computation of the triangle convex relaxation $T_I$ requires checking the properties $\max_{x_0 \in \mathcal{P}_t} (z_{i,j}^a) \leq 0$ and $\min_{x_0 \in \mathcal{P}_t} (z_{i,j}^a) \geq 0$ for each $z_{i,j}^a \in A$ for each $k$. This is computationally expensive. Since $\mathcal{P}_t \subset \mathcal{P}_{t-1}$, $\max_{x_0 \in \mathcal{P}_{t-1}} (z_{i,j}^a) \leq 0 \Rightarrow \max_{x_0 \in \mathcal{P}_t} (z_{i,j}^a) \leq 0$ and $\min_{x_0 \in \mathcal{P}_t} (z_{i,j}^a) \geq 0 \Rightarrow \min_{x_0 \in \mathcal{P}_{t-1}} (z_{i,j}^a) \geq 0$. This allows us to limit the computation of $\max_{x_0 \in \mathcal{P}_t} (z_{i,j}^a)$ and $\min_{x_0 \in \mathcal{P}_t} (z_{i,j}^a)$ to only neurons for which $\min_{x_0 \in \mathcal{P}_{t-1}} (z_{i,j}^a) < 0$ and $\max_{x_0 \in \mathcal{P}_{t-1}} (z_{i,j}^a) > 0$. That is, usually a small subset of neurons allow for large computational gains.

### 6.4 Collecting Counterexamples

We define the worst-case concrete counterexample for $\mathcal{P}_{t-1}$, as a local minimum of

$$[f(x)]_{y_t} - [f(x)]_{(1,\ldots,n_l) \setminus \{y_l\}}$$

(7)

in $\mathcal{P}_{t-1}$, computed using the Frank-Wolfe algorithm. We define the worst-case abstract counterexample for $\mathcal{P}_{t-1}$, as the input for which the LP solver minimizes the verifier objective $O(\mathcal{P}_{t-1})$. Depending on the type of method $m_t$ chosen for collecting $D^-_t$ via the Choose Method method, $x^*$ is either the worst-case concrete or abstract counterexample.

Using the obtained $x^*$, an LP solver is used to compute $x^+ = \text{argmax}_{x \in \mathcal{P}_{t-1}} (||x^* - x||_1)$. Next, our framework computes a predetermined number of equally-spaced points $x^*_i$ on the line segment connecting $x^*$ and $x^+$. For each $x^*_i$, we collect samples from an isotropic Gaussian with covariance $\rho_i^2 I$ centered at $x^*_i$. Each sample generated from the Gaussians is tested for two conditions — whether it is within $\mathcal{P}_{t-1}$ and whether it is a counterexample. $D^-_t$ is then assigned to the set of Gaussian samples that pass both tests.

To determine if a Gaussian sample $x$ is a concrete counterexample, we compute $\text{argmax}_i [f(x)]_i$ and compare it to $y_t$. Determining if $x$ is an abstract counterexample is discussed in the next section. For each individual Gaussian, $\rho_i^2$ is determined using binary search, such that it is maximal and has a counterexample success rate above a certain threshold.
6.5 Approximate Abstract Counterexamples

To determine if a sample \( x \) generated by the Gaussian distributions is an abstract counterexample in \( P_{t-1} \), we need to check if the verifier objective for \( P_{t-1} \), under the additional constraint that \( z_0 = x \), is negative. Exact computation of this verifier objective is possible with an LP solver but is computationally prohibitive to apply to each sample \( x \) individually. In this section, we discuss how to approximate the calculation of the LP objective enabling fast abstract counterexample evaluation.

To compute this objective, the LP assigns values to the variables in \( A \) and \( R \), such that \( z_{l_1,y_t}^a - z_{l_1,\{1,\ldots,n_t\}\setminus\{y_t\}}^a \) is minimal. We define numbers \( g_{l_1,j}^a \) and \( g'_{l_1,j} \), which represent these optimal values for \( z_{l_1,j}^a \) and \( z'_{l_1,j} \), respectively. We approximate \( g_{l_1,j}^a \) and \( g'_{l_1,j} \) by values \( \tilde{g}_{l_1,j}^a \) and \( \tilde{g}'_{l_1,j} \). The computation of \( \tilde{g}_{l_1,j}^a \) and \( \tilde{g}'_{l_1,j} \) is based upon the values \( g_{l_1,j}^a \) and \( g'_{l_1,j} \) assigned to the variables in \( A \) and \( R \) in \( P_{t-1} \) while computing the worst-case abstract counterexample \( x^* \). The values \( \tilde{g}_{l_1,j}^a \) and \( \tilde{g}'_{l_1,j} \) are computed layer by layer, starting with \( \tilde{g}_{l_1,j}^a \) for \( j \in \{1, \ldots, n_t\} \). Each \( \tilde{g}_{l_1,j}^a \) is computed by evaluating \( T_{t}^A \) using the values assigned so far, as follows:

\[
\tilde{g}_{l_1,j}^a = [b_1]_j + \sum_{k=1}^{n_t} [A_1]_{j,k} \cdot \tilde{g}'_{l_1,k}
\]  

(8)

We compute \( \tilde{g}'_{l_1,j} \) based on the set of constraints \( T_{t}^R \). If \( \tilde{T}_{t}^R = \{z_{l_1,j}^a = z_{l_1,j}^a\} \), we compute \( \tilde{g}'_{l_1,j} = \tilde{g}'_{l_1,j}^a \). Similarly, if \( \tilde{T}_{t}^R = \{z_{l_1,j} = 0\} \), we compute \( \tilde{g}'_{l_1,j} = 0 \). In the last case, observe that \( \tilde{T}_{t}^R \) defines a lower bound \( \tilde{b}_{l_1,j} = \max(0, \tilde{g}'_{l_1,j}) \) and an upper bound \( \tilde{u}_{l_1,j} = \lambda_{l_1,j} \tilde{g}'_{l_1,j} + \mu_{l_1,j} \) on \( \tilde{g}'_{l_1,j} \). Similarly, \( \tilde{T}_{t}^R \) also defines a lower bound \( \tilde{b}_{l_1,j} \) and an upper bound \( \tilde{u}_{l_1,j} \) on \( \tilde{g}'_{l_1,j} \) and a lower bound \( \tilde{l}_{l_1,j} \) and an upper bound \( \tilde{u}_{l_1,j} \) on \( \tilde{g}'_{l_1,j} \). When computing \( \tilde{g}_{l_1,j}^a \), the LP solver is free to choose any value in \( [\tilde{b}_{l_1,j}, \tilde{u}_{l_1,j}] \). Similarly, in our approximation, we need to choose the value of \( \tilde{g}_{l_1,j}^a \) in \( [\tilde{b}_{l_1,j}, \tilde{u}_{l_1,j}] \) but without explicitly optimizing the objective. To do so, we mimic the decision taken by \( x^* \) for this variable. We define \( d_{l_1,j}^{lb} = g_{l_1,j}^a - \tilde{b}_{l_1,j}^a \) and \( d_{l_1,j}^{ub} = \tilde{u}_{l_1,j} - g_{l_1,j}^a \) which represent distances from \( g_{l_1,j}^a \) to its lower and upper bounds. We then compute \( \tilde{g}_{l_1,j}^a \) as a linear combination of these bounds:

\[
\tilde{g}_{l_1,j}^a = \tilde{b}_{l_1,j} + \frac{d_{l_1,j}^{lb}}{d_{l_1,j}^{lb} + d_{l_1,j}^{ub}} + \tilde{u}_{l_1,j} - \frac{d_{l_1,j}^{lb}}{d_{l_1,j}^{lb} + d_{l_1,j}^{ub}}
\]

(9)

Samples for which the approximate evaluation achieves \( \tilde{g}_{l_1,y_t}^a - \tilde{g}_{l_1,\{1,\ldots,n_t\}\setminus\{y_t\}}^a < 0 \) are guaranteed to be abstract counterexamples, however it does not provide any guarantees for samples \( x \) for which \( z_{l_1,y_t}^a - z_{l_1,\{1,\ldots,n_t\}\setminus\{y_t\}}^a \geq 0 \). This property of the approximate evaluation guarantees that all samples collected in \( D_t^a \) are abstract counterexamples and thus need to be pruned out of the candidate region \( P_{t-1} \).

6.6 Shrinking the Candidate Region

We next define the shrinking of the candidate regions which is used as a last resort to obtain symbolic adversarial regions when such a region cannot be obtained within \( t_{\text{max}} \) iterations. Given a candidate region \( P_t \), defined by the set of \( m \) inequalities \( W x_0 \leq c \), the shrinking algorithm seeks to choose a new set of biases \( c^* \leq c \) such that the resulting region \( S^* \) can be proven to be adversarial. The algorithm selects a center \( x_c \in \mathbb{R}^m \) based on a coordinate-wise median of the samples in \( D_t^a \).

It then calculates the distances from \( x_c \) to each line in \( P_t \) given by \( d_i = \frac{|\Sigma_{k=1}^m |W|_{k,i} \cdot |x_c|_k - |c|_i|}{\|W\|_2} \) for \( i \in \{1, \ldots, m\} \). For a given \( \theta \in [0, 1] \), we define \( |c^*|_i = |c|_i - \theta \cdot d_i \cdot \|W\|_2 \). Here, \( \theta \) interpolates between the original region \( P_t \) at \( \theta = 0 \) and a region only containing \( x_c \) at \( \theta = 1 \). Finally, \( S^* \) is
chosen via binary search on $\theta$. We next try to verify $S^*$ via the VerifyRegion function, if it fails then the above procedure is repeated.

### 6.7 Replacing Triangle with DeepPoly

So far, we have discussed how to use the triangle convex relaxation to verify candidate regions and generate abstract counterexamples. We can also use the coarser DeepPoly relaxation, which can significantly improve the scalability of our approach. We now discuss how we have extended the algorithm to the DeepPoly convex relaxation. Using DeepPoly allows us to scale our methods to bigger networks in exchange for lower verification precision of symbolic adversarial regions. DeepPoly is a further relaxation of the triangle approximation and as such the algorithms presented here trivially extend to DeepPoly by modifying the triangle relaxation encoding $T_t$. However, a major factor in the speedup provided by DeepPoly is that it is able to substitute the expensive LP encoding of the neural network $T_t$ and to solve the optimization problems involved in the verification process with direct backsubstitution. Therefore, we modified our algorithm to take advantage of this backsubstitution property. The original DeepPoly paper (Singh et al. 2019) describes the backsubstitution algorithm in the case of an input region that is a box. To make it applicable in our setting, we extend the backsubstitution algorithm to allow for general linear inequalities over the input. We do that by terminating the backsubstitution at the input layer to obtain a lower bound and an upper bound of the form $c + \sum_{k=1}^{n_0} w_k \cdot x_{0,k}$ for each neuron. LPs of the form $\min_{x_0 \in P_t} (c + \sum_{k=1}^{n_0} w_k \cdot x_{0,k})$ are then constructed in order to compute the lower bounds of every neuron. Analogously, another set of LPs is constructed to compute the upper bounds. The procedure is efficient since the LPs involved in the process contain only $n_0$ variables and a small number of constraints.

In addition to adapting the verification process itself, we also need to adapt the abstract counterexample evaluation algorithm outlined in Section 6.5. However, the abstract counterexample evaluation can be viewed as an application of the verification process on a box which contains exactly one point — the sample, and thus it is efficiently computed via backsubstitution. To share computation between multiple samples, the backsubstitution can also be precomputed until the input layer, with individual samples being substituted in the resulting linear expression.

### 7 EXPERIMENTAL EVALUATION

We now evaluate the effectiveness of our approach on realistic networks. We compare our framework to Polaris (Zhang et al. 2018), the closest related work, and show that our method scales to larger networks with high-dimensional inputs, while generating regions with large volume.

We implemented our framework in Python and used Tensorflow (Abadi et al. 2015) and CleverHans (Papernot et al. 2018) for generating PGD attacks. We use Gurobi 8.0 (Gurobi Optimization, LLC 2020) for solving LP instances. We rely on Scikit-learn for the logistic regression and ELINA (Singh et al. 2019) for its DeepPoly convex relaxation (Singh et al. 2019).

**Datasets:** We use the standard MNIST (LeCun et al. 1998) and CIFAR10 (Krizhevsky 2009) datasets, as well as the mortgage dataset from Fannie Mae (2017) used by Zhang et al. (2018). The MNIST dataset has grayscale images of size $28 \times 28$ pixels. The CIFAR10 dataset has RGB images of size $32 \times 32 \times 3$. Records in the mortgage dataset consists of 9 categorical features and 12 real-valued features describing the financial information of individuals that were granted a mortgage loan and whether they paid it back.
Table 1. Neural networks used in our experiments.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Model</th>
<th>Type</th>
<th>Neurons</th>
<th>Layers</th>
</tr>
</thead>
<tbody>
<tr>
<td>MNIST</td>
<td>8 × 200</td>
<td>FFN</td>
<td>1,610</td>
<td>9</td>
</tr>
<tr>
<td></td>
<td>ConvSmall</td>
<td>CONV</td>
<td>3,604</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>ConvBig</td>
<td>CONV</td>
<td>48,064</td>
<td>6</td>
</tr>
<tr>
<td>CIFAR10</td>
<td>ConvSmall</td>
<td>CONV</td>
<td>4,852</td>
<td>3</td>
</tr>
<tr>
<td>Mortgage</td>
<td>5 × 200</td>
<td>FFN</td>
<td>1,002</td>
<td>5</td>
</tr>
</tbody>
</table>

Table 2. Polaris vs. our framework with DeepPoly and the triangle relaxations on the mortgage dataset.

<table>
<thead>
<tr>
<th>Metric</th>
<th>Polaris</th>
<th>DeepPoly</th>
<th>Triangle</th>
</tr>
</thead>
<tbody>
<tr>
<td>AvgTime (s)</td>
<td>329</td>
<td>105</td>
<td>396</td>
</tr>
<tr>
<td>MedArea</td>
<td>7.9</td>
<td>7.3</td>
<td>16.5</td>
</tr>
</tbody>
</table>

**Neural Networks**: Table 1 shows the sizes and types of different neural networks we use in our experiments. The network used for the mortgage experiments is taken from Zhang et al. (2018). Remaining networks are taken from Singh et al. (2019). None of the networks are adversarially trained, to allow us to run PGD attacks on them. Our deepest network is the MNIST 8 × 200 fully-connected network (FFN) which has 8 layers with 200 neurons each and another layer with 10 neurons. Our largest network is the MNIST ConvBig network with 6 layers and 48K neurons.

**Experimental Setup**: We ran all our experiments on a 2.2 GHz 12 core Intel Xeon CPU E5-2650 with 64 GB of RAM.

### 7.1 Mortgage Dataset Experiments

Table 2 compares the average time taken (AvgTime) and the median area (MedArea) of the regions on 20 different mortgage samples between Polaris and our framework instantiated with two different certification methods – DeepPoly and the triangle relaxation. We used the 5 × 200 fully connected network (FFN) trained by Zhang et al. (2018). We mimic the evaluation setup of Polaris where 2-D regions based on the Loan-to-Value (LTV) and InterestValue features in the dataset are generated. The low dimensionality enables us to calculate areas exactly. Our framework requires an input regions $S_0$ to start pruning, which we cannot obtain in the non-adversarial Polaris setting. As an alternative to estimating $S_0$, we feed our framework with an overapproximation box containing all linear regions Polaris obtains for the given input. We additionally enlarge that box by 5% in each direction to ensure further pruning of $S_0$ is required. We compare the convex underapproximation Polaris uses for convexifying its final regions with regions pruned by our algorithm. Table 2 shows that our framework using the triangle ReLU approximation creates 2x larger regions than Polaris while being only slightly slower. Table 2 also shows that our framework using the less precise DeepPoly relaxation is 3x faster than Polaris while creating regions that are only slightly smaller.

### 7.2 MNIST and CIFAR10 Dataset Experiments

Table 3 summarizes the results of our experiments on the MNIST and CIFAR10 datasets. For both, we ran our framework on the first 100 test images, while filtering the wrongly-classified ones. In all experiments, we collect 5000 adversarial examples from both PGD and Frank-Wolfe, initialized with different seeds for computing $P_0$. The samples are collected within an $L_\infty$ ball around a test image with the radius $\epsilon$ specified in Table 3. We refer to this as our initial attack method $\alpha$. All experiments in Table 3 use DeepPoly. Further, all experiments use logistic regression with a class
Table 3. Results of our MNIST and CIFAR10 dataset experiments.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Model</th>
<th>$\epsilon$</th>
<th>$t_{max}$</th>
<th>OVER</th>
<th>UNDER</th>
<th>#Regions</th>
<th>#Images</th>
<th>#Failures</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>MNIST</td>
<td>ConvSmall</td>
<td>0.12</td>
<td>50</td>
<td>$10^{441}$</td>
<td>$10^{258}$</td>
<td>64</td>
<td>35</td>
<td>0</td>
<td>399s</td>
</tr>
<tr>
<td></td>
<td>ConvBig</td>
<td>0.05</td>
<td>30</td>
<td>$10^{115}$</td>
<td>$10^{79}$</td>
<td>12</td>
<td>9</td>
<td>5</td>
<td>4310s</td>
</tr>
<tr>
<td>CIFAR10</td>
<td>ConvSmall</td>
<td>0.01</td>
<td>30</td>
<td>$10^{458}$</td>
<td>$10^{265}$</td>
<td>43</td>
<td>22</td>
<td>11</td>
<td>2975s</td>
</tr>
</tbody>
</table>

We define the overapproximation box of a symbolic region as the box generated by the minimum and maximum values of each individual pixel. This box overapproximates the real volume of the region. Similarly, an underapproximation box of a symbolic region gives a lower bound on the region’s volume. We follow the procedure outlined by Gopinath et al. (2019) to compute it. Using these two notions, we calculate the size of a symbolic adversarial example as the number of concrete adversarial examples contained within these two boxes. These are calculated as the number of different discrete values each pixel in the boxes can take.

For each network, in Table 3, we present the number of distinct pairs of an image and a target $(x_0, y_t)$ on which $\alpha$ succeeds (column #Regions), as well as the number of unique images on which $\alpha$ succeeds (column #Images). Table 3 also details the number of regions where our framework fails, that is it finds a symbolic adversarial example whose underapproximation box contains less than the 10000 concrete adversarial examples sampled with $\alpha$ initially. Finally, we report the average running time for the discovered regions, as well as the volume of their median underapproximation and overapproximation boxes. As can be seen, our framework creates symbolic regions with $10^{258}$ and $10^{265}$ concrete examples in the underapproximated box on the MNIST and CIFAR10 ConvSmall networks in $\leq 7$ minutes on average.

Next, we compare our framework to Polaris on the MNIST ConvSmall network. As the implementation by Zhang et al. (2018) does not support convolutional layers, we re-implemented Polaris using ERAN (Singh et al. 2018) and Gurobi (Gurobi Optimization, LLC 2020). We adapt Polaris to search for symbolic adversarial examples by applying its Algorithm 2 on a PGD attack and then adding the LP constraint that the input variables need to be within an $\epsilon$-ball around the original image $x_0$ to the appropriate LP instances. Polaris creates a predetermined number of linear regions based on activation patterns of neurons which are then summarized with a single convex region that underapproximates their union. The algorithms in Polaris for generating the convex underapproximations scale poorly with input dimensionality. Consequently, we do not compare our symbolic examples with these underapproximation regions but directly with the union of individual linear regions collected by Polaris which is the most scalable way of generating regions with Polaris on the image domain.

We compute results for Polaris based on the first 25 MNIST test images for which a PGD attack with $\epsilon = 0.12$ was found. For these images, we generated up to 100 activation regions. For each region, we computed its respective overapproximation and underapproximation boxes. These were then summed over all activation regions retrieved by Polaris, to obtain the final count which is computed as 100. The results show that the actual volume computed via Polaris is much smaller than that of the regions obtained via our framework, as demonstrated by the small number of concrete adversarial examples in the underapproximation boxes.
7.3 Effectiveness of the Gaussian Sampling

We compare our Gaussian sampling heuristic for obtaining counterexamples, against the simple random uniform sampling on the initial hyperbox region $P_0$, for a single MNIST image on the $5 \times 100$ FFN presented in Singh et al. (2019).

After uniformly sampling 100000 samples on $P_0$ and evaluating them on the network, we failed to find a single counter example and, thus failed to cut any volume from $P_0$. In contrast, our sampling finds 4601 samples, which allowed our method to obtain a region after 5 cuts. This behavior of uniform sampling is consistent with our observations on different high-dimensional input spaces.

7.4 Dependence on the Neural Network Architecture

In the next section, we explore the effect of the neural network’s architecture on the process of creating symbolic adversarial examples. In particular, we compare the symbolic adversarial examples created on 3 FNNs – $2 \times 50$, $2 \times 100$ and $5 \times 100$ from Singh et al. (2019) on the same MNIST image ($6^{th}$ test image), the same adversarial target (8) and the same $\epsilon = 0.05$. We explicitly disabled shrinking for this experiment to observe the full complexity of the problem of cutting the volume. Table 4 summarizes the results. We see that, as the size of the network increases, so does the number of cuts required. We conjecture this is due to the finer partition of the input space created by the network. In particular, the size of the partition grows exponentially with the number

---

Table 4. Effects of neural network architecture on symbolic adversarial examples

<table>
<thead>
<tr>
<th>Model</th>
<th>Time</th>
<th>Cuts</th>
<th>Initial Box</th>
<th>Over</th>
<th>Under</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2 \times 50$</td>
<td>88s</td>
<td>1</td>
<td>$10^{285}$</td>
<td>$10^{285}$</td>
<td>$10^{285}$</td>
</tr>
<tr>
<td>$2 \times 100$</td>
<td>2409s</td>
<td>63</td>
<td>$10^{232}$</td>
<td>$10^{232}$</td>
<td>$10^{108}$</td>
</tr>
<tr>
<td>$5 \times 100$</td>
<td>6280s</td>
<td>71</td>
<td>$10^{334}$</td>
<td>$10^{334}$</td>
<td>$10^{88}$</td>
</tr>
</tbody>
</table>

---

Fig. 7. Sensitivity of symbolic adversarial examples on the MNIST ConvBig network.
of neurons. Thus, the input space is partitioned into much smaller chunks, which in turn prevents bigger robust adversarial regions. We also note that the underapproximating volumes of $5 \times 100$ are particularly low. We conjecture this is caused by more complex non-convex decision boundaries associated with the increase in depth.
Fig. 10. Sensitivity of symbolic adversarial examples on the CIFAR10 ConvSmall network. For each subfigure we show from left to right: the original image and the sensitivity in the red, blue and green channel respectively.

8 VISUALISING OUR RESULTS

In this section we show a subset of the symbolic adversarial examples we have obtained for the different neural networks described in Section 7 (Figures 7-10). For all images, colorbars signify how much individual pixel values can change within the underapproximation boxes calculated for the symbolic adversarial examples (out of 256). The pixel colors have the same meaning as in Figure 1. In all figures we show the original test image alongside with the sensitivity image, with the CIFAR10 figure showing a sensitivity image for each color channel separately. We notice common patterns between the adversarial examples obtained for the MNIST networks, where the
background pixels, particularly those on the edges, are green and thus can take several values within our underapproximation boxes. We also see that many foreground pixels are yellow and thus their intensity can vary the highest. For the symbolic adversarial examples obtained on CIFAR10 ConvSmall (Figure 10) we notice a common pattern where the symbolic adversarial examples are invariant to the values of pixels on the bottom rows and right columns. There are few foreground pixels that are also yellow. This is a pattern we observed on most symbolic adversarial examples obtained on this network.

Based on our results for both MNIST and CIFAR10 networks, we conclude that our obtained regions are robust and can capture adversarial examples generated by variations caused when transferring a synthesized adversarial example in real-world conditions.

9 RELATED WORK

The work of Dathathri et al. (2019) uses symbolic interpolation to compute both an under- and an overapproximation of the set of inputs for which a given output property holds. The work of Zhang et al. (2018) explores linear regions specified by the activation patterns of neurons in the network. The regions with different activation patterns are then combined to obtain a final symbolic region. The work of Gopinath et al. (2019) is also based on similar techniques as Zhang et al. (2018). We note that these works do not scale to the larger MNIST and CIFAR10 neural networks used in our experiments. In contrast, our symbolic inference method scales to larger networks and can also be used to address the problems investigated by these works in a more scalable manner.

The work of (Athalye et al. 2018; Kurakin et al. 2016) aims to create adversarial examples that can be reproduced in the real-world. However, both do not generate any continuous region like our work and instead try to find a single adversarial image whose neighbors are likely adversarial.

The work of (Gulshad and Smeulders 2020; Hsieh et al. 2020) utilize adversarial examples for generating feature-based explanations of neural networks. We note that our regions can also produce similar explanations.

10 CONCLUSION

We introduced the concept of a symbolic adversarial example, a convex region containing a large set of concrete adversarial examples. We presented a theoretical analysis showing that the problem of computing optimal symbolic adversarial examples is hard. We presented a scalable method for synthesizing an approximation of the optimal symbolic regions: the method iteratively adds half-space constraints to an initial box region until the region is proved to be adversarial. Our evaluation shows the method scales to larger networks while computing wide regions (10258 concrete adversarial examples) that can be used for producing real-world adversarial examples.

REFERENCES

