Reliable and Trustworthy Artificial Intelligence

Lecture 5: Certified Defenses

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Can certification methods benefit training?

Verifying networks which are not meant to be robust will certainly produce worse results (smaller epsilon provability) than verifying networks which are trained to be provably robust.

Note that there is a difference between training the network to be experimentally robust (e.g., PGD defense) vs. training the network to be provably robust (what we see next).

So, can we then use certification for training the network to be robust?

Recall: PGD Defense

Outer minimization problem

find $\boldsymbol{\theta}$ that minimizes the high loss, aiming to train a robust classifier

find	θ
minimize	$\rho(\theta)$
where	$\rho(\theta) = \mathbf{E}_{(\mathrm{x},\mathrm{y})\sim D}\ [\max\limits_{x' \in S(x)} \ L(\theta, x', y)]$

Inner maximization problem

find $\boldsymbol{x}'$ that achieves high loss

D is the underlying distribution

$\mathbf{E}$ is typically estimated with the empirical risk

$S(x)$ denotes the perturbation region around point x, that is, we want all points in $S(x)$ to classify the same as x . We can pick $S(x)$ to be:

$$S(x) = \{ \boldsymbol{x}' \mid \|\boldsymbol{x} - \boldsymbol{x}'\|_{\infty} < \boldsymbol{\epsilon} \}$$

Madry et.al, 2017

Lets Incorporate Provability

Outer minimization problem

Lets keep this part

find θ

minimize $\rho(\theta)$

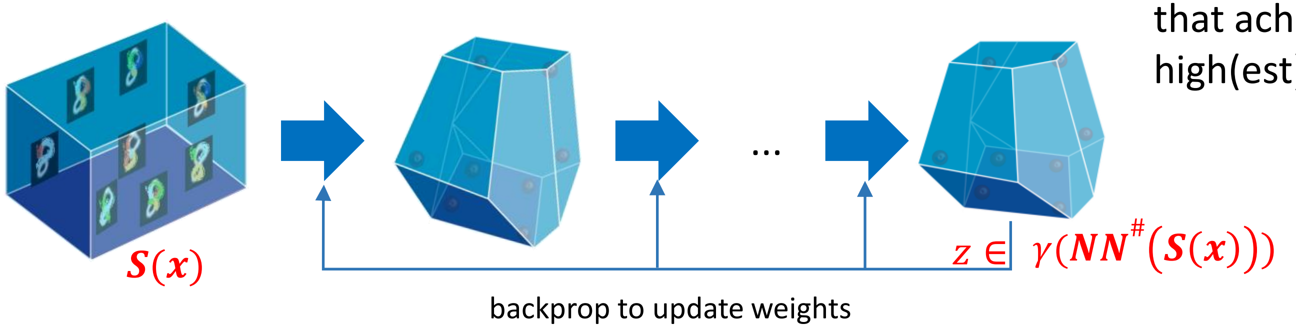
where $\rho(\theta) = \mathbf{E}_{(\mathrm{x},\mathrm{y})\sim D}\left[\max_{z \in \gamma(NN^{\#}(S(x)))} L(\theta, z, y)\right]$

Inner maximization problem

find $\boldsymbol{z}$ that achieves high loss under abstraction

Differentiable Abstract Interpretation for Provably Robust Neural Networks
Mirman, Gehr, V. ICML 2018

Visualization of Certified Training



Essentially: **automatic differentiation of abstract interpretation**

Adversarial Training

find θ
minimize $\rho(\theta)$

where $\rho(\theta) = \mathbf{E}_{(x,y)\sim D}[\max_{\boldsymbol{x}' \in \boldsymbol{S}(\boldsymbol{x})} L(\theta, \boldsymbol{x}', y)]$

Find input $\boldsymbol{x}'$ that achieves high loss

Certified Defense

find θ
minimize $\rho(\theta)$

where $\rho(\theta) = \mathbf{E}_{(\mathrm{x},\mathrm{y})\sim D}[\max_{\boldsymbol{z} \in \gamma(\boldsymbol{NN}^{\#}(\boldsymbol{S}(\boldsymbol{x})))} L(\theta, \boldsymbol{z}, y)]$

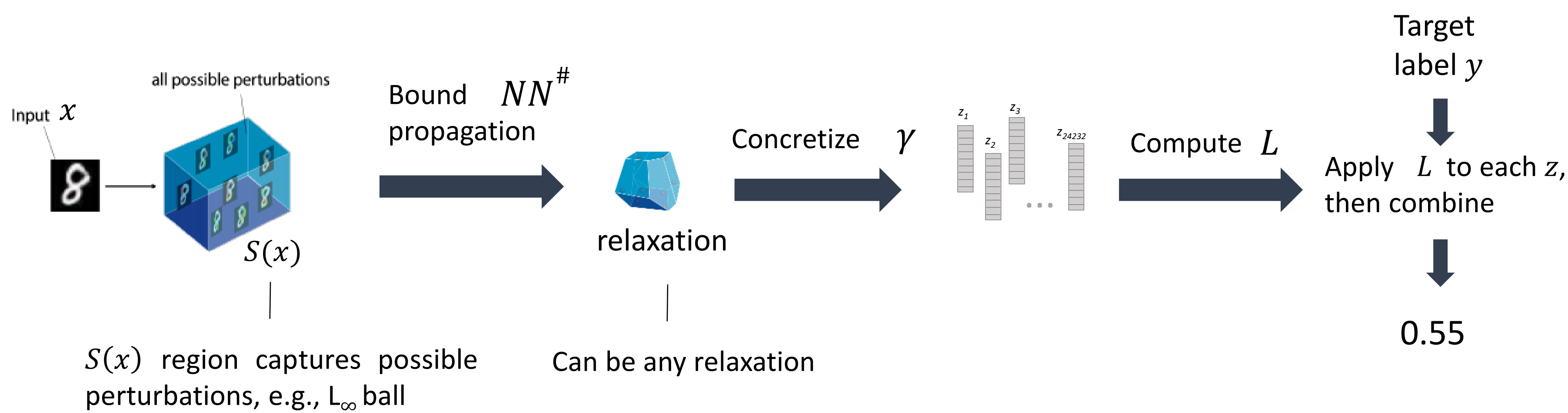
Find output $\boldsymbol{z}$ that achieves high loss (under abstraction)

Certified Defenses: General Method

$$\max_{z \in \gamma(NN^{\#}(S(x)))} L(\theta, z, y)$$

Let us examine the pattern in the concrete first.

The pattern works with any abstract relaxation.



Differentiable Abstract Interpretation for Provably Robust Neural Networks
Mirman, Gehr, V. ICML 2018

Let us now pick a loss function L

$$L(\mathbf{z}, y) = \max_{\mathrm{q} \neq y} (\mathrm{z_q} - \mathrm{z_y})$$

target label

a vector of logits

q ranges over all possible labels

Certified Defenses with a given loss

$$\max_{z \in \gamma(NN^{\#}(S(x)))} L(\theta, z, y)$$

Lets define L to be:

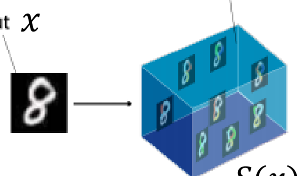
$$L(\mathbf{z}, y) = \max_{\mathrm{q} \neq y} (\mathrm{z_q} - \mathrm{z_y})$$

target label

a vector of logits

Input x

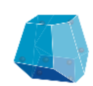
all possible perturbations



$S(x)$

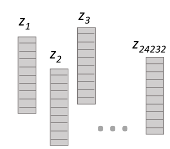
$S(x)$ region captures possible perturbations, e.g., L_∞ ball

Bound $NN^{\#}$ propagation



relaxation

Concretize γ



Compute L

Target label y

Apply L to each z, then take max one

0.55

Differentiable Abstract Interpretation for Provably Robust Neural Networks
Mirman, Gehr, V. ICML 2018

Certified Defenses with a given loss

$$\max_{z \in \gamma(NN^{\#}(S(x)))} L(\theta, z, y)$$

Lets define L to be:

$$L(\mathbf{z}, y) = \max_{q \neq y} (z_q - z_y)$$

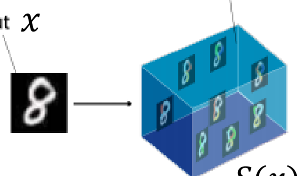
target label

a vector of logits

Target label y

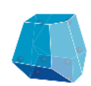
Input x

all possible perturbations



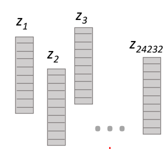
$S(x)$

Bound propagation $NN^{\#}$



relaxation

Concretize γ



Compute L

Apply L to each z, then take max one

0.55

$S(x)$ region captures possible perturbations, e.g., L_∞ ball

Key problem: set of vectors could be infinite or very large, so we cannot just enumerate.

How do we address this?

Certified Defenses in the abstract

$$\max_{z \in \gamma(NN^{\#}(S(x)))} L(\theta, z, y)$$

Lets define L to be:

$$L(\mathbf{z}, y) = \max_{q \neq y} (z_q - z_y)$$

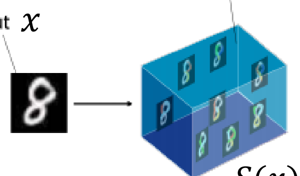
a vector of logits

target label

DeepPoly propagation

Input x

all possible perturbations



$S(x)$

$S(x)$ region captures possible perturbations, e.g., L_∞ ball

Network

$d_0 = z_0 - z_y$

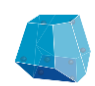
l_0, u_0 for d_0

e.g. [0.1, 0.3]

$\max(box(d_0))$

0.3

...



...

$d_9 = z_9 - z_y$

l_9, u_9 for d_9

e.g. [-0.4, -0.1]

$\max(box(d_9))$

-0.1

0.3

This is an affine transform which is exact for DeepPoly

Compute the maximum

Let us keep the same pattern but now pick a different loss, the cross-entropy loss CE

$$L(\mathbf{z}, y) = CE(\mathbf{z}, y)$$

This is in the concrete, but we need to work in the abstract.

On the Effectiveness of Interval Bound Propagation for Training Verifiably Robust Models, 2018
Gowal, Dvijotham, Stanforth, Bunel, Qin, Uesato, Arandjelovic, Mann, Kohli

Let us keep the same pattern but now pick a different loss, the cross-entropy loss CE

$$L(\boldsymbol{z}, y) = CE(\boldsymbol{z}, y)$$

Abstract $\boldsymbol{z}^{\#}$:

$[l_0, u_0]$
$[l_1, u_1]$
$[l_2, u_2]$
$[l_3, u_3]$
$[l_4, u_4]$
$[l_5, u_5]$
$[l_6, u_6]$
$[l_7, u_7]$
$[l_8, u_8]$
$[l_9, u_9]$

Let $y = 4$

Pick u_i if $y \neq i$

Pick l_i if $y = i$

Concrete (unnormalized) $\boldsymbol{z}$:

u_0
u_1
u_2
u_3
l_4
u_5
u_6
u_7
u_8
u_9

Apply $softmax$

Concrete (normalized) $\boldsymbol{z}$:

u_0'
u_1'
u_2'
u_3'
l_4'
u_5'
u_6'
u_7'
u_8'
u_9'

$CE(\boldsymbol{z}, y)$

0.22

Few additional tricks in practice

- Annealing on the size of $S(x)$ – start with small region around x (small ϵ) and gradually grow it during training. This was found to be most helpful heuristic.

- Even though the whole propagation is done via Box, IBP processes the last linear layer exactly (e.g., zonotope).

- Dynamically weighing-in the standard CE loss and the correctness CE loss.

These and more implemented in the DiffAI certified training system:
https://github.com/eth-sri/diffai

Key observations when using DiffAI scheme in practice

Using cheap relaxations (e.g., Box) scales to large networks. But the problem is, it introduces imprecision (infeasible points) in the final output shape, meaning the deeper the network is, the more the capacity increases (potential for higher accuracy), but the more we are training w.r.t. assigning labels to infeasible points. Thus, typically training with Box scales but accuracy drops substantially.

Naturally we would like to reduce the infeasible points w.r.t to which we are training. However, it turned out that more precise relaxations (e.g., DeepPoly, Zonotope) may lead to worse results than Box! This is an unintuitive pathological situation where more precise relaxations during training do not actually bring better results in provability and where further loss tweaking is not enough.

Why are better relaxations not producing better results?

Hypothesis: More **complex abstractions** lead to more **difficult optimization problems**.

Why? Intuitively, a relatively **small number of weights** in the network need to control complex relaxations with **many more parameters** (than weights). This is quite unlike normal training.

We need a training method that produces a simpler optimization problem

Reminder: optimization problems

Adversarial Training

find θ
minimize $\rho(\theta)$

where $\rho(\theta) = \mathbf{E}_{(x,y)\sim D}[\max\limits_{\boldsymbol{x}' \in \boldsymbol{S}(\boldsymbol{x})} L(\theta, \boldsymbol{x}', y)]$

Find input $\boldsymbol{x}'$ that achieves high loss

Good accuracy

Worse verifiability

Easier optimization

Certified Defense

find θ
minimize $\rho(\theta)$

where $\rho(\theta) = \mathbf{E}_{(x,y)\sim D}[\max\limits_{\boldsymbol{z} \in \boldsymbol{NN}^{\#}(\boldsymbol{S}(\boldsymbol{x}))} L(\theta, \boldsymbol{z}, y)]$

Find output $\boldsymbol{z}$ that achieves high loss (under abstraction)

Worse accuracy

Good verifiability

Harder optimization

Adversarial Training and Provable Defenses: Bridging the Gap

COLT: Balunovic and V, ICLR'20 (oral)

COLT: stands for Convex Layerwise Adversarial Training

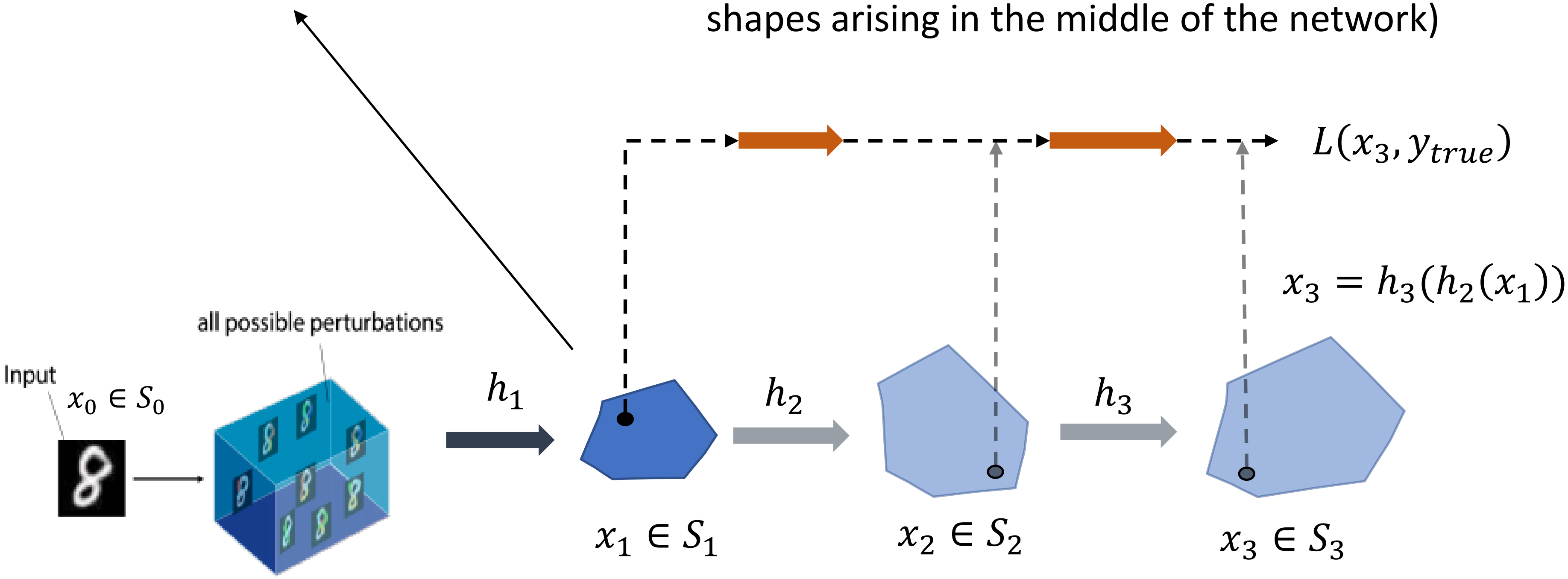
Key challenge:

Find point $x_1 \in S_1$ such that
loss L in the final layer is maximized
Need **projections** again!

Optimization problem (after layer 1):

$$\min_{\theta} \max_{x_1 \in S_1} L(\, h_3(h_2(x_1)), y_{true})$$

(high-level view: PGD training but with shapes arising in the middle of the network)



https://github.com/eth-sri/colt

COLT improved the results on various benchmarks using the Zonotope relaxation, but its drawback is that it requires efficient projection operators for more complex relaxations.

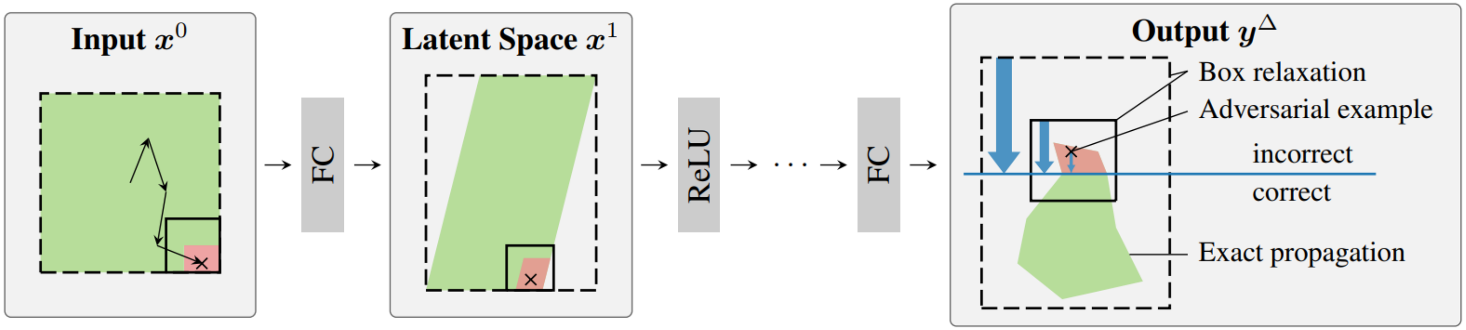
Following the idea of producing simpler optimization problems with tighter bounds, the latest advance in certified training only uses Box but in selective ways.

10 October, 2022: **Latest advance in certified training**

"CERTIFIED TRAINING: SMALL BOXES ARE ALL YOU NEED"

https://arxiv.org/pdf/2210.04871.pdf

Key insight: you can be unsound during forward pass when you train. If you select input sub-boxes carefully, you **can approximate well the worst-case loss on the whole box**.



Leads to state-of-the-art results across all benchmarks

Lecture Summary

Certified defenses: using relaxations during training in order to obtain more provable networks

We introduced the DiffAI method and showed how to instantiate it with two loss functions.

The DiffAI method and its follow-ups can produce complex optimization problems. Towards that, the trend is to seek a balance between easier optimizations problems and sufficient convex approximation precision.