Improving the Certified Robustness of Neural Networks via Consistency Regularization

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Abstract

A range of defense methods have been proposed to improve the robustness of neural networks on adversarial examples, among which provable defense methods have been demonstrated to be effective to train neural networks that are certifiably robust to the attacker. However, most of these provable defense methods treat all examples equally during training process, which ignore the inconsistent constraint of certified robustness between correctly classified (natural) and misclassified examples. In this paper, we explore this inconsistency caused by misclassified examples and add a novel consistency regularization term to make better use of the misclassified examples. Specifically, we identified that the certified robustness of network can be significantly improved if the constraint of certified robustness on misclassified examples and correctly classified examples is consistent. Motivated by this discovery, we design a new defense regularization term called Misclassification Aware Adversarial Regularization (MAAR), which constrains the output probability distributions of all examples in the certified region of the misclassified example. Experimental results show that our proposed MAAR achieves the best certified robustness and comparable accuracy on CIFAR-10 and MNIST datasets in comparison with several state-of-the-art methods.

Introduction

Despite the widespread success of neural network on diverse tasks such as image classification (Krizhevsky, Sutskever, and Hinton 2012), face and speech recognition (Taigman et al. 2014; Hinton et al. 2012). Recent studies have highlighted the lack of robustness in state-of-the-art neural network models, e.g., a visually imperceptible adversarial image can be easily crafted to mislead a well-trained network (Szegedy et al. 2014; Goodfellow, Shlens, and Szegedy 2015). The vulnerability to adversarial examples calls into question the safety-critical applications and services deployed by neural networks, including autonomous driving systems and malware detection protocols.

Considering the significance of adversarial robustness in neural network, a range of defense methods have been proposed. Adversarial training (Goodfellow, Shlens, and Szegedy 2015; Kurakin, Goodfellow, and Bengio 2016) which can be regarded as a data augmentation technique that trains neural networks on adversarial examples are highly robust against the strongest known adversarial attacks such as C&W attack (Carlini and Wagner 2017), but it provides no guarantee — it is unable to produce a certificate that there are no possible adversarial attack which could potentially break the model. To address this lack of guarantees, recent line of work on provable defense (Wong and Kolter 2018; Raghunathan, Steinhardt, and Liang 2018; Mirman, Gebr, and Vechev 2018; Cohen, Rosenfeld, and Kolter 2019) has proposed to train neural networks that no attacks within a certain region will alter the networks prediction. Moreover, recent work (Balunovic and Vechev 2020) combines adversarial training and provable defense methods to train neural network with both high certified robustness and accuracy.

However, recall that the formal definition of certified robustness is conditioned on natural examples that are correctly classified (Balunovic and Vechev 2020; Wong and Kolter 2018). Most provable defense methods treat equally in both correctly classified and misclassified examples during training process while evaluating certified robustness just on correctly classified examples. From this perspec-
the effect of misclassified example on certified robustness is unknown. Therefore, it is not clear for the following questions: (1) Do misclassified examples have effectiveness for improving certified robustness? (2) If yes, how can we make better use of misclassified examples to improve the certified robustness of neural network?

In this paper, we investigate this significant aspect of certified robustness, and find that the misclassified examples do have excellent influence on the certified robustness. To validate this discovery, we conduct a proof-of-concept experiment on CIFAR-10 (Krizhevsky, Hinton et al. 2009) with $L_\infty$ maximum perturbation $\epsilon = 2/255$ based on convex layer-wise adversarial training (COLT) [Balunovic and Vechev 2020].

Different from COLT, which searches the potential adversarial examples on all natural examples within the convex relaxation region for adversarial training layerwisely, we dynamically select two subsets of natural training examples to investigate: 1) a subset of correctly classified examples $C^+$ and 2) a subset of misclassified examples $C^-$. Using these two subsets, we explore different loss functions to re-train the same network $h_\theta$, and evaluate its original accuracy and verified error (The details of these metrics are in Appendix A.4) during the training process. Specifically, let $X$ be natural input of the network with $\{C^+, C^- \in X\}$ and $Y$ be its corresponding ground-truth label. $h_\theta(X)$ is denoted as corresponding output label produced by the network. First, let’s consider the traditional adversarial risk in COLT model:

$$COLT : ADV([C^+]', Y) + ADV([C^-]', Y)$$

where $ADV(\cdot)$ is the adversarial training loss function, $[C^+]', [C^-]'$ are adversarial examples produced by $C^+$ and $C^-$ within the perturbation sets, respectively. As shown in the first part $ADV([C^+]', Y)$ in Equation $1$, the objectives of robustness constraint and original accuracy constraint are the same for correctly classified examples: Constraining the correctly classified examples $C^+$ and all examples within their perturbations $[C^+]'$ to be close enough to the correct labels $Y$. However, for misclassified examples, the constraints on robustness and accuracy in the second part $ADV([C^-]', Y')$ are different: Making the misclassified examples $C^-$ and the examples in the perturbation set $[C^-]'$ close enough to the original labels $Y$ will improve the original accuracy of the network, but it is undeniable that this will destroy the stability of the misclassified examples (the original label is the “wrong label” for misclassified example), thereby reducing the certified robustness of the network. Based on the above observation, we find the constraints of certified robustness between correctly classified and misclassified examples are inconsistent, as shown in Figure 1. To deal with this problem, we firstly propose to use the output label (the output label is the “true label” for misclassified example) of the misclassified example during training process to keep the stability of misclassified examples. The adversarial risk is described as follows, which we call Misclassification Aware Training (MAT):

$$MAT : ADV([C^+]', Y) + ADV([C^-]', h_\theta(C^-))$$

where $h_\theta(C^-)$ denotes the output label corresponding to the input $C^-$. Interestingly, we find it that the misclassified examples have a significant effect on the final certified robustness of network (shown in Figure 2). Compared with COLT (dashed red line), the verified error of MAT (red line) drops drastically. However, the original accuracy of MAT (blue line) is extremely lower than standard COLT (dashed blue line).

In this paper, in order to make better use of misclassified examples, we propose a consistency regularization to constrain the probability distributions of all examples in the certified region of the misclassified example. The regularization term called Misclassification Aware Adversarial Regularization (MAAR) aims to encourage the output of network to be stable against misclassified adversarial examples. In other words, MAAR focuses on solving the inconsistency of certified robustness on correctly classified and misclassified examples, which improves the final certified robustness of network. Meanwhile, MAAR does not change the training label during the training process, which alleviates the decrease of model accuracy.

Our main contributions are:

- We investigate the inconsistency on constraint of certified robustness caused by misclassified examples by a proof-of-concept experiment (i.e., Misclassification Aware Training (MAT)).

- We propose a consistency regularization called Misclassification Aware Adversarial Regularization (MAAR) which improves certified robustness by maintaining the stability of misclassified examples as well as relieving the degree of accuracy decline.

- We show the effectiveness of MAAR by different networks and perturbations on two datasets. Specifically, MAAR achieves the state-of-the-art certified robustness of 62.8% on CIFAR-10 with $2/255$ $L_\infty$ perturbations on 4-layer convolutional network as well as 97.3% on MNIST dataset with $L_\infty$ perturbation 0.1 on 3-layer convolutional network.
Methods

Preliminaries

Base Classifier. For a $K$-class ($K \geq 2$) classification problem, denote a dataset $\{(x_i, y_i)\}_{i=1, \ldots, n}$ with distribution $x_i \in \mathbb{R}^d$ as natural input and $y_i \in \{1, \ldots, K\}$ represents its corresponding true label, a classifier $h_\theta$ with parameter $\theta$ predicts the class of an input example $x_i$:

$$h_\theta(x_i) = \arg \max_{k=1, \ldots, K} p_k(x_i, \theta)$$  \hspace{1cm} (3)

$$p_k(x_i, \theta) = \exp(z_k(x_i, \theta))/\sum_{k=1}^K \exp(z_k(x_i, \theta))$$  \hspace{1cm} (4)

where $z_k(x_i, \theta)$ is the logits output of the network with respect to class $k$, and $p_k(x_i, \theta)$ is the probability (softmax on logits) of $x_i$ belonging to class $k$.

Adversarial Risk. The adversarial risk \cite{Madry2017} on dataset $\{(x_i, y_i)\}_{i=1, \ldots, n}$ and classifier $h_\theta$ output probability $p(x)$ can be defined as follows:

$$\mathcal{ADV}(p(x'), y) = \frac{1}{n} \sum_{i=1}^n \max_{x'\in B_i(x_i)} \mathcal{L}(p(x'_i), y_i)$$  \hspace{1cm} (5)

where $\mathcal{L}$ is the loss function such as commonly used cross entropy loss, and $B_i(x_i) = \{ x : ||x - x_i||_p \leq \epsilon \}$ denotes the $L_p$-norm ball centered at $x_i$ with radius $\epsilon$. We will focus on the $L_\infty$-ball in this paper.

Original Training Risk in COLT. The original training risk in COLT \cite{Balunovic2020} is defined as follows:

$$\mathcal{R}_{COLT}(h_\theta, x_i) := \mathcal{L}_{ori}(p(x_i), y_i) + \mathcal{ADV}(p(x'_i), y_i)$$  \hspace{1cm} (6)

where $\mathcal{L}_{ori}(\cdot)$ is the original training loss function such as cross entropy loss and $x'_i \in B_i(x_i)$.

Misclassification Aware Adversarial Regularization

To differentiate and explore the effect of misclassified examples, we reformulate the training risk based on the prediction of the current network $h_\theta$. Specifically, we split the natural training examples into two subset according to $h_\theta$, with one subset of correctly classified examples ($C_{h_\theta}^+$) and one subset of misclassified examples ($C_{h_\theta}^-$):

$$C_{h_\theta}^+ = \{ i : i \in [n], h_\theta(x_i) = y_i \}$$  \hspace{1cm} (7)

$$C_{h_\theta}^- = \{ i : i \in [n], h_\theta(x_i) \neq y_i \}$$  \hspace{1cm} (8)

With the purpose of avoiding excessive reduction of the original accuracy as well as keeping the consistency of certified robustness on two subsets, we regularize misclassified examples by an additional term (a KL-divergence term that was used previously in \cite{Wang2019} \cite{Zhang2019} \cite{Zheng2016}) rather than changing the training labels. The proposed regularization term aims to constrain the output probability distributions of all examples in the certified region of the misclassified example, thus improving the certified robustness of network. The improved training risk of misclassified examples is formulated as follows:

$$\mathcal{R}^-(h_\theta, x_i) := \mathcal{L}_{ori}(p(x_i), y_i) + \mathcal{ADV}(p(x'_i), y_i) + \kappa \mathcal{KL}(p(x)||p(x'_i))$$  \hspace{1cm} (9)

where

$$\kappa \mathcal{KL}(p(x)||p(x'_i)) = \sum_{k=1}^K p_k(x_i, \theta) \log \frac{p_k(x_i, \theta)}{p_k(x'_i, \theta)}$$  \hspace{1cm} (10)

measures the difference of two distributions.

For correctly classified examples, we simply use original training risk, i.e.,

$$\mathcal{R}^+(h_\theta, x_i) := \mathcal{L}_{ori}(p(x_i), y_i) + \mathcal{ADV}(p(x'_i), y_i)$$  \hspace{1cm} (11)

Finally, by combining the two training risk terms (i.e., Equation (9) and Equation (11)), we train a network that minimizes the following risk:

$$\mathcal{R}(h_\theta, x) := \frac{1}{n} \sum_{x_i \in C_{h_\theta}^+} \mathcal{R}^+(h_\theta, x_i) + \sum_{x_i \in C_{h_\theta}^-} \mathcal{R}^-(h_\theta, x_i)$$

\hspace{1cm} (12)

where $\mathbb{I}(h_\theta(x_i) \neq y_i)$ is the indicator function. $\mathbb{I}(h_\theta(x_i) \neq y_i) = 1$ if $h_\theta(x_i) \neq y_i$, and $\mathbb{I}(h_\theta(x_i) \neq y_i) = 0$ otherwise.

Optimization for Regularization Term. As presented in Equation (12), the new training risk is a regularized adversarial risk with regularization term $\frac{1}{n} \sum_{i=1}^n \mathcal{KL}(p(x)||p(x'_i)) \cdot \mathbb{I}(h_\theta(x_i) \neq y_i)$. However, the indicator function cannot be directly optimized if we conduct a hard decision during the training process. In this study, we propose to use a soft decision scheme by replacing $\mathbb{I}(h_\theta(x_i) \neq y_i)$ with the output probability $1 - p_{y_i}(x_i, \theta)$. The output probability will be large for misclassified examples and small for correctly classified examples, by which we could provide a approximate solution for 0-1 optimization problem.

The Overall Objective. Based on the regularization optimization, the objective function of our proposed Misclassification Aware Adversarial Regularization (MAAR) is formulated as:

$$\mathcal{R}^{MAAR}(\theta) = \frac{1}{n} \sum_{i=1}^n \mathcal{L}^{MAAR}(x_i, y_i, \theta)$$  \hspace{1cm} (13)

where $\mathcal{L}^{MAAR}(x_i, y_i, \theta)$ is defined as:

$$\mathcal{L}^{MAAR}(x_i, y_i, \theta) = \mathcal{L}_{ori}(p(x_i), y_i) + \mathcal{ADV}(p(x'_i), y_i) + \lambda \cdot \mathcal{KL}(p(x)||p(x'_i)) \cdot (1 - p_{y_i}(x_i, \theta))$$  \hspace{1cm} (14)

Here, $\lambda$ is tunable scaling parameters and fixed for all training examples. The sensitivity of $\lambda$ is described in Appendix C.1. For more details on the training procedure, see Appendix A.
Table 1: Comparison with the state-of-the-art methods. Accuracy and certified robustness evaluated with $L_\infty$ perturbation $2/255$ and $8/255$ on CIFAR-10 dataset, $L_\infty$ perturbation 0.1 on MNIST dataset. ACC: Accuracy, CR: Certified robustness.

| Method             | CIFAR-10          | MNIST               |
|--------------------|-------------------|---------------------|
|                    | $\epsilon = 2/255$ | $\epsilon = 8/255$ |
| ACC(%) CR(%)       | ACC(%) CR(%)      |
| Our work (MAAR)    | 77.7 62.8         | 47.6 29.8           |
| COLT (2020)        | 80.0 58.6         | 51.3 26.7           |
| CROWN-IBP (2019a)  | 61.6 48.6         | 48.5 26.3           |
| IBP (2018)         | 58.0 47.8         | 47.8 24.9           |
| Xiao et al. (2018) | 61.1 45.9         | 40.5 20.3           |
| Mirman et al. (2019)| 62.3 45.5        | 46.2 27.2           |
|                   | 99.1 97.3         | 99.2 97.1           |
|                   | 98.7 96.6         | 98.8 95.8           |
|                   | 99.0 95.6         | 98.7 96.8           |

**Results**

![Certified Robustness Plot]

Figure 3: Certified robustness of COLT and MAAR with different perturbations.

**Certification under Different Perturbations.**

We evaluate the effectiveness of MAAR on certified robustness with different perturbations. As shown in Figure 3, the certified robustness of MAAR (orange bar) is obviously higher than COLT (blue bar) during different perturbations. Specifically, MAAR achieves the state-of-the-art certified robustness (i.e., 62.8%) compared with COLT (59.6%) when $\epsilon = 2/255$. We also show the effectiveness of MAAR during laywise training process in Appendix C.2. What’s more, further experimental results show that our MAAR achieves better certified robustness (62.8%) when comparison with giving all examples the same weight (60.8%).

**Comparison with Prior Work.**

We compare our MAAR with COLT (Balunovic and Vechev 2020), CROWN-IBP (Zhang et al. 2019a), IBP (Gowal et al. 2018) in the same network architecture, parameter settings, and certification progress. We also list the results reported in literature of Xiao et al. (2018) and Mirman et al. (2019) in Table 1. The network sizes and training parameters on two datasets (i.e., CIFAR-10 and MNIST) can be found in Appendix B.

**CIFAR-10.** For the $L_\infty$ perturbation $2/255$. Experiment results show that MAAR substantially outperforms its competitors by certified robustness (i.e., 62.8%). Besides, the accuracy of our method also outperforms other works except COLT. This is because one side-effect of our regularization is that it will maintain the distribution around misclassified examples, which will decrease the accuracy in comparison with COLT. Actually, the accuracy–robustness trade-off has been proved to exist in predictive models when training robust models (Tsipras et al. 2018; Zhang et al. 2019b).

We also run the same experiment for $L_\infty$ perturbation $8/255$. When under the same experimental settings, MAAR also achieves the best certified robustness (i.e., 29.8%). Here we do not compare with the certified robustness (i.e., 32.0%) reported in literature of IBP (Gowal et al. 2018) as their results were found to be not reproducible (Mirman, Singh, and Vechev 2019; Zhang et al. 2019b).

**MNIST.** To further evaluate the effectiveness of our method, we also conduct experiments on MNIST dataset with $L_\infty$ perturbation 0.1. We report the full results in Table 1, MAAR also achieve the state-of-the-art certified robustness (i.e., 97.3%) comparable with best results from prior work (i.e., 97.1%).

**Conclusion**

In this paper, we investigated the inconsistent constraint of certified robustness between correctly classified and misclassified and find that misclassified examples have a recognizable impact on the final certified robustness of network. Based on this observation, we designed a consistency regularization term which constrains the output probability distributions of examples in the certified region of the misclassified example. Our method, named Misclassification Aware Adversarial Regularization (MAAR), achieves the state-of-the-art certified robustness of 62.8% on CIFAR-10 with $2/255 L_\infty$ perturbation as well as 97.3% on MNIST dataset with $L_\infty$ perturbation 0.1. The method is general and can be instantiated with most of training risk.

In the future, we plan to investigate the association between accuracy and certified robustness among different neural networks, and apply our method to more provable defense frameworks.
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Appendix A. Algorithmic Details

A.1 MAAR Algorithm

Algorithm 1: Misclassification Aware Adversarial Regularization (MAAR)

\[\text{Input} \ d\text{-layer network } h_\theta, \text{ training set } \{(x, y)\}, \text{ learning rate } \eta, \text{ step size } \alpha, \text{ inner steps } n, \text{ tunable scaling parameters } \lambda, \epsilon.\]

\[\text{for } l \leq d \text{ do}\]

\[\text{for } j \leq n_{\text{epochs}} \text{ do}\]

\[\text{Sample mini-batch:}\]

\[\{(x_1, y_1), (x_2, y_2), \ldots, (x_b, y_b)\} \sim (\mathcal{X}, \mathcal{Y});\]

\[\text{Compute convex relaxations: } \mathcal{C}_l(x_1), \ldots, \mathcal{C}_l(x_b);\]

\[\text{Initialize: } x'_1 \sim \mathcal{C}_l(x_1), \ldots, x'_b \sim \mathcal{C}_l(x_b);\]

\[\text{for } i \leq b \text{ do}\]

\[x'_i \leftarrow \Pi_{\mathcal{C}_l(x_i)}(x'_i + \alpha \nabla x'_i \text{ADV}(h_\theta^{l+1:d}(x'_i), y_i));\]

\[\text{end for}\]

\[L(h_\theta^{l+1:d}(x'_i), y_i) \leftarrow L_{\text{ori}}(p(x_i), y_i) + \text{ADV}(p(x'_i), y_i) + \lambda \cdot K\mathcal{L}(p(x_i)) || p(x'_i) \cdot (1 - p_{y_i}(x_i, \theta))\]

\[\text{Update parameters:}\]

\[\theta \leftarrow \theta - \eta \cdot \frac{1}{b} \sum_{i=1}^b \nabla_{\theta} L(h_\theta^{l+1:d}(x'_i), y_i);\]

\[\text{end for}\]

\[\text{Freeze parameters } \theta_{l+1} \text{ of layer function } h_\theta^{l+1}.\]

\[\text{end for}\]

\[\text{Output} \ \text{Certified robust neural network } h_\theta\]

A.2 Training

The layerwise training (Balunovic and Vechev 2020) has been adopted in our MAAR’s training. Compared with standard adversarial training in (Madry et al. 2017), layerwise training not only performs adversarial attack on the input domain, but also searches potential adversarial examples in the hidden layer of the convex perturbation region. It will freeze the previous layers and stop back-propagation after the update of the current layer.

Each convex region of layer \(i\) is represented as a set \(\mathcal{C}_i(x) = \{a_i + A_i e | e \in [-1, 1]^m\}\) (Wong and Kolter 2018), vector \(a_i\) represents the center of the set and the matrix \(A_i\) represents the affine transformation of the hypercube \([-1, 1]^m\). Propagation of \(a_i, A_i\) through the network can be described as follows:

\[
\begin{align*}
    a_{i+1} &= \left\{ A_{i+1} a_i, \quad \# \text{ReLU Layer} \right. \\
    & \left. \text{s.t.} \quad \frac{1}{2} (x^l + x^u) \right. \\
    & A_{i+1} := \frac{a_{i+1}}{u_i - l_i} \\
    \quad W_{i+1} a_i + b_{i+1}, \quad \# \text{Conv. & FC. layer} \quad \text{and} \quad \text{bias vector} \\
    A_{i+1} &= \left[ \left[ A_{i+1}, M_{i+1} \right], \quad \# \text{ReLU Layer} \right. \\
    & \left. \text{s.t.} \quad \frac{1}{2} I_m (x^u - x^l) \right. \\
    & M_{i+1} := \frac{u_i - l_i}{2} \\
    & W_{i+1} a_i, \quad \# \text{Conv. & FC. layer} \\
\end{align*}
\]

where \(W_{i+1}\) and \(b_{i+1}\) are the weights matrix and bias matrix of layer \(i + 1\), respectively, \(x^l = \max(0, x - \epsilon)\) and \(x^u = \min(1, x + \epsilon)\), \(\epsilon\) is the \(L_\infty\) radius which we are certifying, \([::]\) denotes concatenation of matrices along the column dimension. Specifically, we first compute lower bound \(l_i\) and upper bound \(u_i\) in the set \(\mathcal{C}_i(x)\):

\[
l_i = a_i - |A_i| \quad (17)
\]

\[
u_i = a_i + |A_i| \quad (18)
\]

Then, we need to compute \(|A_i|_1\), which is the \(L_1\) norm of \(A_i\). According to Equation (16), we can get:

\[
A_i = [W_i A_{i-1}, W_{i-2} A_{i-3} \cdots M_0, \cdots, W_i A_{i-1} W_{i-2} M_{i-3}, W_i M_{i-1}] \quad (19)
\]

We use Cauchy random projections to efficiently estimate \(|A_i|_1\) (Wong and Kolter 2018). The method of random projections samples standard Cauchy random matrix \(R\) and split \(R = [R_0, R_1, \cdots, R_{l-1}]\) and compute:

\[
A_i R = W_i A_{i-1} W_{i-2} A_{i-3} \cdots M_0 R_0 + W_i A_{i-1} W_{i-2} M_{i-3} R_{i-3} + W_i M_{i-1} R_{i-1} \quad (20)
\]

Finally, we estimates \(|A_i|_1 \approx \text{median}(|A_i R|)\) and compute \(l_i, u_i\).
Based on these calculations, we search the adversarial examples in layer $i$ as follows:

$$e_n \leftarrow \text{clip}(e_n + \alpha A_i^T \nabla_{x_n} \text{ADV}(x_n', y_n), -1, 1)$$

(21)

$$x_n' \leftarrow a_i + A_i e_n$$

(22)

where $n$ is the iteration steps, clip($\cdot$) is function which thresholds its argument between -1 and 1.

### A.3 Certification

After training completes, we perform certification which is the same as [Balunovic and Vechev 2020] as follows: for every image, we first try to certify it using only linear relaxations. If this fails, we encode the last layer as MILP and try again. Finally, if this fails we encode the ReLU activation after the last convolution using additional up to 50 binary variables and the rest using the triangle formulation [Ehlers 2017]. We consider an image to be not certifiable if we fail to certify it using these methods. We always certify the full test set of 10 000 images. The overall verified pipeline is listed in Algorithm 2.

**Algorithm 2** Verified Pipeline for Provably Robust Certification: $\text{robust}(x_i)$

**Input** $d$-layer network $h_{\theta}$, testing sample $x_i$, perturbation $\epsilon$.

**if** $h_{\theta}(x_i) \neq y_i$ **then** \{##misclassified \}

verified fails; continue

**end if**

**if** $\text{PGD ATTACK success}$ **then**

verified fails; continue

**end if**

**if** $x_i : \text{DIFFAI-v3 verified}$ **then** \{##source code: https://github.com/eth-sri/diffai \}

verified success; continue

**end if**

Perform MILP solver to test $x_i$ layerwisely as follow. \{##source code: https://github.com/eth-sri/colt \}

**for** $l_i : \text{ALL RELU Layers}$ **do**

**if** MILP Solver for $x_i$ in layer $\#l_i$ fails **then**

ENCODER RELU layer $\#l_i$ using additional up to 50 binary variables.

**end if**

**end for**

**if** MILP Solver for $x_i$ success in last layer **then**

verified success

**end if**

**Output** Verified or Not Verified

### A.4 Evaluation Metrics

We use four metrics to evaluate our training models: original accuracy, certified robustness, verified error, and latent robustness. Original accuracy denotes the fraction of a testing set on which a model is correct. It is the standard accuracy metric used to evaluate any DNN, defended or not. Certified robustness denotes the fraction of the testing set on which a certified model predictions are both correct and certified robust for a given prediction robustness threshold. It has become a standard metric to evaluate models trained with certified defenses ([Wong and Kolter 2018], [Raghunathan, Steinhardt, and Liang 2018]). By considering the time consuming for calculating certified robustness during the training process, we define verified error to evaluate the robustness of network in training process. Verified error denotes the fraction of the training set on which the correctly classified examples become to adversarial examples, which is computationally tractable. Latent robustness denotes the fraction of the testing set on which a model predictions are both correct and robust against latent adversarial attacks on a certain layer. Mathematically, the metrics are defined as follows:

- **Original Accuracy (ACC):**

  $$\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(h_{\theta}(x_i) = y_i)$$

  (23)

  where $\mathbb{1}(h_{\theta}(x_i) = y_i)$ denotes a function that will return 1 if the prediction on one testing example $x_i$ returns the correct label $y_i$, and 0 otherwise.

- **Certified Robustness (CR):**

  $$\frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(\text{robust}(x_i) \& (h_{\theta}(x_i) = y_i))$$

  (24)
where \( \text{robust}(x_i) \) represents the network output is certifiable robust to input \( x_i \) (according to Appendix A.3), \( I(\cdot) \) is a indicator function.

- **Verified Error (VE):**
  \[
  \sum_{i=1}^{n} \frac{I((h_\theta(x'_i) \neq y_i) \& (h_\theta(x_i) = y_i))}{\sum_{i=1}^{n} I(h_\theta(x_i) = y_i)}
  \]
  where \( x'_i \in B_\epsilon(x_i) \), \( I(\cdot) \) is an indicator function.

- **Latent Robustness (LR):**
  \[
  \sum_{i=1}^{n} \frac{I((h_d^{\theta}(x'_i) = y_i) \& (h_\theta(x_i) = y_i))}{n}
  \]
  where \( x'_i \in B_\epsilon(x_i) \), \( I(\cdot) \) is an indicator function, \( h_d^{\theta}(\cdot) \) denotes that latent adversarial attack is performed on d-th layer of the network.

**Appendix B. Network Sizes and Training Parameters**

We perform all experiments on a desktop PC using a single GeForce RTX 2080 Ti GPU and 12-core Intel(R) Core(TM) i7-8700 CPU @ 3.20GHz. We implemented training and certification in PyTorch and used Gurobi 9.0 as a MILP solver.

**B.1 CIFAR-10**

The network architecture used for CIFAR-10 is a 4-layer convolutional network: first 3 layers are convolutional layers with filter sizes 32, 32, 128, kernel sizes 3, 3, 4 and strides 1, 2, 2, respectively. Convolutional layers are followed by a fully connected layer consisting of 250 hidden units. After each layer there is a ReLU activation. Final layer is a fully connected layer with 10 output neurons. The model is trained using SGD with momentum 0.9, the initial learning rate is 0.03 and after the initial 60 epochs we multiply the learning rate by 0.5 every 10 epochs. We use 8 steps during the latent adversarial attack and each step size is 0.25 (where perturbations are normalized between -1 and 1). We perform MAAR in 4 stages (i.e., the first convolutional layer (Stage #1), the second convolutional layer (Stage #2), the third convolutional layer (Stage #3), and the fully connected layer (Stage #4)), for 200 epochs per stage, for a total of 800 epochs.

**B.2 MNIST**

For MNIST, we use a 3-layer convolutional network: 2 convolutional layers with kernel sizes 5 and 4, and strides 2 followed by 1 fully connected layer consisting of 100 hidden units. Each of the layers is followed by a ReLU activation function. We use 40 steps for the latent adversarial attack with step size 0.035. We train using Adam [Kingma and Ba 2014] with initial learning rate 0.0001 and after the initial 100 epochs we multiply the learning rate by 0.5 every 10 epochs. We perform MAAR on MNIST in 4 stages (i.e., the first convolutional layer (Stage #1), the second convolutional layer (Stage #2), and the fully connected layer (Stage #3)), for 300 epochs per stage, for a total of 900 epochs.

**Appendix C. Additional Results**

**C.1 Sensitivity of Regularization Parameter \( \lambda \)**

![Figure 4: The network achieves different certified robustness and accuracy across different choices of regularization parameter \( \lambda \).](image-url)
The Consistent Promotion of MAAR in Layerwise Training Mechanism. In addition, we evaluate the final certified robustness of the network on the checkpoint saved after each stage’s training. As shown in Table 2, we can observe that the final certified robustness of our network has been significantly improved in layerwise training fashion (from 54.1% on Stage #1 to 62.8% on Stage #4). Furthermore, the final certified robustness of our proposed MAAR is obviously higher than COLT when evaluated on all stages. Meanwhile, we investigate the latent robustness (LR) of the model. Generally, we run latent adversarial attack (i.e., PGD attack with 150 steps and step size of 0.01) on 3-rd ReLU layer with parameters of each stage. Table 2 indicates the LR of our proposed MAAR improves from 58.3% on Stage #1 to 64.7% on Stage #4, which is also obviously outperforming COLT on all stages. These results demonstrate that MAAR can bring the consistent promotion in layerwise training.