Adversarial Training and Provable Robustness: A Tale of Two Objectives

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Abstract

We propose a principled framework that combines adversarial training and provable robustness verification for training certifiably robust neural networks. We formulate the training problem as a joint optimization problem with both empirical and provable robustness objectives and develop a novel gradient-descent technique that can eliminate bias in stochastic multi-gradients. We perform both theoretical analysis on the convergence of the proposed technique and experimental comparison with state-of-the-arts. Results on MNIST and CIFAR-10 show that our method can consistently match or outperform prior approaches for provable \( \ell_{\infty} \) robustness. Notably, we achieve 6.60\% verified test error on MNIST at \( \epsilon = 0.3 \), and 66.57\% on CIFAR-10 with \( \epsilon = 8/255 \).

Introduction

Vulnerability of deep neural networks to adversarial examples (Szegedy et al. 2014; Goodfellow, Shlens, and Szegedy 2015) has spurred the development of training methods for learning more robust models (Wong and Kolter 2018; Gowal et al. 2018; Zhang et al. 2020; Balunovic and Vechev 2020). Madry et al. (2018) show that adversarial training can be formulated as a minimax robust optimization problem as in (1). Given a model \( f_{\theta} \), loss function \( \mathcal{L} \), and training data distribution \( \mathcal{X} \), the training algorithm aims to minimize the loss whereas the adversary aims to maximize the loss within a neighborhood \( \delta(x, \epsilon) \) of each input data \( x \) as follows:

\[
\min_{\theta} \mathbb{E}_{(x, y) \in \mathcal{X}} \left[ \max_{x' \in \delta(x, \epsilon)} \mathcal{L}(f_{\theta}(x'), y) \right]
\]

In general, the inner maximization is intractable. Most existing techniques focus on finding an approximate solution. There are two main approaches to approximate the inner loss (henceforth referred to as \textit{abstract loss}). One direction is to generate adversarial examples to compute a lower bound of robust loss. The other is to compute an upper bound of robust loss by over-approximating the model outputs. We distinguish these two families of techniques below.

Adversarial training. To improve adversarial robustness, a natural idea is to augment the training set with adversarial examples (Kurakin, Goodfellow, and Bengio 2017). Using adversarial examples to compute the training loss yields a lower bound of \textit{robust loss}, henceforth referred to as \textit{adversarial loss}. Madry et al. (2018) propose to use projected gradient descent (PGD) to compute the adversarial loss and train the neural network by minimizing this loss. Networks trained using this method can achieve state-of-art test accuracy under strong adversaries (Carlini and Wagner 2017; Wang et al. 2018). More recently, Wong, Rice, and Kolter (2020) showed that fast gradient sign method (FGSM) (Goodfellow, Shlens, and Szegedy 2015) with random initialization can be used to learn robust models faster than PGD-based adversarial training. In term of efficiency, FGSM-based adversarial training is comparable to regular training. While adversarial training can produce networks robust against strong attacks, minimizing the adversarial loss alone cannot guarantee that (1) is minimized. In addition, it cannot provide rigorous guarantees on the robustness of the trained networks.

Provable robustness. Verification techniques (Katz et al. 2017; Dvijotham et al. 2018; Ruan, Huang, and Kwiatkowska 2018; Raghunathan, Steinhardt, and Liang 2018; Prabhakar and Aft 2019), on the other hand, can be used to compute a certified upper bound of \textit{robust loss} (henceforth referred to as \textit{abstract loss}). Given a neural network, a simple way to obtain this upper bound is to propagate value bounds across the network, also known as interval bound propagation (IBP) (Mirman, Gehr, and Vechev 2018). Techniques such as CROWN (Zhang et al. 2018), DeepZ (Singh et al. 2018), MIP (Tjeng, Xiao, and Tedrake 2019) and RefineZono (Singh et al. 2019), can compute more precise bounds, but also incur much higher computational costs. Building upon these upper bound verification techniques, approaches such as DIFFAI (Mirman, Gehr, and Vechev 2018) construct a differentiable \textit{abstract loss} corresponding to the upper bound estimation and incorporate this loss function during training. However, Gowal et al. (2018) and Zhang et al. (2020) observe that a tighter approximation of the upper bound does not necessarily lead to a network with low robust loss. They show that IBP-based methods can produce networks with state-of-the-art certified robustness. More recently, COLT (Balunovic and Vechev 2020) proposed to combine adversarial training and zonotope propagation. Zonotopes are a collection of affine forms of the input variables and intermediate vector outputs in the neural network. The idea is to train the network with the so-called latent adversarial examples which are adversarial examples that lie inside these zonotopes.
Table 1: Comparison of different methods for training robust neural networks. We highlight the loss function used in each method. If there is an abstract loss used in training or post-training verification, we also list the corresponding verification method. We categorize the methods along five dimensions, with ✓ indicating a desirable property or an explicit consideration.

| Method          | Loss          | Abstract loss | Efficiency¹ | Empirical Robustness | Provable Robustness | No weight² tuning/scheduling |
|-----------------|---------------|---------------|-------------|----------------------|---------------------|-----------------------------|
| Baseline        | regular loss  | n/a           | ✓           | ✓                    | ✓                   | n/a                         |
| FGSM (2015)     | adversarial loss | n/a           | ✓           | ✓                    | ✓                   | n/a                         |
| FGSM+random init (2020) | adversarial loss | n/a           | ✓           | ✓                    | ✓                   | n/a                         |
| PGD (2018)      | adversarial loss | n/a           | ✓           | ✓                    | ✓                   | n/a                         |
| COLT (2020)     | latent adversarial loss | RefineZono³ | ✓           | ✓                    | ✓                   | n/a                         |
| DIFFAI (2018)   | abstract loss | DeepZ         | ✓           | ✓                    | ✓                   | n/a                         |
| CROWN-IBP (2020) | regular loss+abstract loss | CROWN + IBP | ✓           | ✓                    | ✓                   | n/a                         |
| **AdvIBP**      | adversarial loss + abstract loss | IBP          | ✓           | ✓                    | ✓                   | ✓                           |

¹ The efficiency baseline is the training time for each epoch during regular training. ✓ represents the training time is comparable to the baseline.
² The weights here represent the weights for the different losses if there are multiple of them.
³ RefineZono is not used to construct an abstract loss. Instead, it is used to generate latent adversarial examples and for post-training verification.
⁴ In their experiments, DIFFAI shows that adding regular loss with a fixed weight can achieve better performance.
⁵ DIFFAI can also use IBP for training and verification for improved efficiency. However, the best robustness results are achieved using DeepZ.

This work: a principled framework for combining adversarial loss and abstract loss. We first start with the observation that there is a substantial gap between the provable robustness obtained from state-of-art verification tools and the empirical robustness of the same network against strong adversary in large-scale models. In this paper, we propose to bridge this gap by marrying the strengths of adversarial training and provable bound estimation techniques. Minimizing adversarial loss and minimizing abstract loss can be viewed as bounding the true robust loss from two ends. We argue that simultaneously reducing both losses is more likely to produce a network with good empirical and provable robustness. From an optimization perspective, this amounts to an optimization problem with two objectives and can be solved using gradient descent methods if both objectives are semi-smooth. The challenge is how to balance the minimization of these two objectives during training. In particular, computing the gradient based on a weighted-sum of the objectives can result in biased gradients. Inspired by the work on moment estimates (Kingma and Ba 2016), we propose a novel joint training scheme to compute the weights adaptively and minimize the joint objective with unbiased gradient estimates. For efficient training, we instantiate our framework in a tool called AdvIBP, which uses FGSM and random initialization for computing the adversarial loss and IBP for computing the abstract loss. We validate our approach on a set of commonly used benchmarks demonstrate and demonstrate that AdvIBP can learn provably robust neural networks that match or outperform state-of-art techniques. We summarize and compare the key features of prior methods and AdvIBP in Table 1.

Main contributions.

- A novel framework for training provably robust deep neural networks. The framework marries the strengths of adversarial training and provable upper bound estimation in a principled way.
- A novel gradient descent method for two-objective optimization that uses moment estimates to address the issue of bias in stochastic multi-gradients. We also perform the

Theoretical analysis of the proposed method.

- Experiments on the MNIST and CIFAR-10 datasets show the proposed method can achieve state-of-the-art performance for networks with provable robustness guarantees.

Background

In this paper, we consider an adversary who can perturb an input $x \in \mathcal{X}$ from a data distribution $\mathcal{X}$ arbitrarily within a small $\epsilon$ neighborhood of the input. In the case of $l_\infty$ perturbation, which we experiment with later, we define the allowable adversarial input set as $S(x, \epsilon) = \{ x' \mid \|x' - x\|_\infty \leq \epsilon \}$.

We define a $L$-layer neural network parameterized by $\theta$ as a function $f_\theta$ recursively as:

$$f_\theta(x) = z^{(L)}, \quad z^{(l)} = W^{(l)} h^{(l-1)} + b^{(l)}, \quad h^{(l)} = \sigma^{(l)}(z^{(l)})$$

where $l \in \{1, \cdots, L-1\}$. $z$ represent the pre-activation neuron values, $h$ represent post-activation neuron values and $\sigma$ is an element-wise activation function. We denote $h_\theta^{(l)}$ the mapping applied at layer $l$ with parameter $\theta_l$ and the network can be represented as $f_\theta = h_\theta^{(L)} \circ h_\theta^{(L-1)} \cdots \circ h_\theta^{(1)}$.

In classification, the provable robustness seeks for the lower bounds of the margins between the ground-truth logit and all other classes. Let vector $m$ be the margins between the ground-truth class and all other classes. Each element in $m$ is a linear combination of the output (Wong and Kolter 2018): $c^T f_\theta(x)$, where $c$ is set to compute the margin. We define the lower bound of $m$ in $S(x, \epsilon)$ as $m(x, c; \theta)$. When all elements of $m(x, c; \theta) > 0$, $x$ is verifiably robust for any perturbation with $l_\infty$-norm less than $\epsilon$.

Interval bound propagation (IBP). Interval bound propagation uses a simple bound propagation rule. For the input layer we define element-wise upper and lower bound for $x$, $z^{(l)}$ and $h^{(l)}$ as $x_L \leq x_L \leq x_U$, $z^{(l)} \leq z^{(l)} \leq z^{(l)}$ and $h^{(l)} \leq h^{(l)} \leq h^{(l)}$. For affine layers, we have:

$$z^{(l)} = W^{(l)} h^{(l-1)} + b^{(l)}$$

$$h^{(l)} = \sigma^{(l)}(z^{(l)})$$

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where \( W^{(l)} = \min(0, W^{(l)}) \) and \( W^{(l)} = \max(0, W^{(l)}) \). Note that \( \hat{h}^{(0)} = x_U \) and \( \hat{h}^{(1)} = x_L \). For monotonic increasing activation functions \( \sigma \), we have \( \hat{h}^{(1)} = \sigma (x^{(1)}) \) and \( h^{(1)} = \sigma (x^{(1)}) \).

We define \( m_{\text{IBP}}(x; c; \theta) \) as the lower bound of the margin obtained by IBP which is an underapproximation of \( m(x; c; \theta) \). More generally, we use \( m_{\text{abstract}}(x; c; \theta) \) as the lower bound of the margin obtained by abstract methods. When \( m_{\text{abstract}}(x; c; \theta) \geq 0, \) \( x \) is verifiably robust by the abstract method for any perturbation with \( l_{\infty} \)-norm less than \( \epsilon \). Additionally, [Wong and Kolter 2018] showed that for cross-entropy (CE) loss:

\[
\max_{x^* \in \mathcal{B}(x, \epsilon)} \mathcal{L}(f(x^*), y) \leq \mathcal{L}(-m_{\text{abstract}}(x; c; \theta); y; \theta) \tag{2}
\]

IBP or other abstract methods gives a tractable upper bound of the inner-max in (1) and we refer it as abstract loss. In practice, solely minimizing abstract loss can be unstable and hard to tune [Mirman, Gehr, and Vechev 2018; Gowal et al. 2018]. To mitigate this instability, prior works [Mirman, Gehr, and Vechev 2018; Gowal et al. 2018; Zhang et al. 2020] propose to stabilize the minimization of the abstract loss by adding normal robust loss in the objective. More specifically, the new objective can be formed as follows:

\[
\mathcal{L}(\theta) = \kappa_1 \mathcal{L}(f_\theta(x), y) + \kappa_2 \mathcal{L}(-m_{\text{abstract}}; y; \theta) \tag{3}
\]

The coefficients \( \kappa_1 \) and \( \kappa_2 \) are hand-tuned to balance the minimization between robust loss and abstract loss. The goal is to improve the robustness of the trained model while avoiding the instability caused by loose abstract loss with respect to the true robust loss. Among different abstract methods, computing IBP bounds only requires two simple forward passes through the network and is thus computationally efficient. The downside of IBP, however, is that it can lead to loose upper bounds. [Mirman, Gehr, and Vechev 2018; Gowal et al. 2018] propose to combine regular loss and IBP abstract loss as \( \frac{1}{2} \). CROWN-IBP [Zhang et al. 2020] uses a mixture of linear relaxation and IBP to compute the abstract loss and jointly minimize it with the regular loss. While the approaches based on \( \frac{1}{2} \) produce state-of-the-art results on a set of benchmarks, this type of works rely on an \( ad \) hoc scheduler to tune the weights between the regular loss and the abstract loss during training. In addition, regular loss is a loose lower bound of robust loss and minimizing the regular loss does not directly guide the training to a robust model. In this paper, we show that it is better to combine adversarial loss and abstract loss while leveraging the efficiency of IBP. Moreover, we can eliminate weight tuning and scheduling in a principled manner.

**Methodology**

**Overview.** Let the perturbed input be \( x_{\text{adv}} \). The relations among adversarial loss, robust loss and IBP abstract loss are as follows.

\[
\mathcal{L}(f_\theta(x_{\text{adv}}), y) \leq \max_{x^* \in \mathcal{B}(x, \epsilon)} \mathcal{L}(f_\theta(x^*), y) \leq \mathcal{L}(-m_{\text{IBP}}(x, \epsilon); y; \theta) \tag{4}
\]

We note that (4) holds for general adversarial training and provable robustness methods. Specifically adversarial loss provides a lower bound of robust loss and minimizing this loss can result in good empirical robustness. Latent adversarial examples [Balunovic and Vechev 2020], for instance, can be used to construct a different adversarial loss. However, a smaller latent adversarial loss does not necessarily indicate better certified robustness. COLT [Balunovic and Vechev 2020] uses multiple regularizers to mitigate this issue. On the other hand, minimizing the abstract loss can help to train a network with certified robustness. In this case, the choice of verification methods used in computing the abstract loss can significantly influence the final training outcome. For instance, training with the IBP abstract loss can result in a network that is amenable to IBP verification. The true robustness of the network or the robustness attainable under the given neural network architecture, however, could still be far away from this bound. In fact, a small gap between empirical robustness and provable robustness does not necessarily indicate the attainment of good robustness (the extreme case would be a ReLU network with only positive weights). Thus, the tightness of both losses relative to robust loss is critical to improving the model’s true robustness.

We consider the joint minimization of adversarial loss and abstract loss as a two-objective optimization problem. A straightforward way to solve this joint optimization problem is to optimize a weighted sum of the objectives. This leads to the following objective similar to \( \frac{1}{2} \):

\[
\mathcal{L}(\theta) = \kappa_1 \mathcal{L}(f_\theta(x_{\text{adv}}), y) + \kappa_2 \mathcal{L}(-m_{\text{IBP}}; y; \theta) \tag{5}
\]

However, this simple linear-combination formulation is only sensible when the two objectives are not competing, which is rarely the case. The conflicting objectives require modeling the trade-off between objectives, and are generally handled by adaptive weight updates [Sener and Koltun 2018]. This approach, however, faces the issue that even though the stochastic gradients for each objective are unbiased estimates of the corresponding full gradients, the weighted sum of the stochastic gradients is a biased estimate if the weights are associated with the sampled gradients. This bias can cause instability and local optima issues [Liu and Vicente 2019]. In this paper, we leverage moment estimates to compute the weights adaptively and ensures their independence from the corresponding sampled gradients to eliminate the bias. Minimizing the two objectives jointly tightens the approximation of robust loss from both ends. For efficient training, we develop \textit{AdvIBP} using FGSM+random init to compute adversarial loss and IBP to compute abstract loss.

**Joint Training as Two-Objective Optimization**

We propose a two-objective optimization method inspired by [Fan et al. 2019; Zhang, Yu, and Turk 2019] to choose the gradient descent direction that reduces adversarial loss and abstract loss simultaneously. Let the adversarial loss be \( \mathcal{L}_{\text{adv}}(\theta) \) and IBP abstract loss be \( \mathcal{L}_{\text{IBP}}(\theta) \). Their gradients with respect to \( \theta \) are denoted by

\[
g_{\text{adv}} = \nabla_\theta \mathcal{L}_{\text{adv}}(\theta), \quad g_{\text{IBP}} = \nabla_\theta \mathcal{L}_{\text{IBP}}(\theta)
\]

To balance between the two objectives, we update the network parameters in the direction of the angular bisector of the two
Then, we average the projected vectors of the two gradients on this direction. If \((g_{\text{adv}}, g_{\text{IBP}}) > 0\), this results in an update that is expected to reduce both losses to improve the adversarial accuracy and tighten IBP. If \((g_{\text{adv}}, g_{\text{IBP}}) \leq 0\), taking the angular bisector direction results in an update that improves the objective functions little or not at all for either objective. In this case, we project one of the gradients onto the hyperplane that is perpendicular to the other gradient. The idea is that when two gradients disagree with each other, we prioritize the minimization of one of the objectives. The final gradient guides the search in the direction that reduces the prioritized objective while avoiding increasing the other objective. We use Algorithm 1 to illustrate this computation.

To decide which direction to prioritize, the tightness of adversarial loss and abstract loss relative to the ground-truth robust loss can be the determining factor. \cite{Wang2019} propose the First-Order Stationary Condition (FOSC) to quantitatively evaluate the adversarial strength of adversarial examples. In general, the adversarial loss is closer to robust loss with stronger adversarial examples. Let \(c(x_{\text{adv}})\) be FOSC value of \(x_{\text{adv}}\) and \(c_t\) be the threshold that indicates the desired adversarial strength at the \(t\)-th epoch. Smaller FOSC values would indicate stronger adversarial examples. With strong attacks \((c(x_{\text{adv}}) \leq c_t)\), adversarial training leads to robust models. Thus, we prioritize the gradient of adversarial loss in this case. The idea is to drive the search to the region of robust models with high accuracy and stabilize the minimization of abstract loss. With weak attacks \((c(x_{\text{adv}}) > c_t)\), minimizing adversarial loss does not necessarily imply better robustness. However, minimizing abstract loss makes solving \(c(x_{\text{adv}})\) tractably. We prioritize the gradient of abstract loss in this case. Figure 1 provides a visualization of the final gradient computation in different cases.

![Figure 1: Three cases of computing \(g_{\text{final}}\) from \(g_{\text{adv}}\) and \(g_{\text{IBP}}\).](image)

**Stochastic gradients.** Since the data distribution \(\mathcal{X}\) is unknown in practice, it is impossible to get the full gradients, \(g_{\text{adv}}\) and \(g_{\text{IBP}}\). We denote the realizations of the stochastic objectives at subsequent training epochs as \(L_{\text{adv,t}}(\theta^0), \ldots, L_{\text{adv,t-1}}(\theta^{T-1})\) and \(L_{\text{IBP,t}}(\theta^0), \ldots, L_{\text{IBP,t-1}}(\theta^{T-1})\). The stochastic gradients \(g_{\text{adv,t}}\) and \(g_{\text{IBP,t}}\) are the evaluations of data points from mini-batches and provide unbiased estimation of the full gradients. However, the stochastic gradient of the weighted-sum objective at the \(t\)-th epoch becomes a biased estimate of the final gradient, \(g_{\text{final}}\). The bias is the result of dependence between the weights and the corresponding stochastic gradients.

**Unbiased weights computation.** To eliminate this bias, we propose to compute the weights from the estimates of the first and norm moments of the gradients instead of the stochastic gradients. The goal is to ensure the independence of stochastic gradients and the corresponding weights. Let \(m_{1,t}, m_{2,t}, v_{1,t}\) and \(v_{2,t}\) represent the moment estimates for \(g_{\text{adv,t}}, g_{\text{IBP,t}}\). We modify the moment estimate in \cite{Kingma2015} to meet the independence requirement. In Algorithm 2, the \(t\)-th moment estimates are the exponential moving averages of the past stochastic gradients from epoch 0 to epoch \(t - 1\), where the hyper-parameters \(\beta_1, \beta_2 \in [0, 1)\) control the exponential decay rates. The moving averages themselves, \(m_{1,t}, m_{2,t}, v_{1,t}, v_{2,t}\), are estimate of the first moment and the norm moment of the true gradients. The independent mini-batch sampling guarantees the independence of stochastic gradients. Thus, the moment estimates are independent from the current sampled stochastic gradient. Then, we calculate the weights using the moment estimates in Algorithm 1 and update the model parameters with unbiased gradient estimates.

The overall joint training algorithm is shown in Algorithm 2. The regularization term \(\kappa_{\text{reg}}\) in line 11 is only used when prioritizing the minimization of abstract loss. The regularizer helps to bound the convergence rate of training.

**Leveraging FOSC in joint training.** In Algorithm 2, we use similar dynamic criterion FOCS as in \cite{Wang2019}. In the early stages of training, \(c_t\) is close to the maximum FOCS value \(c_{\text{max}}\), which can be satisfied with weak adversarial examples. Thus, the early stages of training will mostly prioritize the minimization of adversarial loss. This helps to avoid the instability caused by a loose abstract loss. However, prioritizing the adversarial loss does not necessarily improve
Algorithm 2 Joint Training

1: **Input** Warm-up epochs $T_{nat}$ and $T_{adv}$, $c_{\text{train}}$ ramp-up epochs $R$, maximum FOSC value $c_{\text{max}}$
2: $f_{\theta_0} \leftarrow \text{WARM-UP}(f_{\theta_0}, T_{nat}, T_{adv})$
3: for $t = 0$ to $T - 1$
4:     $c_t = c_{\text{train}} - (t - R) \cdot c_{\text{max}} / T'$, $0, c_{\text{max}}$
5:     Sample $B = \{(x_1, y_1), \ldots, (x_B, y_B)\} \sim (X, Y)$
6:     for $i = 0$ to $|B| - 1$
7:         $\epsilon_i \leftarrow \text{RAMPUP_SCHEDULER}(t, \epsilon_{\text{train}}, R)$
8:     $x_{\text{adv}}, \gamma \leftarrow \text{FGSM+RANDOM_INIT}(x_i, y_i, \epsilon_i)$
9:     end for
10: $\kappa_{\text{adv}}, \kappa_{\text{IBP}}, \kappa_{\text{reg}} \leftarrow \text{COMPUTE_WEIGHTS}(x_{\text{adv}}, t, \epsilon_t)$
11: $\ell \leftarrow \kappa_{\text{adv}} \ell_{\text{adv}}(\theta_t') + \kappa_{\text{IBP}} \ell_{\text{IBP}}(\theta_t') + \kappa_{\text{reg}} \| \ell_{\text{IBP}}(\theta_t') \|^2_2$
12: $\theta_{t+1} = \theta_t - \eta_t \gamma_{\text{final}}(\theta_t') \circ \gamma_{\text{final}}(\theta_t')$; stochastic gradient
13: end for
14: procedure **WARMUP**($f_{\theta_0}, T_{nat}, T_{adv}$) \triangleright Warm-up phase
15:     for $t = 0$ to $T_{nat} - 1$
16:         Train on the regular loss $\mathcal{L}(f_{\theta_t'}, (x, y))$
17:     end for
18: end procedure
19: for $t = T_{nat}$ to $T_{nat} + T_{adv} - 1$
20:     Train on the adversarial loss $\mathcal{L}(f_{\theta_t'}(x_{\text{adv}}), y)$
21: end for
22: return $f_{\theta_T}$
23: end procedure

The verified robustness of the models. Thus, we design the FOSC value $c_t$ so that it decreases linearly towards zero as training progresses. As a result, in the later training stages, the joint training scheme will mostly prioritize the minimization of the abstract loss to improve provable robustness.

Theoretical Analysis

We provide a theoretical analysis of our proposed joint training scheme to train IBP certified robust networks. It aims to provide insights on how the ground-truth robust loss changes during training by our joint training scheme. The gradient update and the prioritization scheme provide an approximate maximizer for the inner maximization. Below, we provide theoretical analyses on how robust loss changes when two gradients agree with each other and how abstract loss changes when two gradients disagree with each other.

In detail, let $x^*(\theta) = \arg\max_{x \in (x, e)} \mathcal{L}(f_{\theta}(x'), y)$. $\hat{x}(\theta)$ is a $\delta$-approximation solution to $x^*$, if it satisfies that ($\text{Wang et al.}^{2019}$)

$$c(\hat{x}(\theta)) = \max_{x \in \tilde{B}^+(x, e)} \langle x' - \hat{x}(\theta), \nabla x \mathcal{L}(f_{\theta}(\hat{x}(\theta)), y) \rangle \leq \delta (6)$$

Let the robust loss in (1) be $\mathcal{L}(\theta)$, and its gradient be $\nabla \mathcal{L}(\theta) = \mathbb{E}[\nabla \theta \mathcal{L}(f_{\theta}(x^*(\theta)), y)]$. We denote the stochastic gradient of $\mathcal{L}(\theta)$ as $g(\theta) = 1 / |B| \sum_{i \in B} \nabla \theta \mathcal{L}(f_{\theta}(x_i^*(\theta)), y_i)$. We denote the stochastic gradient of $\mathcal{L}(\theta)$ as $\tilde{g}(\theta) = \mathbb{E}[\nabla \theta \mathcal{L}(\mathcal{M}(x, e); y)]$. Note that $\mathbb{E}[g(\theta)] = \nabla \mathcal{L}(\theta)$ and $\mathbb{E}[\tilde{g}(\theta)] = \nabla \tilde{\mathcal{L}}(\theta)$. The adversarial loss, $\mathcal{L}_{adv}(\theta)$, is $\mathbb{E}[\mathcal{L}(f_{\theta}(\hat{x}(\theta)), y)]$ and its stochastic gradient is $\hat{g}(\theta) = 1 / |B| \sum_{i \in B} \nabla \theta \mathcal{L}(f_{\theta}(\hat{x}(\theta)), y_i)$. We make assumptions similar to those in ($\text{Wang et al.}^{2019}$) and present the theoretical analysis of our method below.

**Assumption 1.** The function $\mathcal{L}(\theta; x)$ and $\mathcal{L}(\theta; x)$ satisfies the gradient Lipschitz conditions s.t.

$$\sup_x \| \nabla \theta \mathcal{L}(\theta; x) - \nabla \theta \mathcal{L}(\theta'; x) \|_2 \leq L_{\theta \theta} \| \theta - \theta' \|_2$$
$$\sup_x \| \nabla \theta \mathcal{L}(\theta; x) - \nabla \theta \mathcal{L}(\theta; x') \|_2 \leq T_{\theta x} \| x - x' \|_2$$
$$\sup_x \| \nabla \theta \tilde{\mathcal{L}}(\theta; x) - \nabla \theta \mathcal{L}(\theta; x') \|_2 \leq L_{\theta \tilde{\theta}} \| x - x' \|_2$$
$$\sup_x \| \nabla \theta \mathcal{L}(\theta; x) - \nabla \theta \tilde{\mathcal{L}}(\theta; x) \|_2 \leq L_{\theta \tilde{\theta}} \| x - x' \|_2$$

where $L_{\theta \theta}, L_{\theta x}, L_{\theta \tilde{\theta}}, L_{\theta \tilde{\theta}}$ are positive scalars. Assumption[1] was made in ($\text{Wang et al.}^{2019}$) to assure the smoothness of the loss function. Recent studies ($\text{Du et al.}^{2019}$) help justify it by showing that the loss function of overparameterized neural networks is semi-smooth. Let $\Delta = \mathcal{L}(\theta) - \min_0 \mathcal{L}(\theta)$ and $\Delta = \mathcal{L}(\theta) - \min_0 \mathcal{L}(\theta)$. Under Assumption[1], we have the following theoretical results.

**Theorem 1.** If the dot product of the gradients of the two objectives is greater than 0 and the step size of the training is set to $\eta_\theta = \eta \min(1/6L, \sqrt{\Delta / T \Delta^2})$, then the expectation of the gradient of robust loss satisfies

$$\frac{1}{T} \sum\limits_{t=0}^{T-1} \mathbb{E}[\| \nabla \mathcal{L}(\theta_t') \|^2_2] \leq 8\sigma \sqrt{\frac{L_{\Delta \Delta}}{T}} + \frac{7L_{\Delta \Delta}^2}{3\mu}$$

**Theorem 2.** If the dot product of the gradients of the two objectives is smaller or equal to 0, adversarial loss is not tight enough ($c(x_{\text{adv}}) > c_t$), and the step size of training is set to $\eta_\theta = \eta \min(2 \times \mathbb{E}[\| \ell_{\text{IBP}}(\theta_t') \|_2 - 1 / L, \sqrt{\Delta / T \Delta^2})$ with $\mathbb{E}[\| \ell_{\text{IBP}}(\theta_t') \|_2] > 1/2$, then the expectation of the gradient of IBP abstract loss satisfies

$$\frac{1}{T} \sum\limits_{t=0}^{T-1} \mathbb{E}[\| \nabla \tilde{\mathcal{L}}(\theta_t') \|^2_2] \leq 2\sigma \sqrt{\frac{L_{\Delta \Delta}}{T}} (1 + \sum\limits_{t=0}^{T-1} (1 + \mathbb{E}[\| \ell_{\text{IBP}}(\theta_t') \|_2^2]))$$

The complete proof can be found in the Appendix. If the two gradients agree with each other (i.e. their dot product is greater than 0), Theorem[1] suggests that the robust loss minimization can converge to a first-order stationary point at a sublinear rate with sufficiently small $\delta$. Using FOSC ensures that the adversarial loss approximates the robust loss up to a precision less than $\delta$ as in (6). Note that it is difficult
for the perturbed input $x_{adv}$ to reach the maximum adversarial strength (minimum FOSC value which is 0) as the model becomes more robust during training. Algorithm 2 will mostly prioritize the abstract loss minimization when the two gradients disagree with each other since $c_t$ is decreasing to 0. In this case, Theorem 2 suggests that the abstract loss (as obtained by IBP) minimization can converge to a first-order stationary point at a sublinear rate. Although $L_{IBP}$ is not guaranteed to converge, our joint training scheme actively reduces the abstract loss to avoid its divergence. In practice, potential divergence of the $L_{IBP}$ is controlled with a stable training process in our method. Although Theorem 2 requires $E[\mathcal{L}_{IBP}(\theta^t)]>1/2$, the abstract loss will be sufficiently small if the condition does not hold. With Theorem 1 and 2, the robust loss or its upper bound abstract loss can be minimized at a sublinear convergence rate. These results provide theoretical support for our approach.

Experiment

Experiment setup. We evaluate AdvIBP on all the network model structures used in (Gowal et al. 2018, Zhang et al. 2020) on the MNIST and CIFAR-10 datasets with different $l_\infty$ perturbation bounds, $\epsilon$. We denote these models as DM-Small, DM-Medium and DM-Large. We perform all experiments on a desktop server using at most 4 GeForce GTX 1080 Ti GPUs. All models are trained using a single GPU except for DM-Large which requires all 4 GPUs.

Metrics. We use the following metrics to compare the trained neural networks: (i) IBP verified error, which is the percentage of test examples that are not verified by IBP; (ii) standard error, which is the test error evaluated on the clean test dataset; and (iii) PGD error, which is the test error under 200-step PGD attack. Verified errors provide the worst-case test error against $l_\infty$ perturbations. PGD errors provide valid lower bounds of test errors against $l_\infty$ perturbations.

![Figure 2: Comparison with the baseline.](image)

Baseline comparison. We consider a baseline method that uses the same warm-up strategy in Algorithm 2 but fixes the coefficients to $\kappa_{adv}=1.0$ and $\kappa_{IBP}=1.0$ (effectively using the weighted sum method). As shown in Figure 2 (b) AdvIBP, which automatically adapts the coefficients, reduces the IBP verified errors by 9.1% to 31.9% compared with the baseline.

Comparison with prior works. Table 4 and 5 shows the standard, verified and PGD errors under different $\epsilon$ on CIFAR-10 and MNIST. On CIFAR-10, our method outperforms the state-of-art methods on verified errors obtained from IBP. In addition to CROWN-IBP, we also present the best errors reported by IBP method (Gowal et al. 2018), MIP (Xiao et al. 2019) and COLT (Balunovic and Vechev 2020). Note that MIP (Xiao et al. 2019) reports the verified error obtained by mixed integer programming, which is able to compute the exact value of robust loss. COLT (Balunovic and Vechev 2020) uses RefineZono to compute the verified errors and RefineZono is supposed to a much higher precision than IBP. On both MNIST and CIFAR-10, even though our method does not use regular loss, we still achieve lower standard errors across different models in most cases. The verified errors obtained by AdvIBP on MNIST can match the prior state-of-art results. The result of $l_\infty$ perturbation 2/255 outperforms existing approaches except for the results in (Zhang et al. 2020; Singh et al. 2019). However, we note here that both methods in (Zhang et al. 2020; Singh et al. 2019) use over-approximation methods with better precision in both training and verification, which may result in significant computation overhead and memory requirement. We hypothesize that the main reason for this performance gap is that with a relatively small $l_\infty$ perturbation, the minimization of IBP abstract loss reduces the capacity of the models to learn well as reflected by the higher standard errors.

Additionally, we compare AdvIBP with CROWN-IBP across a wide range of neural network models (Table 1) rather than on a few hand-selected models. In Table 3, we present the best, median and worst verified and standard test errors for models trained on MNIST and CIFAR-10 using CROWN-IBP (with default settings) and AdvIBP respectively. AdvIBP’s best, median and worst verified errors outperform those of CROWN-IBP in almost all cases.

AdvCROWN-IBP. In our joint training scheme, one can replace IBP with a more precise method for computing the abstract loss. We present here the results of AdvCROWN-IBP which uses CROWN-IBP to compute the abstract loss on the MNIST dataset. CROWN-IBP uses a linear combination of CROWN bounds and IBP bounds to compute the abstract loss during the warm-up period. After the warm-up period, the abstract loss is computed solely with IBP bounds. In Table 4 we can observe that with a more precise abstract loss, our joint training scheme outperforms CROWN-IBP and AdvIBP in IBP verified errors consistently across different model structures. In fact, to the best of our knowledge, AdvCROWN-IBP achieves the best verified error rates compared to those reported in existing literature on the MNIST dataset across different choices of network models for these $\epsilon$ bounds.

Conclusion

We propose a new certified adversarial training framework that bridges the gap between adversarial training and provable robustness from a joint training perspective. We formulate the joint training as a two-objective optimization problem, which facilitates the balance between adversarial loss and abstract loss. We show that our joint training framework outperforms prior certified adversarial training methods in both standard and verified errors, and achieves state-of-the-art verified test errors for $l_\infty$ robustness.
Table 2: Evaluation on the CIFAR-10 dataset between models trained by AdvIBP and those by CROWN-IBP. AdvIBP outperforms the state-of-art, CROWN-IBP, and other best reported results under all perturbation and model settings if IBP is used to compute the verified errors. If different network architectures and more precise verification methods are also considered, our IBP verified errors still outperform the best prior results for both $\epsilon = \frac{8}{255}$ and $\epsilon = \frac{10}{255}$.

| $\epsilon$ (\textit{L}_\infty norm) | Training Method | DM-Small model’s err. (%) | DM-Medium model’s err. (%) | DM-Large model’s err. (%) | Best errors reported in literature(\%)
|---|---|---|---|---|---|
| $\epsilon = \frac{2}{255}$ | CROWN-IBP | 38.15 | 52.57 | 50.35 | 32.78 | 49.57 | 44.22 | 28.48 | 46.03 | 40.28 | IBP method (Gowal et al. 2018) | 39.22 | 55.19 | 28.88 | 54.07 |
| | AdvIBP | 42.33 | 56.00 | 50.08 | 35.36 | 52.27 | 43.75 | 40.61 | 51.66 | 46.97 | COLT (Balunovic and Vechev 2020) | 21.60 | 39.50 |
| $\epsilon = \frac{8}{255}$ | CROWN-IBP | 59.94 | 70.76 | 69.65 | 58.19 | 68.94 | 67.72 | 54.02 | 66.94 | 65.42 | IBP method (Gowal et al. 2018) | 58.43 | 70.81 | 59.55 | 79.73 |
| | AdvIBP | 57.88 | 70.34 | 66.52 | 54.20 | 68.21 | 61.21 | 52.86 | 66.57 | 61.66 | COLT (Balunovic and Vechev 2020) | 48.30 | 72.50 |
| $\epsilon = \frac{16}{255}$ | CROWN-IBP | 67.42 | 78.41 | 76.86 | 67.94 | 78.46 | 77.21 | 66.06 | 76.80 | 75.23 | IBP method (Gowal et al. 2018) | 68.97 | 78.12 | n/a | n/a |
| | AdvIBP | 67.32 | 78.12 | 73.44 | 66.26 | 77.79 | 73.52 | 64.40 | 76.05 | 71.78 | COLT (Balunovic and Vechev 2020) | n/a | n/a | n/a | n/a |

1. The verified error of CROWN-IBP in this setting is computed using CROWN.
2. Some of the best errors from literature are obtained from models with different architectures from ours. Some of the verified errors are also obtained using more precise verification methods.
3. The results are reproduced by [Zhang et al. 2020] on the same perturbation settings and models used by our method and CROWN-IBP. The verified error is obtained from IBO.

Table 3: Standard, verified and PGD test errors for a wide range of models trained on MNIST and CIFAR-10 datasets using CROWN-IBP and AdvIBP. The purpose of this experiment is to compare model performance statistics on a wide range of models, rather than a few selected models. For each setting, we report 3 statistics, the smallest, median and largest verified errors. We also report the standard and PGD errors in the same way.

| Dataset | $\epsilon$ (\textit{L}_\infty norm) | Training Method | Standard Error (%) | Verified Error (%) | PGD Error (%) | Number of AdvIBP models with lower verified errors among all trained model structures |
|---|---|---|---|---|---|---|
| MNIST | $\epsilon = 0.2$ | CROWN-IBP | 2.49 | 3.50 | 5.39 | 4.81 | 6.33 | 8.82 | 3.42 | 4.94 | 7.33 | 9/10 |
| | AdvIBP | 2.41 | 3.36 | 5.29 | 4.76 | 6.13 | 8.52 | 3.31 | 4.70 | 7.01 | |
| | $\epsilon = 0.3$ | CROWN-IBP | 2.49 | 3.50 | 5.39 | 7.19 | 9.12 | 11.58 | 3.85 | 5.47 | 8.46 | 8/10 |
| | AdvIBP | 2.41 | 3.36 | 5.29 | 7.21 | 8.86 | 11.32 | 4.04 | 5.40 | 8.80 | |
| CIFAR-10 | $\epsilon = \frac{1}{255}$ | CROWN-IBP | 57.25 | 59.84 | 63.46 | 60.02 | 71.32 | 72.40 | 65.56 | 67.57 | 70.17 | 7/7 |
| | AdvIBP | 57.03 | 58.85 | 60.97 | 68.50 | 69.36 | 71.40 | 65.08 | 66.90 | 68.74 | |

Table 4: Evaluation on the MNIST dataset between models trained by AdvIBP, AdvCROWN-IBP and those by CROWN-IBP. The CROWN-IBP result is from Table C. in [Zhang et al. 2020]. AdvIBP achieves competitive performance compared to CROWN-IBP on MNIST. AdvCROWN-IBP outperforms CROWN-IBP under all settings, and achieves state-of-the-art verified errors on MNIST dataset for $l_\infty$ robustness.

| $\epsilon$ (\textit{L}_\infty norm) | Training Method | DM-Small model’s err. (%) | DM-Medium model’s err. (%) | DM-Large model’s err. (%) | Best errors reported in literature(\%) |
|---|---|---|---|---|---|
| $\epsilon = 0.1$ | CROWN-IBP | 1.67 | 3.44 | 3.09 | 1.14 | 2.64 | 2.23 | 0.97 | 2.25 | 2.18 |
| | AdvIBP | 1.63 | 3.69 | 2.70 | 1.41 | 3.24 | 2.26 | 1.03 | 2.28 | 2.53 |
| | AdvCROWN-IBP | 1.52 | 3.19 | 2.39 | 1.23 | 2.88 | 2.18 | 1.22 | 2.19 | 1.57 |
| $\epsilon = 0.2$ | CROWN-IBP | 2.96 | 6.11 | 5.74 | 2.37 | 5.35 | 4.90 | 1.62 | 3.87 | 3.81 |
| | AdvIBP | 4.15 | 7.68 | 5.81 | 2.33 | 5.37 | 3.54 | 1.58 | 4.70 | 2.59 |
| | AdvCROWN-IBP | 3.22 | 6.02 | 4.50 | 2.45 | 5.16 | 3.27 | 1.31 | 3.87 | 1.98 |
| $\epsilon = 0.3$ | CROWN-IBP | 3.55 | 9.40 | 8.50 | 2.37 | 8.54 | 7.74 | 1.62 | 6.68 | 8.58 |
| | AdvIBP | 4.15 | 10.80 | 6.83 | 2.33 | 8.73 | 4.35 | 1.58 | 8.23 | 3.17 |
| | AdvCROWN-IBP | 3.22 | 9.03 | 5.42 | 2.45 | 8.31 | 3.81 | 1.90 | 6.60 | 2.87 |
| $\epsilon = 0.4$ | CROWN-IBP | 3.78 | 15.21 | 13.34 | 3.16 | 14.19 | 11.31 | 1.62 | 12.46 | 9.47 |
| | AdvIBP | 4.15 | 17.57 | 8.48 | 2.72 | 16.18 | 5.58 | 1.88 | 16.57 | 3.21 |
| | AdvCROWN-IBP | 3.22 | 14.42 | 6.69 | 2.98 | 13.88 | 6.38 | 1.90 | 12.30 | 3.46 |

1. To further probe the true robustness of the trained models, we verify the robustness of the AdvIBP trained models with a more precise method, RetinaZono. The results are shown in Table B. in the Appendix.
2. We have also tested three model structures similar to DM-Small, DM-Medium and DM-Large. Results are reported in Table C. in the Appendix. For these models, AdvIBP already outperforms CROWN-IBP in all settings.
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Ethics Statement

Broad acceptance and adoption of large-scale deployments of deep learning systems rely critically on their trustworthiness which, in turn, depends on the ability to assess and demonstrate the safety of such systems. Concerns like adversarial robustness already arise with today’s deep learning systems and those that may be exacerbated in the future with more complex systems. Our research has the potential to enable the efficient training of robust deep learning systems. It can help unlock deep learning applications that are currently not deployable due to safety, robustness or resource concerns. These applications range from autonomous driving to mobile devices, and can benefit the society at large.

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Appendix

Additional Experiment Results

Table C presents the verified and standard errors for three model architectures in A and perturbation settings used in (Zhang et al. 2020). On these three new models, AdvIBP outperform CROWN-IBP on the verified and standard errors in all settings.

Table A: Model structures used in the experiments. "Conv \( k \times h + s \)" represents a 2D convolutional layer with \( k \) filters of size \( w \times h \) using a stride of \( s \) in both dimensions. "FC \( n \)" represents a fully connected layer with \( n \) outputs. The last fully connected layer is omitted. All networks use ReLU activation functions.

| Dataset       | DM-Small model (s) | DM-Model model (s) | DM-Large model (s) |
|---------------|--------------------|--------------------|--------------------|
| MNIST         | 6683               | 43024              | 128747             |
| CIFAR-10      | 63570              | 292863             | 527667             |

For a mini-batch \( B \), we compute the average of the FOSC values, \( c(x) = \sum_{i=0}^{|B|-1} c(x_{adv,i}) \), and compare it with \( c_t \) to determine the prioritization direction (line 12 in Algorithm 1).

Training Time

In terms of runtime compared to the baseline method in Figure 2, the training times of the baseline method for the three models were 5942, 38290, and 108683 seconds. On the same models and hardware, AdvIBP took 6683, 43024, and 128747 seconds respectively. This shows that the automatic coefficient computation in AdvIBP does not significantly increase training time. Furthermore, since AdvIBP primarily combines FGSM-AT and IBP training, the efficiency of AdvIBP is comparable to those of FGSM-AT and IBP.

In Table B, we present the training time of AdvIBP for the models used in our experiments. The hyperparameters are chosen as stated in . We perform layer-wise training for each model and report the total training time here. All experiments are measured on a single GeForce GTX 1080 Ti GPU with 11 GB RAM except DM-Large models where we used 4 GeForce GTX 1080 Ti GPUs to speed up training.

The Computation of FOSC Value

We use Eq.(4) in Wang et al. (2019) to compute the FOSC value for \( x_{adv} \) generated by FGSM+random initialization. Specifically, for an allowable perturbation input set \( S(x, \epsilon) \), the FOSC value of \( x_{adv} \in S(x, \epsilon) \) is computed as follows.

\[
c(x_{adv}) = \epsilon \| \nabla_x L(f_\theta(x_{adv}), y) \|_1 - (x_{adv} - x, \nabla_x L(f_\theta(x_{adv}), y))
\]
Table C: The standard and verified errors for trained models on MNIST.

| $\epsilon (l_\infty \text{ norm})$ | Training Method | CNN-Small model’s err. (%) | CNN-Medium model’s err. (%) | CNN-Large model’s err. (%) |
|-----------------------------------|-----------------|-----------------------------|-----------------------------|-----------------------------|
|                                   |                 | Standard | Verified | Standard | Verified | Standard | Verified |
| $\epsilon = 0.1$                  | CROWN-IBP       | 1.44     | 2.85     | 1.19     | 2.65     | 1.07     | 2.56     |
|                                   | AdvIBP          | 1.09     | **2.63** | 1.12     | **2.60** | 1.01     | **2.50** |
| $\epsilon = 0.2$                  | CROWN-IBP       | 2.81     | 5.79     | 2.57     | 4.93     | 2.34     | 4.71     |
|                                   | AdvIBP          | 2.38     | **5.22** | 2.33     | **4.66** | 2.04     | **4.37** |
| $\epsilon = 0.3$                  | CROWN-IBP       | 2.81     | 8.55     | 2.57     | 7.78     | 2.34     | 7.22     |
|                                   | AdvIBP          | 2.38     | **8.52** | 2.33     | **7.58** | 2.04     | **6.87** |
| $\epsilon = 0.4$                  | CROWN-IBP       | 2.81     | 13.74    | 2.57     | 13.53    | 2.34     | 12.00    |
|                                   | AdvIBP          | 2.38     | **13.24**| 2.33     | **13.36**| 2.04     | **11.98**|

Table D: Evaluation on the MNIST dataset between models trained by AdvIBP and those by CROWN-IBP. We verify the networks with RefineZono (Singh et al. 2019) for 1000 images randomly sampled from the test dataset. The IBP verified errors are in parentheses. The CROWN-IBP results are from Table C in (Zhang et al. 2020).

| $\epsilon (l_\infty \text{ norm})^2$ | Training Method | DM-Small model’s err. (%) | DM-Medium model’s err. (%) | DM-Large model’s err. (%) |
|--------------------------------------|-----------------|---------------------------|---------------------------|---------------------------|
|                                      |                 | Verified | PGD     | Verified | PGD     | Verified | PGD     |
| $\epsilon = 0.1$                     | CROWN-IBP       | 3.44     | 3.09    | 3.26     | 2.82    | 2.10 (2.24) | 1.81 |
|                                      | AdvIBP          | **2.90** (3.69) | 2.70     | **2.80** (3.24) | 2.26    | **1.90** (2.28) | 1.53 |
| $\epsilon = 0.2$                     | CROWN-IBP       | 6.11     | 5.74    | 5.35     | 4.90    | 4.00 (3.87) | 3.81 |
|                                      | AdvIBP          | 6.80 (7.68) | 5.81    | **4.50** (5.37) | 3.54    | **3.80** (4.70) | 2.59 |
| $\epsilon = 0.3$                     | CROWN-IBP       | 9.40     | 8.50    | 8.54     | 7.74    | 6.20 (6.68) | 5.85 |
|                                      | AdvIBP          | 9.30 (10.80) | 6.83    | **6.80** (8.73) | **4.35** | **5.70** (8.23) | 3.17 |

1 The models reported in (Zhang, Yu, and Turk 2019) were unavailable except DM-Large at the time when this paper was written. As a result, we only report the verified errors obtained by RefineZono for the DM-Large models trained using CROWN-IBP.
2 We do not present the result of RefineZono at $\epsilon=0.4$ due to the intensive GPU memory request. This configuration is not reported in related works (Balunovic and Vechev 2020, Mirman, Gehr, and Vechev 2018, Singh et al. 2018) on similar-scale models.
3 The computation of the verified error under this setting uses DeepZ on a single TESLA V100 GPU with 16GB memory and costs 5 hours. RefineZono will take days to verify 1000 inputs.
Models and Hyperparameters

The models structures (DM-Small, DM-Medium and DM-Large) used in Table 2 and 3 are listed in Table 4. These three model structures are the same as those in (Gowal et al. 2018; Zhang et al. 2020). The large models are trained on 4-GPUs. For small and medium sized models, we train them on a single GPU. The model structures used in Table 2 are listed in Table 3. These models are all trained on a single GPU. Training hyperparameters are detailed below:

- For MNIST AdvIBP with $\epsilon_{\text{train}} = 0.2$ and $\epsilon_{\text{train}} = 0.4$ in Table 4, we set warm-up epochs as $T_{\text{nat}} = 10$ and $T_{\text{adv}} = 40$. We use Adam optimizer and set learning rate to $5 \times 10^{-4}$. After warm-up phase, we train 200 epochs with a batch size of 256 and gradually ramp up $\epsilon$ from 0 to $\epsilon_{\text{train}}$ in $R = 50$ epochs with extra 10 epochs training at $\epsilon_{\text{train}}$. We control the linear decay rate of $c_t$ with $T'$. We set $T' = 50$ starting with $c_{\text{max}} = 1e-4$ for $\epsilon_{\text{train}} = 0.4$ and $c_{\text{max}} = 1e-5$ for $\epsilon_{\text{train}} = 0.2$. We reduce the learning rate by $4 \times$ at epoch 150 and 200. At the layer-wise training stage, we start with learning rate $1.25 \times 10^{-4}$ and train 250 epochs each layer. We reduce the learning rate by $4 \times$ at 50, 100 and 200 epoch. The exponential decay rates for computing the weights are set to $\beta_1 = 0.9$ and $\beta_2 = 0.99$.

- For CIFAR-10 AdvIBP, we set $\epsilon_{\text{train}} = 1.1c$ and train 3200 epochs each layer with a batch size of 256. We set the first 800 epochs as warm-up phase with $T_{\text{nat}} = 400$ and $T_{\text{adv}} = 410$. Then, we ramp up $\epsilon$ for $R = 1000$ epochs with extra 20 epochs training at $\epsilon_{\text{train}}$. We set $T' = 280$ starting with $c_{\text{max}} = 1e-3$ for $\epsilon_{\text{train}} = 0.8$ and $c_{\text{max}} = 1e-5$ for $\epsilon_{\text{train}} = 0.2$. Learning rate is reduced by $10 \times$ at epoch 2200 and 2700 from $5 \times 10^{-4}$. At the layer-wise training stage, we start with learning rate $5 \times 10^{-5}$ and train 3200 epochs each layer. We reduce the learning rate by $10 \times$ every 1000 epochs. The exponential decay rates for computing the weights are set to $\beta_1 = 0.9$ and $\beta_2 = 0.99$.

Table E: Model structures used in the experiments. ”Conv k $w \times h \times s$” represents a 2D convolutional layer with k filters of size $w \times h$ using a stride of s in both dimensions. ”FC n” represents a fully connected layer with n outputs. The last fully connected layer is omitted. All networks use ReLU activation functions.

| DM-Small | DM-Medium | DM-Large |
|----------|-----------|----------|
| Conv 16 4 x 4 + 2 | Conv 32 3 x 3 + 1 | Conv 64 3 x 3 + 1 |
| Conv 32 4 x 4 + 1 | Conv 64 3 x 3 + 1 | Conv 64 3 x 3 + 1 |
| FC 100 | Conv 64 3 x 3 + 1 | Conv 128 3 x 3 + 2 |
| Conv 64 4 x 4 + 2 | Conv 128 3 x 3 + 1 | Conv 128 3 x 3 + 1 |
| FC 512 | Conv 128 3 x 3 + 1 | Conv 512 |

Hyperparameters $c_{\text{max}}$ and $\beta$. The hyperparameters unique to AdvIBP are the initial bound for adversarial strength (FOSC value) and the exponential moving average decay rate in moment estimates.

We choose the $c_{\text{max}}$ based on the adversarially trained networks. Let us assume that we fix the adversarial attack strategy to generate the perturbed inputs. For arbitrary networks without adversarial training, it is easy for a perturbed input to flip the output. Though the adversarial strength of the perturbed input is high (small FOSC value), the true robustness of the network is low. For adversarially trained networks, it becomes hard to find a perturbed input that can flip the output since these networks have strong empirical robustness. The adversarial loss computed based on the generated perturbed inputs cannot approximate the robust loss tightly. As a result, a perturbed input can have low adversarial strength. The FOSC value of a perturbed input against an adversarially trained network provides an estimate of the largest FOSC value that an perturbed input can achieve under the specified perturbation against a robust model. At the beginning of training, this estimate allow us to train on weak adversarial examples to stabilize the training process. Wang et al. (2019) observes that training on adversarial examples of higher adversarial strength at later stages leads to higher robustness. Thus, we set $c_{\text{max}}$ to the FOSC value based on the adversarially trained network initially. Then, after the warm-up phase, we gradually decrease $c_t$. Decreasing $c_t$ requires stronger and stronger adversarial examples to fulfill the condition $c(x_{\text{adv}}) \leq c_t$ where the optimization prioritizes the minimization of adversarial loss.

Our choice of exponential average decay rate is inspired by the choices made in (Kingma and Ba 2016). The decay rate for the first order moment estimate is set to $\beta_1 = 0.9$. The decay rate for the 2-norm moment estimate is set to $\beta_2 = 0.99$. In the future, we plan to experiment with more choices for the decay rates to investigate how they influence the training process.

Layer-wise Training

We investigate the role of latent adversarial examples plays in our training process. Recall that adversarial loss and latent adversarial loss are obtained from random initialized FGSM. We freeze the current layer where attacks apply and train the rest of the network layer by layer. In Figure A we show the verified errors achieved when the parameters of the corresponding layer are frozen. Note that while layer-wise latent adversarial loss helps with improving certified robustness, AdvIBP already produces competitive results in terms of verified error at layer 0 (i.e. adversarial examples in the inputs). In addition, the layer-wise training strategy produces most
of the improvement in the first two layers. One major difference between Adversarial Loss and Abstract Loss is that we consider the tightness of over-approximation explicitly and model the trade-off between latent adversarial loss and abstract loss without requiring weight tuning. COLT (Balunovic and Vechev 2020) does not explicitly consider abstract loss but use multiple regularization terms to control the over-approximation. Adding these regularization terms does not guarantee tighter over-approximation and the coefficient for each regularization term needs to be picked manually.

During the experiments, we also observed that strong latent adversarial examples are easy to be found if the over-approximation is loose. These latent adversarial examples are far from the boundary of the over-approximation. This indicates that minimizing the latent adversarial loss alone cannot guarantee better precision of over-approximation. This observation further motivates the need to explicitly consider the minimization of the abstract loss and our proposed joint training scheme.

**Proof of Theorem 1 and 2**

**Assumption 2.** The robust loss and abstract loss are locally strongly concave with respect to \( \mu \) and \( \bar{\mu} \) in allowable adversarial attack set \( \mathcal{S}(x, \epsilon) \). With the result of Lemma 1 in Wang et al. (2019), we have for any \( \theta_1 \) and \( \theta_2 \) the following holds

\[
\mathcal{L}(\theta_1) \leq \mathcal{L}(\theta_2) + \langle \nabla \mathcal{L}(\theta_2), \theta_1 - \theta_2 \rangle + \frac{L}{2} \| \theta_1 - \theta_2 \|_2^2, \quad \mathcal{Z}(\theta_1) \leq \mathcal{Z}(\theta_2) + \langle \nabla \mathcal{Z}(\theta_2), \theta_1 - \theta_2 \rangle + \frac{L}{2} \| \theta_1 - \theta_2 \|_2^2
\]

where \( L = (L_{\theta x} L_{\mu x} / \mu + L_{\mu x}) \) and \( \mathcal{L} = (L_{\theta x} L_{\mu x} / \mu + L_{\mu x}) \).

The relation between (1) and distributional robust optimization (Sinha, Namkoong, and Duchi 2018; Lee and Raginsky 2018) supports the strongly concave assumption. The last assumption is common in stochastic gradient based optimization algorithms.

**Assumption 3.** The variances of stochastic gradients \( g(\theta) \) and \( \bar{g}(\theta) \) are bounded by constants \( \sigma, \sigma > 0 \):

\[
\mathbb{E}[\| \nabla \mathcal{L}(\theta) \|_2^2] \leq \sigma^2, \quad \mathbb{E}[\| \nabla \mathcal{Z}(\theta) \|_2^2] \leq \sigma^2
\]

where \( \nabla \mathcal{L}(\theta) \) and \( \nabla \mathcal{Z}(\theta) \) are full gradients.

The proof is inspired by Wang et al. (2019). Before we prove the theorems, we need the following lemma from Wang et al. (2019) to bound the difference between the gradient of adversarial loss and that of robust loss.

**Lemma 1.** Under Assumptions 1 and 2 the approximate stochastic gradient \( \hat{g}(\theta) \) satisfies

\[
\| \hat{g}(\theta) - g(\theta) \|_2 \leq L_{\theta x} \sqrt{\frac{\delta}{\mu}}
\]

(7)
Proof of Theorem 1: We first prove Theorem 1 under the case where \(\langle m_{1,t} \cdot m_{2,t} \rangle > 0\).

\[
L(\theta^{t+1}) \leq L(\theta^t) + \langle \nabla L(\theta^t), \theta^{t+1} - \theta^t \rangle + \frac{L}{2} \| \theta^{t+1} - \theta^t \|^2
\]

\[
= L(\theta^t) - \eta_t \left( \frac{1}{v_{1,t}} \frac{1}{v_{2,t}} \frac{1}{v_{1,t}} \| \nabla L(\theta^t) \|^2 + \frac{L \eta^2}{2} \| \nabla L(\theta^t) \|^2 + \frac{L \eta^2}{2} \| \theta^t \| \right)
\]

\[
= L(\theta^t) - \eta_t \left( \frac{1}{v_{1,t}} \frac{1}{v_{2,t}} \frac{1}{v_{1,t}} \| \nabla L(\theta^t) \|^2 + \frac{L \eta^2}{2} \| \nabla L(\theta^t) \|^2 + \frac{L \eta^2}{2} \| \theta^t \| \right)
\]

\[
\leq L(\theta^t) - \frac{\eta_t}{2} \| \nabla L(\theta^t) \|^2 + \frac{\eta_t}{2} (1 + 3 \eta \| \nabla L(\theta^t) \|) + \frac{\eta_t}{2} (1 + L \eta) \frac{L \eta^2 \| \theta^t \|}{\mu}
\]

Assume the same condition \(g_{adv} \cdot g_{IBP} > 0\) holds and \(\eta_t = \| \nabla L(\theta^t) \| \cdot \eta\)

\[
E[\| \nabla L(\theta^t) \|^2] \leq \frac{\eta_t}{2} (1 - 3 \eta \| \nabla L(\theta^t) \|) + \frac{\eta_t}{2} (1 + L \eta) \frac{L \eta^2 \| \theta^t \|}{\mu}
\]

Taking telescope sum of \(E[\| \nabla L(\theta^t) \|^2] \) over \(t = 0, \ldots, T - 1\), we obtain

\[
\sum_{t=0}^{T-1} \frac{\eta_t}{2} (1 - 3 \eta \| \nabla L(\theta^t) \|) \leq E[\| \nabla L(\theta^t) \|^2] + \frac{\eta_t}{2} (1 + L \eta) \frac{L \eta^2 \| \theta^t \|}{\mu} + L \eta^2 \sigma^2
\]

Choosing \(\eta = \min(1/6L, \sqrt{\Delta/TL \sigma^2})\), we can show that

\[
\frac{1}{T} \sum_{t=0}^{T-1} E[\| \nabla L(\theta^t) \|^2] \leq 8 \frac{\sqrt{\Delta L}}{T} \frac{7L \eta^2 \| \theta^t \|}{3 \mu}
\]

which completes the proof.
Proof of Theorem 2

Now we prove Theorem 2 under the case where \( \langle m_{1,t} \cdot m_{2,t} \rangle \leq 0 \).

\[
\mathcal{L}(\theta^{t+1}) \leq \mathcal{L}(\theta^t) + \langle \nabla \mathcal{L}(\theta^t), \theta^{t+1} - \theta^t \rangle + \frac{T}{2} \| \theta^{t+1} - \theta^t \|^2 \\
= \mathcal{L}(\theta^t) - \eta_t (1 + \mathcal{L}(\theta^t)) \mathcal{g}(\theta^t) + \eta_t \frac{\langle m_{1,t}, m_{2,t} \rangle}{v_{1, t}} \mathcal{g}(\theta^t) \\
+ \frac{T \eta_t^2}{2} \| \frac{\langle m_{1,t}, m_{2,t} \rangle}{v_{1, t}} \mathcal{g}(\theta^t) - (1 + \mathcal{L}(\theta^t)) \mathcal{g}(\theta^t) \|_2^2 \\
= \mathcal{L}(\theta^t) - \eta_t (1 + \mathcal{L}(\theta^t))(\nabla \mathcal{L}(\theta^t), \mathcal{g}(\theta^t)) + \frac{T \eta_t^2}{2} (1 + \mathcal{L}(\theta^t))^2 \| \mathcal{g}(\theta^t) \|^2 \\
+ \frac{\eta_t \langle m_{1,t}, m_{2,t} \rangle}{v_{1, t}} (\nabla \mathcal{L}(\theta^t), \mathcal{g}(\theta^t)) + \frac{T \eta_t^2 \langle m_{1,t}, m_{2,t} \rangle^2}{2 v_{1, t}^2} \| \mathcal{g}(\theta^t) \|^2 \\
- \frac{T \eta_t^2 \langle m_{1,t}, m_{2,t} (1 + \mathcal{L}(\theta^t)) \rangle}{v_{1, t}^2} (\mathcal{g}(\theta^t), \mathcal{g}(\theta^t))
\]

Taking expectation on both sides of the above inequality conditioned on \( \theta^t \), we have

\[
\mathbb{E}[\mathcal{L}(\theta^{t+1})] - \mathcal{L}(\theta^t) \leq - \eta_t (1 + \mathcal{L}(\theta^t))(1 - \frac{T \eta_t (1 + \mathcal{L}(\theta^t))}{2}) \| \nabla \mathcal{L}(\theta^t) \|^2 \\
+ \frac{T \eta_t^2 (1 + \mathcal{L}(\theta^t))^2}{2} \| \mathcal{g}(\theta^t) \|^2 \\
= - \eta_t (1 + \mathcal{L}(\theta^t)) - \frac{T \eta_t}{2} \| \nabla \mathcal{L}(\theta^t) \|^2 \\
+ \frac{T \eta_t^2 (1 + \mathcal{L}(\theta^t))^2}{2} \| \mathcal{g}(\theta^t) \|^2 \\
(9)
\]

Taking telescope sum of (9) over \( t = 0, \ldots, T - 1 \), we obtain

\[
\sum_{t=0}^{T-1} \eta_t (\mathbb{E}[\mathcal{L}(\theta^t)]) - \frac{T \eta_t}{2} \mathbb{E}[\| \nabla \mathcal{L}(\theta^t) \|^2_2] \leq \mathbb{E}[\mathcal{L}(\theta^0) - \mathcal{L}(\theta^T)] + \sum_{t=0}^{T-1} \frac{T \eta_t^2 (1 + \mathcal{E}[\mathcal{L}(\theta^t)])^2}{2} \sigma^2
\]

Choosing \( \eta_t = \min(2 * \mathbb{E}[\mathcal{L}(\theta^t)] / \mathcal{L} - 1 / \mathcal{L}, \sqrt{\Delta_T / T \sigma^2}) \), if \( \mathbb{E}[\mathcal{L}(\theta^t)] > 1 / 2 \), then we can show that

\[
\frac{1}{T} \sum_{t=0}^{T-1} \mathbb{E}[\| \nabla \mathcal{L}(\theta^t) \|^2_2] \leq 2
\]

which completes the proof.