Voting based ensemble improves robustness of defensive models

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Abstract

Developing robust models against adversarial perturbations has been an active area of research and many algorithms have been proposed to train individual robust models. Taking these pretrained robust models, we aim to study whether it is possible to create an ensemble to further improve robustness. Several previous attempts tackled this problem by ensembling the soft-label prediction and have been proved vulnerable based on the latest attack methods. In this paper, we show that if the robust training loss is diverse enough, a simple hard-label based voting ensemble can boost the robust error over each individual model. Furthermore, given a pool of robust models, we develop a principled way to select which models to ensemble. Finally, to verify the improved robustness, we conduct extensive experiments to study how to attack a voting-based ensemble and develop several new white-box attacks. On CIFAR-10 dataset, by ensembling several state-of-the-art pre-trained defense models, our method can achieve a 59.8% robust accuracy, outperforming all the existing defensive models without using additional data.

1. Introduction

Despite achieving human-level performance in many important tasks, it has been discovered that deep networks are vulnerable to adversarial perturbations—a small but human imperceptible perturbation can easily alter the prediction of a neural network [34, 4, 35, 13]. Since deep neural networks are being deployed in many safety-critical applications, it becomes important to develop robust defence mechanisms to make them robust against adversarial perturbations. Adversarial training [13, 20] has become one of the key techniques to develop defenses against adversarial attacks. [21] showed that adversarial training can be formulated as solving a minimax objective function, where one conducts Projected Gradient Descent (PGD) to find an adversarial example to maximize the loss, and then update the neural network weights based on this adversarial example. After that, many variations of adversarial training has been proposed by improving the minimax objective, including TRADES [45], MART [41], MMA [11] and many others [40, 46, 44]. The family of adversarial training-based defense methods have become state-of-the-arts under the current strongest white-box attacks [10].

Many of these adversarially trained models, despite having different objectives, achieving similar level of robust accuracy under white-box attacks. This naturally leads to the following important question: Can we ensemble these robust models to further boost the performance? Surprisingly, this fundamental question has not been properly answered in the literature, and previous ensemble-based methods often fail to improve the performance under white-box attacks. For example, [24], [31], and [39] suggested a special loss function, different architectures, and different DNNs output representation respectively to increase the ensemble diversity but were proven non robust [37].

In contrast to previous works that blending softmax probabilities or logit outputs of the base models (which failed to improve robustness), we consider a majority-vote ensemble mechanism in this paper. To investigate whether majority-vote ensemble can improve robust accuracy, we need to answer the following questions: 1) How can we properly evaluate the robustness of a majority-vote ensemble? 2) How can we choose a proper set of base models to achieve the best performance? To answer the first question, we conduct a comprehensive study on how to best attack a majority-vote ensemble, using both existing and newly developed techniques. For the second question, we show that a majority-vote ensemble can boost robust accuracy when the loss landscape of these base models are diverse enough. We verify this empirically and propose a novel framework to automatically select which base models should be included in the ensemble.

Our contributions can be summarized below:

• We show that voting-based ensemble can improve robustness over each individual robust model, if the loss is diverse enough. Taking a pool of 3 recently proposed defensive models, including Trades [45], MART [41] and PGD [21], we show that the majority-vote ensemble can achieve 57.32% robust accuracy.
on CIFAR-10 against $8/255 \ell_\infty$ perturbation, significantly outperforming the best base model (54.86%).

- We propose a novel algorithm to select which models to ensemble given a pool of defenses. Our algorithm is able to automatically select the best 3 models among a total set of 7 state-of-the-art models to further boost robust accuracy to 59.8% on CIFAR-10 against $8/255 \ell_\infty$ perturbation, achieving the state-of-the-art performance without using additional data.\footnote{Based on the snapshot of \url{https://github.com/fra31/auto-attack} when we finish this paper, the best publicly available model trained on CIFAR-10 achieves 56.17\% robust accuracy. Note that all the methods achieving robust accuracy beyond 59\% are using additional unlabeled data.}

- To verify that the voting based ensemble is truly robust, we carefully test existing attack methods as well as developing several novel attack algorithms to attack the ensemble. The proposed model is still robust under these adaptive attacks.

The rest of the paper is arranged as follows. In Section 2, we cover the related work to adversarial defense and ensemble based defense. In Section 3, we first introduce some basic notions and explain different ensemble types we consider. We then discuss choosing between a logits-summed ensemble and a voting-based ensemble. In Section 3.3, we study when given a pool of different defense methods, how to choose which ones to use to form an ensemble. Then we introduce several novel techniques for a white-box attacks on a majority-vote ensemble. The experimental results are delivered in Section 4.

2. Related Work

Since the discovery of adversarial examples \cite{Szegedy2013}, many algorithms have been proposed to improve the robustness against adversarial examples \cite{Goodfellow2014, Carlini2017, Madry2017, Kurakin2016, Szegedy2013a, Tramer2017b, Carlini2017a, Kurakin2017, Athalye2018, Papernot2016}. However, many previous techniques have shown vulnerable under stronger adaptive attacks \cite{Athalye2018, Papernot2016}. Among them, adversarial training has become one of the most reliable approaches. In this paper, we will focus on ensembling adversarially trained models.

**Adversarial training** To enhance the adversarial robustness of a neural network model, the most popular method is adversarial training which iteratively uses the generated adversarial examples back into the training process. Specifically, Goodfellow et al. \cite{Goodfellow2014} first uses adversarial examples generated by FGSM method to augment the training data, while later Kurakin et al. \cite{Kurakin2016} uses a multi-step FGSM to further improve adversarial robustness. Madry et al. \cite{Madry2017} formalize this iterative data augmentation process into a min-max optimization problem and propose to use PGD attack (similar to multi-step FGSM) to find adversarial examples for each batch. It shows the adversarial trained model could achieve a relatively good adversarial robustness even facing with very strong attacks \cite{Athalye2018}. Based on the min-max framework, Zhang et al. \cite{Zhang2019} proposes TRADES, a theoretical based framework to adjust the trade-off between adversarial robustness and generalization. Wang et al. \cite{Wang2018} later introduce label correctness into the TRADES and propose MART to improve the overall performance. Recently, Schmidt et al. \cite{Schmidt2018} finds the sample complexity of robust learning can be significantly larger than that of standard learning. Since then, several works \cite{Athalye2018, Papernot2016} have been introduced to use unsupervised or semi-supervised method to introduce more data into training process and shows it could further push the limit on the robustness. Many other recent defense methods also follow this min-max optimization framework \cite{Schmidt2018, Zhang2019, Athalye2018, Papernot2016}.

**Previous research on ensemble-based defense** There has been some work on using ensemble to boost the robustness of DNNs but most of them have been shown to fail under different attacks. Liu et al. \cite{Liu2015} added random noise to form an ensemble and showed that it could achieve a better robustness. He et al. \cite{He2019} considered several ensemble methods using weak individual models and showed them non-robust. Tramèr et al. \cite{Tramer2017b} used ensemble adversarial training by collecting adversarial examples from different models to train a single robust model. Elaborate black-box attack which enhanced transferability showed \cite{Tramer2017b} non-robust though. Strauss et al. \cite{Strauss2019} studied popular ensemble methods like bagging, adding gaussian noise during training, and using different training architecture. But their analysis are under weak attacks and they don’t consider majority-vote ensembles. Liu et al. \cite{Liu2015} proposed random self-ensemble for defense, but it is based on ensembling a set of randomized models with different random seed, and their method cannot be used to blend several different models. Pang et al. \cite{Pang2019} suggested training an ensemble using a specially crafted loss function to increase the robustness. Sen et al. \cite{Sen2020} use architectures with different precisions to form a majority-vote ensemble. Verma and Swami \cite{Verma2020} aimed at introducing enough diversity in models forming an ensemble and use ideas from error correcting code for robust classification. However, these all three ensemble defenses were shown in Tramer et al. \cite{Tramer2017b} to be ineffective under several attacks.

3. Robustness of Ensemble Defense

In this section, we will first introduce the proposed majority-vote ensemble and provide empirical evidences showing it outperforms sum-of-logit based ensembles. Then we discuss how to select the right subset of models
to ensemble in Section 3.3. Finally, we discuss existing and newly proposed ways to attack majority-vote ensemble in Section 3.4.

3.1. Ensemble methods

We consider a C-way classification problem and assume there are n neural network models that we want to ensemble. We denote an input as (x, y) where x ∈ ℝ^d is the input image and y ∈ [C] is the class label. The logits of ith neural network is defined by f_i(x) ∈ ℝ^C, i ∈ [n]. The inputs to the softmax function are called logits. The label assigned by each network is denoted by

\[ F_i(x) := \arg \max_{c=1,...,C} f_i(x)_c. \]

**Logits-summed ensemble** Given n networks in the ensemble, most of the previous methods use the logits-summed ensemble [24, 43], where the decision function f(x) is defined as

\[ f(x) := \sum_{i=1}^{n} f_i(x). \]

Informally, the logit output by the ensemble is the sum of logits by individual networks comprising the ensemble.

**Majority-vote ensemble** Given n networks in the ensemble, we define the majority-vote ensemble as a network with output F(x) ∈ ℝ^C as

\[ F(x) := \arg \max_{c=1,...,C} \sum_{i=1}^{n} F_i(x). \]

If more than one components have max value then we assign 1 to any one of them arbitrarily. Informally, the majority-vote ensemble outputs a one-hot vector with prediction as the class having maximum vote by comprising individual networks in the ensemble.

3.2. Shifting from logits-summed ensemble to majority-voting ensemble:

We started by asking ourselves the natural first question: Is it sufficient to just take few (differently initialized) models of the same defense type and make a logits-summed ensemble? We conduct experiments for ensembling 3 models and the robustness improvement was only marginal. For example, against one of the most effective adversarial attack, Autoattack [10], TRADES [45] robust accuracy improved from 54.08% of an individual TRADES model to 56.4% of the logits-summed ensemble. For MART [41], the improvement was less (from 54.86% to 55.7%).

The natural question we asked next was: Can we take different defense models and ensemble them rather? We formed a logits-summed ensemble of MART, TRADES, and PGD [21] model and found the robust accuracy 51.9%, which is lesser than before. Upon inspection, we found that most of the points were able to only fool just one of the three models. The individual robust accuracy on each of the TRADES, MART, and PGD model against the adversarial points generated for their logits-summed ensemble was 65.5%, 66.8%, and 48.8% respectively. This means that PGD model logits were driving the sum of the logits towards the wrong class. As two of the three models were still predicting correct for most of the examples, we rather decide to use majority-vote ensemble. Using the later developed (Section 3.4) white-box attacks for voting-based ensemble, the worst accuracy we got for TRDAES, MART, PGD voting-based ensemble is 57.4% — much higher than 51.9% when using logits-summed ensemble.

This led to the following intuition: Do models trained with different loss functions have diverse decision boundaries? At first, this looks reasonable because loss functions have a direct implication on the geometry of decision boundary. We took pairs of models, attacked them individually with the same attack, and measured the average cosine of angle between perturbations generated for the pair of models. Let θ represent this angle for a given point x. We'd expect that if indeed models trained on different loss functions are more diverse, their adversarial perturbations will be more diverse too (hence smaller average \( \cos(\theta) \)) compared to a pair of models which are trained on the same loss function (hence larger average \( \cos(\theta) \)). We took 5 recently proposed state-of-the-art defenses (mentioned in Table 1).

We trained 2 (differently initialized) models of each defense method, attacked them using PGD attack [21] and C&W attack [6], and measured average (taken over points) \( \cos(\theta) \) of the perturbations for all 5 * 5 = 25 pairs of models. We report the numbers in Table 1 and notice the results in alignment to our intuition. We believe this is some metric, if not the perfect metric, to show the difference in diverseness of decision boundary for pairs of models trained on the same loss function compared to different loss functions.

Another question that could be asked is: What if we rather use a pool of similarly-robust defenses? In this case, one could expect the logits-summed ensemble to perform well. In order to answer this, we considered the following 5 recently proposed state-of-the-art defenses which have robust accuracies within 0.7% of each other (Table 2): TRADES [45], MART [41], TRADES+SAT [16], ATES [32], and PGD+HE [23]. We formed 3 network ensembles, hence \( 5^3 = 125 \) possibilities (remember all models in an ensemble are differently randomly initialized). Testing these many ensembles is tough, hence we tested a big and good representative subset of them. This includes all possible

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\[ ^2 \text{we would have taken more but could find training code available for only 5 of them} \]
Table 1: Average $\cos(\theta)$ where $\theta$ is the angle between adversarial perturbation on pair of models under the same attack. Left (a) is on PGD-CE attack, right (b) is on C&W attack. We take TRADES [45], MART [41], TRADES-AWP [42], PGD [21], and PGD+HE [23] and represent them as 0, 1, 2, 3, 4 respectively, for brevity.

| Defense | 0    | 1    | 2  | 3  | 4  |
|---------|------|------|----|----|----|
| 0       | 0.485| 0.365| 0.435| 0.2 | 0.265|
| 1       | 0.365| 0.477| 0.36 | 0.203| 0.328|
| 2       | 0.435| 0.36  | 0.51 | 0.21 | 0.27 |
| 3       | 0.2  | 0.203| 0.21 | 0.24 | 0.203|
| 4       | 0.265| 0.328| 0.27  | 0.203| 0.49 |

\(\binom{n}{3} = 10\) ensembles consisting three models all of different defense methods, 7 ensembles consisting 2 models of one defense type and 1 of another defense type, and 3 ensembles consisting all three models of same defense type. The highest accuracy against Autoattack we got was 57.9%. However, just considering the \(\binom{n}{3} = 10\) possible majority-vote ensembles consisting three models all of different defense methods, we got 59.17% robust accuracy. The majority-vote ensemble accuracy is measured using WA-autoattack, the strongest white-box attack we found as discussed later in Sections 3.4, 4.4.

In order to take advantage of diverse decision boundaries, majority-vote ensembles seem to be the natural fit compared to a logits-summed ensemble. It has been widely observed that DNNs predict the wrong class with high confidence against an adversarial example [36, 22]. Hence, the sum of logits could be driven to wrong class due to a single model being non-robust on a given point, even if the other models in the ensemble may be predicting correct (as we saw in PGD, MART, TRADES logits-summed ensemble). All the above observations motivate us to investigate majority-vote ensemble over a logits-summed ensemble.

3.3. Model Selection for majority-vote ensemble

Given \(n\) individual defenses, our aim is to select \(k\) defenses out of the \(n\) available to form a majority-vote ensemble. This problem isn’t easy to solve as it requires selecting models based on how individually robust they are, as well as how diverse they are with respect to each other. In the following, we model this problem from an optimization point of view and derive an algorithm for model selection. Let \(g_i(\cdot)\), where \(i \in \binom{[n]}{k}\) and \(g_i(\cdot) \in \mathbb{R}^C\) denote the \(i^{th}\) ensemble formed of \(k\) models. We assume data follow the distribution \((x, y) \sim D\) and use \(B\) to denote the allowed perturbation set. For example, a typical \(\ell_p\) norm threat model assumes \(B = \{\delta \mid \|\delta\|_p \leq \epsilon\}\), where \(\epsilon\) is preset threshold. So the adversary is allowed to perturb an original point \(x\) to any point \(x'\) such that \(x' - x \in B\).

Let \(sc(g_i, B, D)\) denote robust accuracy of \(i^{th}\) ensemble defined as

\[
sc(g_i, B, D) = \mathbb{E}_{(x, y) \sim D} \min_{\delta \in B} \mathbb{I}_{g_i(x + \delta) = y},
\]

where the inner minimization corresponds to the adversary that finds the worst-case perturbation within set \(B\) for each input, and \(y\) is the correct label. Finding the best ensemble can then be formally written as finding the best \(i\) from all the \(\binom{n}{k}\) cases to maximize robust accuracy:

\[
\max_i sc(g_i, B, D). \tag{1}
\]

However, solving (1) is intractable because to (approximately) solving the inner minimization, a strong adversarial attack is required to be conducted for all the \(\binom{n}{k}\) ensembles, and a large-enough subset of samples needs to be tested in order to obtain a good estimation of robust accuracy. Even if we use a simple PGD-based attack, it is computational infeasible to run it on all the \(O(\binom{n}{k})\) cases.

Hence, we propose a novel algorithm to approximately solve (1) in tractable time. The main idea is to use the adversarial examples generated by base models instead of ensemble models to evaluate robust accuracy. We take \(r\) random test/validation points \(\{x_1, \ldots, x_r\}\) with true labels \(\{y_1, \ldots, y_r\}\) from \([C]\). We generate perturbation for each point by attacking any one of the \(n\) models. To maintain uniformity, we use the first model to generate perturbations for the first \(r/n\) points, the second model for next \(r/n\) points, and so on. Let \(\{x_1', \ldots, x_r'\}\) denote these \(r\) adversarial examples. For each \(\binom{n}{k}\) possible ensembles, we calculate its score as the number of adversarial points predicted correctly by at least \(\lceil k/2 \rceil\) out of the \(k\) models in the ensemble. This is because we’re focusing on majority-vote ensemble and so using its definition to calculate the ensemble’s score. Finally, we choose the ensemble with the highest score. The algorithm is also presented in appendix A.1.

The approximate evaluation scheme introduced above can reduce the number of attacks from \(r \times \binom{n}{k}\) to \(r \times n\), which makes model selection feasible. In our current implementation, there are only few models to ensemble so we
will evaluate the approximate score for each of \( \binom{n}{k} \) models and select the best. If \( n \) goes larger, we can further use a genetic algorithm to conduct model selection based on this approximate scoring function.

Intuitively, testing a model on adversarial points captures the model’s robustness. And testing the adversarial points generated by one model on another tests transferability and hence the diverseness of different models with respect to each other. We later show this heuristic gives a reasonable approximation to the actual eq. (1) objective in Section 4.5 by considering a pool of 7 different defenses.

3.4. How to attack a majority-vote ensemble?

As we want to objectively test the robustness, we perform white-box attacks on all the ensembles. Since the voting mechanism is a discrete process, the gradient of ensemble does not exist and it is nontrivial to attack a voting based ensemble. Currently the only method used in the literature for attacking voting-based ensemble is to approximate it by a logits-summed ensemble. This method, called logis-summed attack in our paper, has been used in [37] to break the defense in [31] and was also mentioned in [3]. On the other hand, although BPDA attack [3] can handle some discrete models, they only cover discrete processes that can be approximated by an identity mapping and applied a straight-through estimator for attack, which is not applicable for majority-vote ensemble.

There hasn’t been any systematic study on developing white-box attacks to test majority-vote ensemble. Here, in addition to the logits-summed attack, we propose three other attack techniques which could be used on top of any existing white-box attacks to test majority-vote ensemble.

3.4.1 Weakest-attacked attack

Let the point in consideration be \((x, y)\). Let there be \( n \) networks in the ensemble. The attacker calculates logits \( f_i(x) \) for all \( n \) networks. If the majority vote \( F(x) \) for majority-vote ensemble (as defined in Section 3.1) is already the nontrue class, then the attacker is done. Otherwise, among the individual models (also referred to networks in this work) which predict correct label \( y \), the attacker chooses the weakest model and performs a local small step attack on it. The weakest model among those which predict the true class \( y \) is determined by calculating the probability of individual models on true class \( y \) and choose the one with lowest probability. Let \( y \in \mathbb{R}^C \) represent the one-hot vector with 1 at component \( y \) and 0 otherwise. Mathematically the weakest model output can be represented as \( f_k(x) \) where

\[
k = \arg \min_{i \in [n]} (1_{F_i(x)=y} \cdot (p_i(x))_y + 1_{F_i(x) \neq y} \cdot 1),
\]

where \( p_i(x) = \text{Softmax}(f_i(x)) \)

and \( 1 \) is an indicator variable and \( (p_i(x))_y \) refer to the \( y \)th component of vector \( p_i(x) \).

Take an example of an ensemble consisting of three models \( \{m_1, m_2, m_3\} \). Let the clean data point be \( x \) and its true class be \( y \). The attacker checks if the majority vote is already a non-true class. If so, the attacker is done. Let’s say this is not the case and \( \{m_1, m_2\} \) predict the true class \( y \). Also let the probability of class \( y \) predicted by \( m_1 \) be less than that predicted by \( m_2 \). Most of the existing white-box based attacks happen by taking multiple small steps towards final perturbation. In this case, the attacker performs a local attack on \( m_1 \) and moves \( x \) to \( x + \epsilon \). The attacker again passes this \( x + \epsilon \) through all three models \( \{m_1, m_2, m_3\} \). Let’s say still \( \{m_1, m_2\} \) predict the true class \( y \) but this time probability of class \( y \) by \( m_2 \) is less than that of \( m_1 \). In this step, the attacker performs a local attack on \( m_2 \) to get \( x + \epsilon + \epsilon' \). This is repeated until either the number of steps are over or the majority vote becomes a non-true class. Intuitively, the attacker performs a greedy attack over the three models to turn the majority vote to a non-true class. We present the attack formally in appendix A.2.

Note that similar to logits-summed attack technique, this attack technique could also use any existing white-box attack. We never fixed what attack is applied on the locally weakest model. In this work we consider PGD with CE loss attack [20], FAB-attack [9], autoattack [10], and \( l_\infty \) B&B attack [5] with this attack technique.

3.4.2 Objective-summed attack

Most of the existing white-box attacks decrease/increase a particular objective. For example, PGD attack with CE loss function maximizes the CE loss, C&W attack minimizes the C&W loss [6]. Therefore another attack technique is to take sum of this attack objective values on individual models of the ensemble and decrease/increase it. Notice that just like previous techniques, even this method can work with any white-box attack. In this work, we particular consider C&W loss objective. That is, we sum the C&W loss over all the models comprising the ensemble, and decrease it using PGD.

3.4.3 majority-attack

Rather than using the previous three introduced attack technique over the entire ensemble, one can use them over just a subset of \( \binom{n}{n/2} \) models among the \( n \) models comprising the ensemble. Intuitively, as majority-vote ensemble needs to misclassify any \( \binom{n}{n/2} \) models, the attacker focuses on doing just that. One needs to consider all possible \( \binom{n}{n/2} \) combination though, hence this attack technique isn’t very efficient. But for small \( n \) one can use it. In this work, we use Objective-summed attack technique (Section 3.4.2).
with C&W attack on an ensemble consisting 3 models and attack all possible \( \binom{3}{2} \) pairs of models of the ensemble.

4. Experimental Evaluations

In this section, we select various existing defenses and perform extensive experimentation on them. We first introduce certain notations, then ensemble 3 (hand-picked) defenses and perform a more thorough analysis on them. We then use the algorithm mentioned in Section 3.3 on the entire pool of 7 models, form various ensembles, and test them under strong attacks.

4.1. Ensemble models

We select a pool of 7 state-of-the-art defenses: PGD [21], TRADES [45], MART [41], TRADES-AWP [42], PGD+HE [25], TRADES+SAT [15], and ATES [32]. We pick 3 models to form the ensemble, each model being one of the above 7 defense types. Every individual model in all the ensembles is differently initialized when training. The final ensemble output is the majority vote of individual models. If there’s no majority vote, the ensemble outputs one of the model predictions randomly.

We report as a baseline the individual model accuracy against PGD attack with CE loss, FAB attack, and C&W attack in Table 3(a). The parameters for these attacks are mentioned in Section 3.2. We later in Sections 3.4.4, 3.4.5 test a few ensembles against stronger attacks. Specifically, in Table 3(b) we test the above 7 models accuracy against these stronger attacks. We trained TRADES, MART, and PGD model from scratch hence they might be slightly different in performance compared to the ones available online.

Notations In tables and a few other places, for brevity, we represent TRADES model with the letter T, MART model with letter M, and PGD trained model with letter P. T=r/M=r represents a TRADES/MART model trained with \( \beta = r \). TRADES and MART loss function is based on a mix of clean accuracy and robustness term, where robustness is controlled by the parameter \( \beta \). Unless otherwise specified, T=T-6 and M=M-6. Logits-summed-PGD-CE attack is represented by LS-PGD, Logits-summed-FAB is represented by LS-FAB, Weakest-attacked-PGD-CE is represented by WA-PGD, and Weakest-attacked-FAB is represented by WA-FAB. Every experiment on an ensemble is repeated 2–4 times. We report the mean values in the table.

4.2. Attacks

We use the following 5 white-box attacks: 1) logits-summed-CE (LS-CE): PGD attack with CE loss function using logits-summed attack technique (Section 3.4.1 [37]); 2) logits-summed-FAB (LS-FAB): FAB attack using logits-summed attack technique (Section 3.4.1 [37]); 3) weakest-attacked-CE (WA-CE): PGD attack with CE loss using the technique as explained in Section 3.4.1; 4) weakest-attacked-FAB (WA-FAB): FAB attack using the technique in Section 3.4.1; 5) C&W attack using objective-summed attack technique, as mentioned in Section 3.4.2.

We consider \( l_{\infty} \) attack with \( \epsilon = 0.03 \). For PGD-CE attack, we set the number of iterations as 150 and the learning rate to be 0.007. For FAB attack [9] we run for 25 iterations and keep the rest of the parameters default from advertorch implementation [12]. For C&W attack [6], we set the number of iterations to be 150, learning rate 0.007, and \( \kappa = 0 \).

4.3. Ensemble of models trained with same objective function but different hyper-parameters

Before testing models with different training objectives, we first conduct experiments to investigate whether ensembling models trained with varied hyper-parameters on the same objective function can improve robustness. We form 3 ensembles all forming by three TRADES models but trained with different \( \beta \) parameter. Among the three individual models in each of these 3 ensembles, two of the models are fixed as T-6 models, while the third one is kept either of T-4, T-2, and T-1. Though individual TRADES model accuracy goes down with \( \beta \), we notice a consistent improvement in accuracy of the ensemble (Table 3). We believe this is because as \( \beta \) takes lower values, the overall loss functions becomes more and more different than the one with \( \beta = 6 \). Hence, even though the individual model accuracy is decreasing, the ensemble diversity increases by small margins leading to an overall better ensemble defense. A similar trend is observed across most of the attacks by using MART with different \( \beta \) (s). That is, two of the models in the ensemble is fixed at \( \beta = 6 \) while the third model is chosen among \( \beta = 4/2/1 \) (Table 3). We see later in Table 4 that ensembles [T,T,P] and [M,M,P] have a more pronounced increase because this third model is trained on a completely different loss function like the [20] min-max loss function with CE loss.

4.4. Ensemble of models trained with different objective functions

Next we hand-pick some sets of base models trained with different objective functions to demonstrate a significant boost of robust accuracy when ensemble a set of diverse models. Table 4 show accuracy of ensembles having three similar models, two similar and one different model, and all three different models (last row). The last column denotes the worst accuracy among the 5 attacks. We notice a consistent improvement in accuracy of any ensemble comprising three similar model to when replaced by one different model and the rest remaining same, to all three different models, on all the attacks.

\[ \text{https://github.com/BorealisAI/advertorch} \]
Table 2: Mean accuracy of individual models. Left (a) attacks have parameters as mentioned in Section 4.2, while right (b) are stronger attacks with parameters mentioned in Section 4.4.

| Ensemble | PGD-CE | FAB | C&W |
|----------|--------|-----|-----|
| T (T-6)  | 55.7%  | 53.97% | 54.08% |
| T-4      | 54.5%  | 53.3% | 53.65% |
| T-2      | 52.9%  | 52.09% | 52.3% |
| T-1      | 50.28% | 50.06% | 50.5% |
| M (M-6)  | 57.9%  | 54.13% | 54.86% |
| M-4      | 57.99% | 54.31% | 54.8% |
| M-2      | 57.17% | 53.8% | 54.54% |
| M-1      | 56.42% | 53.38% | 54.56% |
| P        | 49.1%  | 50.2% | 49.2% |

(b)

| Ensemble | Strong-FAB | autoattack |
|----------|------------|------------|
| PGD [21] | 48.72%     | 46.94%     |
| TRADES [45] | 53.97% | 54.08% |
| MART [41] | 54.13%     | 54.86%     |
| ATES [32] | 53.56%     | 53.93%     |
| TRADES-AWP [42] | 58.09% | 57.6% |
| TRADES+SAT [16] | 55.27% | 54.65% |
| PGD+HE [25] | 55.24% | 54.59% |

Table 3: Ensemble robust accuracy of Trades and Mart trained with diff β

| Ensemble | LS-PGD | LS-FAB | C&W | WA-PGD | WA-FAB | acc. against best attack |
|----------|--------|--------|-----|--------|--------|--------------------------|
| T-6,T-6,T-4 | 56.89% | 69.86% | 58.16% | 58.99% | 57.36% | 56.89% |
| T-6,T-6,T-2 | 57.17% | 70.87% | 58.35% | 59.13% | 57.52% | 57.17% |
| T-6,T-6,T-1 | 57.55% | 71.1% | 58.96% | 59.5% | 57.87% | 57.55% |
| M-6,M-6,M-4 | 57.38% | 69.36% | 58.2% | 61.01% | 56.94% | 56.94% |
| M-6,M-6,M-2 | 57.5% | 69.05% | 58.92% | 61.5% | 57.4% | 57.4% |
| M-6,M-6,M-1 | 57.73% | 69.72% | 58.55% | 61.7% | 57.55% | 57.55% |

Table 4: Robust accuracy of ensembles of different models. Note that T,T,T indicate an ensemble of three Trades models trained with different random initializations.

| Ensemble | LS-PGD | LS-FAB | C&W | WA-PGD | WA-FAB | acc. against best attack |
|----------|--------|--------|-----|--------|--------|--------------------------|
| T,T,T | 57.18% | 70.1% | 58.6% | 58.88% | 57.14% | 57.14% |
| M,M,M | 57.4% | 69.17% | 57.77% | 60.93% | 57% | 57% |
| P,P,P | 55.1% | 70.37% | 56.56% | 54.15% | 55.67% | 54.15% |
| T,T,M | 57.74% | 70.3% | 59.33% | 61.78% | 58.39% | 57.74% |
| T,T,P | 62.82% | 76.92% | 60.46% | 59.8% | 58.2% | 58.2% |
| M,M,T | 58.22% | 69.69% | 59.17% | 61.44% | 57.47% | 57.47% |
| M,M,P | 65.28% | 76.79% | 61% | 61.79% | 57.69% | 57.69% |
| P,M,T | 63.18% | 77.05% | 61.26% | 63.29% | 59.63% | 59.63% |

Table 5: Robust accuracy of selected ensembles against stronger attacks

| Ensemble | Strong WA-FAB | RayS | WA-B&B | C&W over 2 | LS-autoattack | WA-autoattack |
|----------|---------------|------|--------|------------|---------------|---------------|
| T,T,T | 56.62% | 62.6% | 56.9% | 58.28% | 58.85% | 54.9% |
| T,T,P | 57.54% | 61.6% | 57.56% | 58.83% | 64.95% | 56.03% |
| P,M,T | 59.03% | 62.57% | 58.68% | 60.59% | 65.22% | 57.32% |

**Stronger attacks to validate robust accuracy**: We further test a selected representative 3 ensembles - [T,T,T], [T,T,P], and [P,M,T] against stronger attack to validate robust accuracy and the accuracy trend. We take these particular ensembles for the following reasons: 1) TRADES is a strong defense hence forms a good baseline of using three similar model ensemble; 2) Replacing one of the TRADES by MART would not support our claim as strongly as replacing it with PGD. This is because PGD is substantially less robust (refer Table 2) compared to TRADES, being almost 5 – 6% less robust across various attacks. While MART is still almost similar robust to TRADES across various attacks (Table 2). Hence, still observing an improvement in the ensemble of [T,T,P] compared to [T,T,T] sup-
ports our hypothesis strongly; 3) [P,M,T] consists of all three individual models trained on different loss functions, inducing the highest diversity.

We test the above ensembles against 1) a stronger WA-FAB attack with default parameters from advertorch\(^2\) in order to show that there’s no gradient masking involved we test against RayS\(^6\), a blackbox attack, on \(\approx 2500\) random samples; 3) WA-B&B attack: L-inf B&B attack\(^5\) on the locally weakest model technique as mentioned in Section 3.4.1. We use the foolbox implementation\(^3\)\(\Delta\(\approx 35\) with default parameters, making it a strong attack; 4) C&W attack as introduced in Section 3.4.3. We report the worst accuracy obtained among the possible \(\binom{7}{3}\) subsets over which C&W loss objective is summed and optimized. We refer to this attack as “C&W over 2” in Table 5. 5) LS-autoattack: Autoattack\(^10\) using logits-summed attack technique (Section 3.4); 6) WA-autoattack: Autoattack using the weakest-attacked technique as mentioned in Section 3.4.1. Autoattack\(^10\) introduces an ensemble of different attacks including an improved version of PGD (APGD or apgd-ce for improved PGD-CE), a targeted PGD attack with a new loss function (apgd-t), FAB, and square attack\(^2\). The authors suggest to use ‘standard’ attack with an ensemble of [‘apgd-ce’, ‘apgd-t’, ‘FAB’, ‘square’] attacks. But we noticed using auto attack with these constituent attacks was quite slow to evaluate the entire testset. Furthermore, taking a random sample of 1000 points we noticed that [‘FAB’, ‘square’] could introduce only 1 extra successful adversarial example compared to what [‘apgd-ce’, ‘apgd-t’] could generate. Hence, we use a custom autoattack using ensemble of [‘apgd-ce’, ‘apgd-t’] with better params than standard ensemble attack - apgd.n_restarts = 2, apgd.targeted.n_restarts = 2, apgd.targeted.n_target_classes = 9, while other parameters being same as default\(^6\).

We report the ensemble accuracy against above mentioned strong attacks in Table 5. We still observe the same trend consistent across all the attacks supporting our claim that individual models trained on different loss function have diverse decision boundary thus possibly leading to more diversity when formed an ensemble. Also notice that WA-autoattack and WA-FAB are two of the strongest attacks, which we’ll use to test more ensembles in the next subsection.

### 4.5. Selecting individual models from a pool to form an ensemble

We test the algorithm described in Section 3.4 to select individual models that forms the strongest ensemble. We show empirically that this heuristic works with reasonable approximation. As mentioned, we choose \(n = 7\) different defense models: PGD\(^{\Delta21}\), TRADES\(^{\Delta45}\), MART\(^{\Delta41}\), Trades-AWP\(^{\Delta42}\), PGD+HE\(^{\Delta25}\), TRADES+SAT\(^{\Delta15}\), and ATES\(^{\Delta32}\). We fix \(k = 3\), and choose \(r \approx 4500\) random points. We ran the WA-autoattack and WA-FAB attack on all \(\binom{7}{3}\) = 35 ensembles. We measure the effectiveness of the algorithm using Kendall’s \(\tau\) statistic of predicted score by the algorithm and the actual accuracy of the ensembles. Kendall’s \(\tau\) is used to measure ordinal association between two quantities. The kendall’s \(\tau\) average value over three runs of the algorithm is +0.53 and +0.503 for WA-autoattack and WA-FAB attack respectively. Note that the range of kendall’s \(\tau\) is \([-1, +1]\), where 0 indicates zero correlation, and \(> 0.5\) typically indicates a moderate positive correlation. Moreover, in each run we got the highest accuracy ensemble within the top 3 ranked/scored by our algorithm. We provide the supporting figures in appendix A.1. Finally, we report accuracy on few of the best ensembles among these \(\binom{7}{3}\) ensembles in Table 6 against WA-autoattack and WA-FAB attack. We represent PGD by P, MART by M, TRADES by T, TRADES-AWP by TA, PGD+HE by PH, TRADES+SAT by TS, and ATES by A for brevity in Table 6.

| Ensemble | Strong WA-FAB | WA-autoattack |
|----------|---------------|---------------|
| PTA,PH   | 61.57%        | 59.84%        |
| TA,TS,PH | 61.42%        | 59.78%        |
| P,A,T    | 60.86%        | 59.42%        |
| P,TS,PH  | 60.97%        | 59.2%         |
| A,TS,PH  | 60.89%        | 59.17%        |

It’s worth mentioning that TRADES-AWP (TA) is much more robust than other models in our pool. Majority-vote ensemble accuracy is a factor of individual model robustness forming the ensemble, and their diverseness. As the rest of the models are comparatively quite less robust, adding them with TRADES-AWP to form an ensemble leads to comparatively less increase over the individual TRADES-AWP model (57.6% to 59.84%). However, just restricting to other models in the pool except TRADES-AWP leads to much higher increase. The highest base model robust accuracy is 54.86% of MART, to 59.2% of the best ensemble formed out of the remaining 6 models, thereby an increase of \(\approx 4.34\%\).

### 5. Conclusion

We show voting-based ensemble can improve the robustness over a set of adversarially trained base models. Furthermore, we propose an algorithm to automatically select an ensemble from a pool of models. Using our algorithm, we achieve an ensemble with state-of-the-art robust accuracy on CIFAR-10 dataset, and the performance is verified by both existing and several newly proposed strong attacks.

\(^2\)https://github.com/BorealisAI/advertorch
\(^3\)https://foolbox.jonasrauber.de/
\(^4\)https://github.com/fra31/auto-attack
\(^5\)https://github.com/foolbox
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A. Appendix

A.1. Algorithm for choosing models to ensemble

We present CHOOSE_ENSEMBLE in Algorithm 1 for selecting models for majority-vote ensemble mentioned in Section 3.3. We denote by \( A(\cdot) \) a generic white-box attacks which takes a model and a point \( x_i \) and generates an adversarial example. We don’t include other details like perturbation bound and other hyperparameters for brevity.

![Figure 1](image)

Figure 1: Average accuracy vs rank (correspondingly score order) of the heuristic proposed. The shaded area represents the error region.

We use this algorithm in Section 4.3 on a pool of 7 models to form 3 model ensembles, hence \( \binom{7}{3} = 35 \) ensembles. We plot the output ranks (in decreasing scores) with the actual accuracy of the ensemble in Figure 1. We take three runs of the algorithm over random \( \sim 4500 \) points and plot the mean accuracy for each rank. The shaded area represents the error region (mean_accuracy - std_dev_of_accuracy to mean_accuracy + std_dev_of_accuracy). We observe that our algorithm performs reasonably well with the best ensemble always in top 3 scored, and an overall consistent trend of accuracy-vs-rank. Recall that the average (over 3 runs) Kendell’s \( \tau \) statistic of predicted score by the algorithm and the actual accuracy of the ensembles is +0.53 and +0.503 for WA-autoattack and WA-FAB attack respectively.

A.2. Algorithm for weakest-attacked attack technique

We present WEAKEST_ATTACKED(\cdot) in Algorithm 2. This is the weakest-attacked attack strategy mentioned in Section 3.4.1.

```
Algorithm 1 CHOOSE_ENSEMBLE(A(\cdot), X, Y, M, k)
1: Input: Attack function A(\cdot), test points (X, Y), M = \{f_0, \cdots, f_{n-1}\} base models, size of ensemble to form k
2: set G = \{g_i(\cdot) \mid i \in \binom{[n]}{k}\} \triangleright Form a set of all possible \binom{[n]}{k} ensembles
3: for \( x_i \) in X do
4: set \( x'_i \leftarrow A(f_{i\%n}, x) \triangleright Attack (i\%n)^{th} model\)
5: end for
6: for \( g_i \) in G do
7: set \( sc(g_i) \leftarrow \sum_{j=1}^{n} \mathbb{1}_{g_i(x'_j)==y_j}\)
8: end for
9: return \( \{sc(g_i) \mid i \in \binom{[n]}{k}\}\)
```

```
Algorithm 2 WEAKEST_ATTACKED(A(\cdot), g(\cdot), lr, ss, s, B, x, y)
1: Input: Attack function A(\cdot), data point and true label (x, y), learning rate lr, step size ss, number of steps s, allowed perturbation set B, and the majority-vote ensemble g(\cdot).
2: set \( x_{\text{adv}} \leftarrow x \)
3: for i in s do
4: if \( g(x_{\text{adv}}) \neq y \) then
5: Break
6: end if
7: min_prob \leftarrow 1
8: for model in g do
9: set \( p \leftarrow \text{Softmax}(\text{model}(x_{\text{adv}}))\)
10: if \( \text{arg max}_j p_j == y \) and \( p_y \leq \text{min_prob} \) then
11: min_prob = \( p_y \)
12: model_to_attack \leftarrow model
13: end if
14: end for
15: \( x_{\text{adv}} \leftarrow A(\text{model_to_attack}, lr, ss, s = 1, x_{\text{adv}}, y) \)
16: \( x_{\text{adv}} \leftarrow g(x_{\text{adv}} - x) \triangleright Project the perturbation on allowed perturbation set\)
17: end for
18: return \( x_{\text{adv}} \)
```