Learning Diverse-Structured Networks for Adversarial Robustness

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Abstract

In *adversarial training* (AT), the main focus has been the objective and optimizer while the model has been less studied, so that the models being used are still those classic ones in *standard training* (ST). Classic *network architectures* (NAs) are generally worse than searched NAs in ST, which should be the same in AT. In this paper, we argue that NA and AT cannot be handled independently, since given a dataset, the optimal NA in ST would be *no longer optimal* in AT. That being said, AT is time-consuming itself; if we directly search NAs in AT over large *search spaces*, the computation will be practically infeasible. Thus, we propose a *diverse-structured network* (DS-Net), to significantly reduce the size of the search space: instead of low-level operations, we only consider predefined *atomic blocks*, where an atomic block is a time-tested building block like the residual block. There are only a few atomic blocks and thus we can weight all atomic blocks rather than find the best one in a searched block of DS-Net, which is an essential trade-off between *exploring* diverse structures and *exploiting* the best structures. Empirical results demonstrate the advantages of DS-Net, i.e., weighting the atomic blocks.

1. Introduction

Safety-critical areas, such as autonomous driving, healthcare and finance, necessitate deep models to be adversarially robust and generalize well (Goodfellow et al., 2015). Recently, *adversarial training (AT)* has been shown effective for improving the robustness of different models (Madry et al., 2018). Compared with *standard training (ST)* on natural data, AT is a new training scheme, which generates adversarial examples on the fly and employs them to update model parameters (Madry et al., 2018; Zhang et al., 2019b; 2020b; Wong et al., 2020; Pang et al., 2021).

Table 1. Performance misalignment for different NA in terms of robustness (PGD-20) and standard accuracy. Models which perform better after ST are not necessarily more robust after AT. AdaRKNet denotes dynamic system-inspired network (Kim et al., 2020). AT is performed by PGD-10 with a perturbation bound of 0.031. Robustness is evaluated with the same perturbation bound of 0.031.

Model	Standard Acc.	Ranking	Robustness	Ranking
WRN-28-10	0.9646	1	0.4872	3
ResNet-62	0.9596	2	0.4855	4
DenseNet-121	0.9504	3	0.4993	2
MobileNetV2	0.9443	4	0.4732	6
AdaRKNet-62	0.9403	5	0.5016	1
ResNet-50	0.9362	6	0.4807	5

The research focus of AT has mainly been the *objective* and *optimizer* while the *model* has been less studied. Therefore, it is urgent to explore the influence of network architectures (NAs) for adversarial robustness. Some emerging studies imply that the classic human-designed NAs (e.g., ResNet (He et al., 2016)), specified for ST, may not be suitable for AT. For example, Li et al. (2020a) and Kim et al. (2020) argued that the forward propagation of ResNet can be explained as an explicit Euler discretization of an ordinary differential equation (ODE), which leads to unstable predictions given perturbed inputs. They proposed to change NAs according to more stable numerical schemes and thus obtained higher model robustness. Meanwhile, Xie et al. (2020a) discovered that the ReLU activation function weakens AT due to its non-smooth nature. They replaced ReLU with its smooth approximations to improve robustness.

In addition, we show in Tab. 1 a *misalignment phenomenon* for different NA in terms of their robustness after AT and standard accuracy after ST. This phenomenon further demonstrates a fact that *manually-crafted NAs for ST may not be suitable for AT*. Specifically, among various architectures, a clear trend can be observed that models which perform better in terms of standard accuracy may not be more robust. Moreover, a newly-designed AdaRKNet-62 (Kim et al., 2020) has the *biggest misalignment*, which inspires us to rethink NAs for AT. Namely, all intriguing results

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Proceedings of the 38th International Conference on Machine Learning, PMLR 139, 2021.

suggest improving adversarial robustness requires carefully modified structures. Nevertheless, designing an optimal architecture for AT is still a challenging problem.

One straightforward remedy is to search robust NAs (Guo et al., 2020; Dong et al., 2020a), where the key to success is *exploring* diverse structures. However, it suffers from computational inefficiency and is sometimes not effective. Specifically, AT is inherently time-consuming, and searching NAs over large spaces with AT drastically scales up the computation overhead (Guo et al., 2020). Besides, searching over a large space (denoted as the search phase) requires pruning less useful operations and retraining the model from scratch (denoted as the evaluation phase), which naturally leads to an optimization gap between these two phases. As claimed in Xie et al. (2020b), the search phase seeks to optimize a large network, but a well-optimized large network does not necessarily produce high-quality sub-architectures. Thus, the searched architecture may not always be more robust or generalizing better. This motivates us to find an effective architecture for AT which is easy to build and efficient to train while encouraging flexible NA exploration.

In this paper, we introduce a novel network design strategy which trades off *exploring* diverse structures and *exploiting* the best structures. Concretely, we propose a Diverse-Structured Network (DS-Net) as a novel solution to the trade-off (see Fig. 1). Specifically, DS-Net consists of a sequence of modules. To significantly reduce the fine-grained search space, each module contains a few off-the-shelf time-tested building blocks (i.e., predefined atomic blocks in Section 3.3), which are either human-designed or search-based blocks that can be flexibly chosen. To encourage structure exploration, besides block parameters, we introduce a set of learnable attention weights to weight the outputs of these atomic blocks rather than finding the best one. The weights are concurrently optimized with the block parameters by the robust training objective and are fixed for evaluation.

Our end-to-end design strategy is analogous to manual design, which operates on a fixed set of atomic blocks but leverages attention weights to flexibly explore their relationship. It is different from searching robust NAs that determines the local structures inside each block by two-stage training. Additionally, the structure of DS-Net is consistent during AT, which does not require the operation of pruning that causes the optimization gap during searching NAs. Thus, our main contributions are summarized as follows:

- We propose a novel DS-Net that trades off *exploring* diverse structures and *exploiting* the best structures. DS-Net remains the computational efficiency and effectiveness, which are limited in existing methods.
- DS-Net allows for a flexible choice among powerful off-the-shelf atomic blocks including human-designed and search-based blocks, which are easy to understand, build, and robustify/generalize well.
- DS-Net learns attention weights of predefined atomic blocks based on the objective of AT. It empirically performs better than powerful defense architectures with less parameters on CIFAR-10 and SVHN.

2. Related Work

Adversarial defense. Existing literature on the adversarial defense of neural networks can be roughly divided into two categories, namely certified robustness (Tsuzuku et al., 2018; Zhang & Liang, 2019) and empirical robustness (Cai et al., 2018; Madry et al., 2018; Zhang et al., 2020a). The former one focuses on either training provably robust models (Wong & Kolter, 2018) or obtaining certified models via random smoothing (Cohen et al., 2019), but often with a limited robustness compared to the latter approach. Empirical approaches usually rely on different techniques, such as input transformation (Dziugaite et al., 2016), randomization (Xie et al., 2018) and model ensemble (Liu et al., 2018).

However, most of them are evaded by adaptive attacks (Athalye et al., 2018), while the most effective approaches till now are AT (Madry et al., 2018) and its variants (Zhang et al., 2019b; Wang et al., 2020b). Based on it, many improvements were proposed, e.g., by metric learning (Li et al., 2019), self-supervised learning (Naseer et al., 2020), model-conditional training (Wang et al., 2020a), weight perturbation (Wu et al., 2020), generative models (Wang & Yu, 2019) and semi-supervised learning (Zhai et al., 2019). Besides, several works attempted to speed up AT, such as computation reuse (Zhang et al., 2019a), adaptive inner maximization steps (Wang et al., 2019b; Zhang et al., 2020b) and one-step approximation (Wong et al., 2020; S. & Babu, 2020). Note DS-Net improves AT from the viewpoint of network structure.

Several works attempted to improve adversarial robustness by diversity (Pang et al., 2019; Dong et al., 2020b; Abbasi et al., 2020; Kariyappa & Qureshi, 2019), but neither of them focused on learning diverse-structured networks.

Robust network architecture. To obtain robust NAs, researchers developed smooth activation functions (Xie et al., 2020a), channel activation suppressing (Bai et al., 2021), dynamical system-inspired networks (Li et al., 2020a; Kim et al., 2020), model ensemble (Wang et al., 2019a), sparse coding (Cazenavette et al., 2020) and regularization (Bui et al., 2020; Rahnama et al., 2020) to enhance robustness. Besides, several works explored searching robust architectures (Cubuk et al., 2018; Li et al., 2020b; Hosseini et al., 2020; Vargas & Kotyan, 2019; Yue et al., 2020; Chen et al., 2020; Ning et al., 2020). Note DS-Net attempts to trade off *exploring* diverse structures and *exploiting* the best structures, which is orthogonal to these approaches.

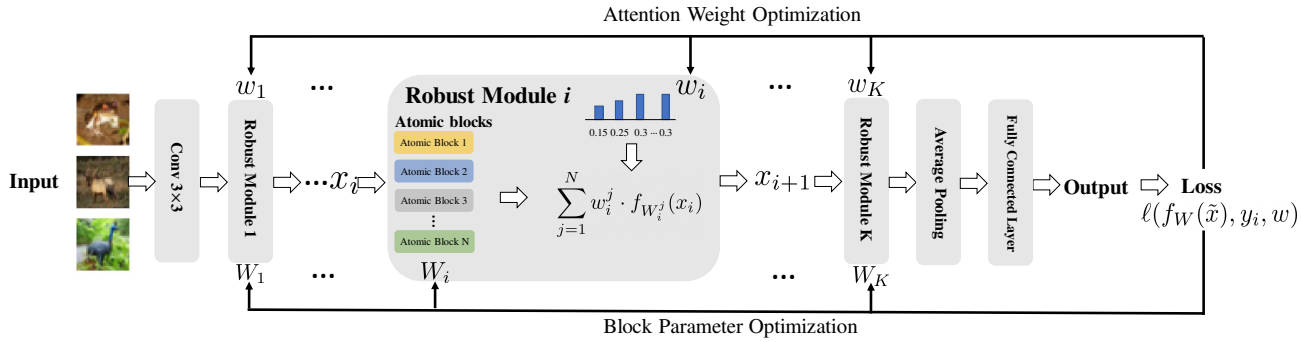

Figure 1. The network structure of DS-Net, where $\tilde{x}$ means the perturbed data and $f_W(\cdot)$ denotes the DS-Net with parameter W. The output from the i-th module x_i goes through every atomic block and outputs x_i^j. The output x_{i+1} is calculated by multiplying attention weights w_i^j $(j = 1, ..., N)$ and the corresponding outputs in a block-wise fashion. Here, N is the number of atomic blocks, K is the number of robust modules in sequence, and W_i denotes the block parameter for the i-th module.

3. Proposed Approach

3.1. Preliminaries

In this section, we briefly introduce the background for AT.

Standard AT. For each input x, let the input feature space $\mathcal{X}$ with the infinity distance metric $d_{\inf}(x,x') = \|x-x'\|_\infty$ be $(\mathcal{X}, d_\infty)$, the closed ball of radius $\varepsilon > 0$ centered at x in $\mathcal{X}$ be $\mathcal{B}_\varepsilon[x] = \{x' \in \mathcal{X} \mid d_{\inf}(x,x') \le \varepsilon\}$, and the function space be $\mathcal{F}$. Given a dataset $S = \{(x_i, y_i)\}_{i=1}^n$ where $x_i \in \mathcal{X}$ and $y_i \in \mathcal{Y} = \{0, 1, \ldots, C-1\}$, the objective function of the standard adversarial training (Madry et al., 2018) is

$$\min_{f_W \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \left\{ \max_{\tilde{x} \in \mathcal{B}_\varepsilon[x_i]} \ell\left(f_W(\tilde{x}), y_i\right) \right\}, \tag{1}$$

where $\tilde{x}$ is the adversarial data centered at x within the ε-ball, $f_W(\cdot) : \mathcal{X} \to \mathbb{R}^C$ is a score function with parameters W and $l(\cdot) : \mathbb{R}^C \times \mathcal{Y} \to \mathbb{R}$ is the loss function that is composed of a base loss $\ell_{\mathrm{B}} : \Delta^{C-1} \times \mathcal{Y} \to \mathbb{R}$ (e.g., the cross-entropy loss) and an inverse link function $\ell_{\mathrm{L}} : \mathbb{R}^C \to \Delta^{C-1}$ (e.g., the soft-max activation). Here Δ^{C-1} is the corresponding probability simplex. In other words, $\ell(f(\cdot), y) = \ell_{\mathrm{B}}(\ell_{\mathrm{L}}(f(\cdot)), y)$. Denote $x^{(0)}$ as the starting point and $\alpha > 0$ as the step size, standard AT generates the most adversarial data by Projected Gradient Descent (PGD) as follows:

$$x^{(t+1)} = \Pi_{\mathcal{B}[x^{(0)}]}\left(x^{(t)} + \alpha \operatorname{sign}\left(\nabla_{x^{(t)}} \ell\left(f_W\left(x^{(t)}\right), y\right)\right)\right), \forall t \ge 0, \tag{2}$$

until a certain stopping criterion is satisfied to get the adversarial data $\tilde{x}$. Π is the projection operator. It then minimizes the classification loss on $\tilde{x}$, which is agnostic to NAs.

TRADES. To trade off natural and robust errors, Zhang et al. (2019b) trained a model on both natural and adversarial data and changed the min-max formulation as follows:

$$\min_{f_W \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \left\{ \ell\left(f_W(x_i), y_i\right) + \beta \ell_{\mathrm{KL}}\left(f_W(\tilde{x}_i), f_W(x_i)\right) \right\}, \tag{3}$$

where ℓ_{KL} is the Kullback-Leibler loss. β is a regularization parameter that controls the trade-off between standard accuracy and robustness. When β increases, standard accuracy will decease while robustness will increase, and vice visa. Meanwhile, the adversarial examples are generated by

$$\tilde{x}_i = \arg \max_{\tilde{x} \in \mathcal{B}_\varepsilon[x_i]} \ell_{KL}(f_W(\tilde{x}), f_W(x)). \tag{4}$$

Friendly adversarial training. Friendly AT (Zhang et al., 2020b) is a novel formulation of adversarial training that searches for least adversarial data (i.e., friendly adversarial data) minimizing the inner loss, among the adversarial data that are confidently misclassified. It is easy to implement by just stopping the most adversarial data searching algorithms such as PGD (projected gradient descent) early. The outer minimization still follows Eq. (1). However, instead of generating adversarial data via inner maximization, friendly AT generates $\tilde{x}_i$ as follows:

$$\begin{aligned} \tilde{x}_i = & \arg\min_{\tilde{x} \in \mathcal{B}_\varepsilon[x_i]} \ell\left(f_W(\tilde{x}), y_i\right) \\ & \text{s.t. } \ell\left(f_W(\tilde{x}), y_i\right) - \min_{y \in \mathcal{Y}} \ell(f(\tilde{x}), y) \ge \rho, \end{aligned} \tag{5}$$

where there is a constraint on the margin of loss values ρ (i.e., the misclassification confidence). This constraint firstly ensures $\tilde{x}$ is misclassified and secondly ensures for $\tilde{x}$ the wrong prediction is better than the desired prediction y_i by at least ρ in terms of the loss value.

There are other AT styles, such as misclassification-aware AT (Wang et al., 2020b) and Fast AT (Wong et al., 2020).

3.2. Diverse-Structured Network

The overview of our DS-Net is demonstrated in Fig. 1, which starts with a stem layer (e.g., a convolutional layer for images) for feature transformation. It then stacks K sequential robust modules and ends with an average pooling layer

and a fully connected layer. Each module has N atomic blocks and two sets of variables for optimization, namely the attention weights w and the block parameters W. We denote the attention weight for the j-th atomic block at the i-th module as w_i^j, which is randomly initialized before training. The feature transformation function of the j-th block at the i-th module is denoted as $f_{W_i^j}(\cdot)$ with the parameter W_i^j. During AT, DS-Net alternates between adversarial data generation (with the attention weights fixed) and classification loss minimization. For convenience, the following contents are described in the context of standard AT.

Forward propagation. Denote x_i as the output feature of the $(i-1)^{\text{th}}$ module and $g(\cdot)$ as the first stem layer, given an input x or its adversarial counterpart $\tilde{x}$, the forward propagation of DS-Net is formulated as follows:

$$x_{i+1} = \sum_{j=1}^{N} w_i^j \cdot f_{W_i^j}(x_i), x_1 = g(\tilde{x}), \tag{6}$$

where the output of each module is calculated as the weighted sum of outputs of different atomic blocks. Each atomic block in a robust module has the same number of input and output channels.

Backward propagation. During the backward propagation to generate adversarial examples, DS-Net fixes attention weights w and uses PGD to generate adversarial data as

$$x^{(t+1)} = \Pi_{\mathcal{B}[x^{(0)}]}\left(x^{(t)} + \alpha \operatorname{sign}\left(\nabla_{x^{(t)}} \ell\left(f_W\left(x^{(t)}\right), y, w\right)\right)\right), \forall t \geq 0, \tag{7}$$

which is similar to Eq. (2) but with a set of attention weights.

During classification loss minimization, the attention weights w and the atomic block parameters W are optimized by Stochastic Gradient Descent (SGD) as:

$$\begin{aligned} w' &= w - \alpha_w \nabla_w \ell\left(f_W(\tilde{x}), y_i, w\right), \\ W' &= W - \alpha_W \nabla_W \ell\left(f_W(\tilde{x}), y_i, w\right), \end{aligned} \tag{8}$$

where $\alpha_w, \alpha_W > 0$ are the learning rate for the two set of variables.

Under standard AT, the minimax formulation is changed as

$$\min_{w, f_W \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \left\{ \max_{\tilde{x} \in \mathcal{B}_\varepsilon[x_i]} \ell\left(f_W(\tilde{x}), y_i, w\right) \right\}, \tag{9}$$

where f_W means DS-Net with the full set of atomic block parameters W. W is simultaneously optimized with the block weights w by the classification loss on the generated adversarial data. Therefore, DS-Net is able to automatically learn to weight different atomic blocks so as to improve architecture exploration and diversity. The training and evaluation outline of DS-Net is presented in Algorithm 1.

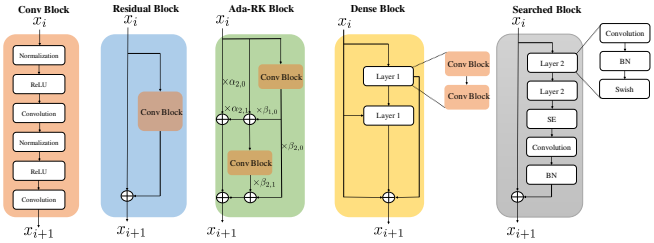

Figure 2. The atomic blocks (except for the Conv block) in DS-Net. SE means the Squeeze-and-Excitation Layer (Hu et al., 2018). Swish is an activation function (Ramachandran et al., 2018).

Algorithm 1 Diverse-Structured Network.

Input: input data $x \in \mathcal{X}$ with label $y \in \mathcal{Y}$, model f_W with block parameters W, loss function ℓ, maximum PGD steps K, perturbation bound ε, step size α, and randomly initialized attention weights w.
Output: learned model f_W and attention weights w.
while *not eval* **do**
  Step 1: Fix w and W, generate $\tilde{x}$ by Eq. (7).
  Step 2: Update w and W by Eq. (8).
end
while *eval* **do**
  Step 3: Fix w and W, generate $\tilde{x}$ by Eq. (7).
  Step 4: Calculate output by Eq. (6) and report accuracy.
end

3.3. Predefined Atomic Blocks

DS-Net allows for a flexible choice of the atomic blocks. We implement DS-Net by using four powerful atomic blocks in Fig. 2, which are either human-designed, such as the residual block (He et al., 2016), dense block (Huang et al., 2017) and Adaptive Runge Kutta (Ada-RK) block (Kim et al., 2020), or searched-based block (Tan et al., 2019). Most blocks have been theoretically or empirically validated to improve ST instead of AT. Although Ada-RK aims at AT, its generalization ability is not satisfactory (Kim et al., 2020). To trade off robustness and generalization, we simultaneously leverage four predefined atomic blocks via the learnable attention weights. Note that there are other potential candidates except the above four predefined blocks, which is a promising future work beyond the scope of our study.

Importantly, using atomic blocks avoids costly structure search for AT while exploiting powerful architectures in literature. Besides, building a robust model by these blocks is easier while retaining sufficient diversity, which is important for AT.

3.4. Robustness Analysis

We provide a robustness analysis of our DS-Net. Previous works (Weng et al., 2018; Hein & Andriushchenko, 2017) usually connected Lipschitz smoothness w.r.t. the input with

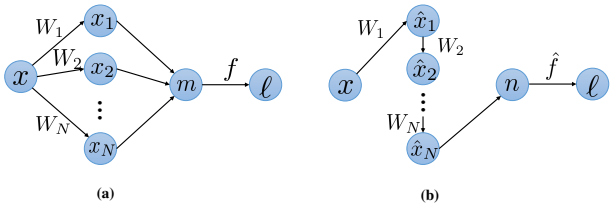

Figure 3. Two different architectures. (a) The robust module for DS-Net. (b) The common network architecture, which covers many human-designed models and searched models. $x_i, \hat{x}_i$ denote the intermediate outputs (atomic block outputs for DS-Net). $f, \hat{f}$ denote the training objective functions. m, n denote the outputs.

network robustness, which suggests that a small input perturbation will not lead to large change of the output. Formally, we give its definition.

Definition 3.1 (Paulavičius & Žilinskas, 2006) Given a model f and a perturbation δ within the ε-ball of the input x. The Lipschitz smoothness of f is represented as

$$|f(x) - f(x+\delta)| \leq L_f \|\delta\|_p \leq L\varepsilon, \tag{10}$$

where $p \geq 0$ is the norm of interest and L_f is the Lipschitz constant. Thus, a robust model holds a small value of L_f.

We fist provide Lemma 3.2 that decomposes the global Lipschitz constant into the value for each atomic block and then propose our main proposition (Proposition 3.3).

Lemma 3.2 *Denote the attention weight and the Lipschitz constant of the j-th block at the i-th module for DS-Net f as w_i^j and L_i^j, and the Lipschitz constant of the j-th block in the common network architecture $\hat{f}$ as L_j. If the number of layers and atomic blocks in DS-Net are K and N, the Lipschitz constants can be decomposed as*

$$L_f = \prod_{i=1}^{K} \sum_{j=1}^{N} w_i^j \cdot L_i^j, \quad L_{\hat{f}} = \prod_{j=1}^{NK} L_j. \tag{11}$$

Proposition 3.3 *Denote the Lipschitz constants for DS-Net with learnable or fixed attention weights as L_f and L'_f, and those of the common network architectures as $L_{\hat{f}}$, we get $L_f \leq L_{\hat{f}}$ and $L_f \leq L'_f$.*

Remark: From Proposition 3.3, we conclude two results: 1) A common network architecture $\hat{f}(\cdot)$ (Fig. 3(b)) with the same number of parameters as DS-Net (Fig. 3(a)) always holds a larger Lipschitz constant $L_{\hat{f}}$. 2) The Lipschitz constant L_f of DS-Net with learnable attention weights is smaller than that of DS-Net with an arbitrary fixed set of attention weights. The proof can be found in Appendix A.

3.5. Convergence Analysis

We provide a convergence analysis of DS-Net for solving the min-max optimization problem in Eq. (9). Due to the nonlinearities in DNNs such as ReLU (Nair & Hinton, 2010) and pooling operations, the exact assumptions of Danskin's theorem (Danskin, 2012) do not hold. Nonetheless, since adversarial training only computes approximate maximizers of the inner problem, we can still provide a theoretical guarantee of convergence. The several necessary assumptions for the analysis are given as follows.

Assumption 3.4 *Let L_{WW}, L_{Wx}, L_{xW} be positive constants, the function $f_W(x,y)$ satisfies the gradient Lipschitz conditions as follows*

$$\begin{aligned}
&\sup_x \|\nabla_W f_W(x,y) - \nabla_W f_{W'}(x,y)\|_2 \leq L_{WW} \|W - W'\|_2; \\
&\sup_W \|\nabla_W f_W(x,y) - \nabla_W f_W(x',y)\|_2 \leq L_{Wx} \|x - x'\|_2; \\
&\sup_x \|\nabla_x f_W(x,y) - \nabla_x f_{W'}(x,y)\|_2 \leq L_{xW} \|W - W'\|_2.
\end{aligned} \tag{12}$$

Assumption 3.4 requires that the loss function satisfies the Lipschitzian smoothness conditions. Despite the non-smoothness of the ReLU activation function, recent studies (Allen-Zhu et al., 2019; Du et al., 2019; Cao & Gu, 2019) justify the loss function of overparamterized networks are semi-smooth. Thus this assumption is satisfied.

Assumption 3.5 *The variance of the stochastic gradient of $f_W(x)$ is bounded by a constant $\sigma^2 > 0$ as*

$$\mathbb{E}\left[\|g(x_k, \xi_k) - \nabla f_W(x_k)\|^2\right] \leq \sigma^2, \tag{13}$$

where $g(x_k, \xi_k)$ is an unbiased estimator of $\nabla f_W(x_k)$ as $\mathbb{E}[g(x_k, \xi_k)] = \nabla f_W(x_k)$. $\xi_k, k \geq 1$ are random variables.

Assumption 3.5 is commonly used in stochastic gradient based optimization algorithms (Wang et al., 2019b).

Then we introduce the convergence analysis of non-convex optimization with the randomized stochastic gradient method (Ghadimi & Lan, 2013) as follows:

Theorem 3.6 *(Ghadimi & Lan, 2013) Suppose the technical assumptions 3.4 and 3.5 hold. Let f be L-smooth and non-convex function and f^* be the optimal value of the optimization problem (9). Given repeated, independent accesses to stochastic gradients with variance bound σ^2, let SGD start with initial network parameters W_0, iterations $N > 0$ and step size $\gamma_k < \frac{1}{L}$, then it converges to the following point by randomly choosing W_k as the final output W_R with probability $\frac{\gamma_k}{H}$. For $H = \sum_{k=1}^{N} \gamma_k$:*

$$\mathbb{E}\left[\|\nabla f_{W_R}(x)\|^2\right] \leq \frac{2\left(f_{W_0}(x) - f^*\right)}{H} + \frac{L\sigma^2}{H} \sum_{k=1}^{N} \gamma_k^2, \tag{14}$$

where f is the robust network in our case.

From this theorem, we can see that the convergence speed and stability of the optimization problem heavily depend on the Lipschitz smoothness L and the gradient variance σ^2

given the fixed number of iterations N and SGD step size (i.e., learning rate) γ_k.

In the following theorem, we explain that DS-Net has a smaller Lipschitz smoothness constant and gradient variance than common NAs. We also conduct an empirical analysis on these two factors to support our claim (Section 4.7).

Due to the complexity of global Lipschitz smoothness, we instead use the block-wise Lipschitz smoothness (Beck & Tetruashvili, 2013) in the following. Consider two architectures in Fig. 3 with the same number of parameters, then we have the following theorem.

Theorem 3.7 *Following Fig. 3, let λ_i be the largest eigenvalue of the network parameters $W_i, i = 1,\dots,N$. $f, \hat{f}$ are the objective functions for DS-Net and common network architectures, respectively. For any two possible assignments W_i^1, W_i^2 of W_i, the block-wise Lipschitz smoothness w.r.t. the network parameters and the gradient variance of the common network architectures are represented as*

$$\begin{aligned} \frac{\|\nabla_{W_i^1}\hat{f} - \nabla_{W_i^2}\hat{f}\|}{\|W_i^1 - W_i^2\|} &\leq L_i \cdot \prod_{k=1}^{i-1}\lambda_k, \\ \mathbb{E}\|\nabla_{W_i}\hat{f} - \mathbb{E}\nabla_{W_i}\hat{f}\|^2 &\leq N\sum_{k=i}^{N}\left(\frac{\sigma_k}{\lambda_i}\prod_{j=1}^{k}\lambda_j\right)^2, \end{aligned} \tag{15}$$

by assuming the two properties of DS-Net satisfy: $\|\nabla_{W_i^1} f - \nabla_{W_i^2} f\| \leq L_i \left\|W_i^1 - W_i^2\right\|$, $\mathbb{E}\left\|\nabla_{W_i} f - \mathbb{E}\nabla_{W_i} f\right\|^2 \leq \sigma_i^2$. N is the number of intermediate layers or atomic blocks.

Remark: From Theorem 3.7, we conclude two results: 1) The common network architectures hold a Lipschitz smoothness constant, namely, $\prod_{k=1}^{i-1}\lambda_k$ times that of DS-Net. Note most of the largest eigenvalues of neural networks are bigger than 1 to prevent vanishing gradients (Pascanu et al., 2013). Therefore, the convergence of Problem (9) is slower than that of DS-Net. 2) The bound of the gradient variance in common network architectures is scaled up by the largest eigenvalue of network parameters and the network depth, which hurts the convergence speed and stability of AT. The proof can be found in Appendix B, which is adapted from Shu et al. (2020). Overall, Theorem 3.7 tells us DS-Net (Fig. 3 (a)) converges faster and more stably than common network architectures (Fig. 3 (b)).

4. Experiments and Results

In this section, we present empirical evidence to validate DS-Net on benchmarks with three AT styles. The code is available at https://github.com/d12306/dsnet.

4.1. Experimental Setting

We evaluated DS-Net on CIFAR-10 and SVHN using: Projected Gradient Descent (PGD) (Madry et al., 2018), Fast Gradient Sign Method (FGSM) (Goodfellow et al., 2015), Carlini & Wagner (C&W) (Carlini & Wagner, 2017) and AutoAttack (AA) (Croce & Hein, 2020). We compared with human-designed models, such as ResNet (He et al., 2016), WideResNet (Zagoruyko & Komodakis, 2016), IE-skips (Li et al., 2020a), AdaRK-Net (Kim et al., 2020) and SAT (Xie et al., 2020a). We also compared with searched NAs for AT, i.e., RobNet (Guo et al., 2020). We used three training styles, i.e., AT (Madry et al., 2018), TRADES (Zhang et al., 2019b) and MART (Wang et al., 2020b).

For CIFAR-10, during training, we set the perturbation bound ε to 0.031 and step size α to 0.007 with 10 steps. We used SGD optimizer with a momentum of 0.9 and weight decay of 5e-4. The initial learning rate is 0.1. We trained for 120 epochs for standard AT and the learning rate is multiplied by 0.1 and 0.01 at epoch 60 and 90. For TRADES, we trained for 85 epochs and the learning rate is multiplied by 0.1 at epoch 75. We tested the performance when the model is trained with regularization factor $\beta = 1$ and $\beta = 6$. For MART, we trained for 90 epochs and the learning rate is multiplied by 0.1 at epoch 60. We set $\beta = 6$. The batch size is set to 128. For SVHN, the step size is set to 0.003 with $\varepsilon = 0.031$. The training epochs including the epoch for learning rate decay is reduced by 20 for AT, TRADES and MART. We trained on one Tesla V100 and used mixed-precision acceleration by apex at O1 optimization level[1]. We select all models 1 epoch after the 1st learning rate decay point following Rice et al. (2020) because robust overfitting also happens for DS-Net. We have tried to use 1,000 images from the training set as validation set to determine the stopping point, which aligns with our selection point.

We used Adam optimizer (Kingma & Ba, 2014) with a learning rate of 1e-3 and a weight decay of 1e-3 to optimize the attention weights, which is then normalized by softmax function. The comparison with using other optimizers is shown in Appendix E. We set the number of layers to 15 and the initial channel number to 20. We used two residual layers at the $\frac{1}{3}$ and $\frac{2}{3}$ of the total depth of the DS-Net to increase the channels by a factor of k and 2, respectively. Meanwhile, the spatial size of the feature map is reduced by a half. We set $k = 4/6$ and obtain a small and large DS-Net in our experiments, denoted as DS-Net-4/6-softmax.

The evaluation ε is set to 0.031. We used PGD attack with 20 steps and CW attack with 30 steps. The step size is set to 0.031 for FGSM attack. For non-FGSM attack, we set the step size to 0.003 on TRADES while the evaluation step size on AT and MART is 0.008. We reported the best accuracy for comparison. Due to the complexity, we reported the accuracy of AA by randomly sampling 12.5% of the test set. Each experiment is repeated by 3 times with three random seeds. The results are averaged for comparisons.

[1] https://github.com/NVIDIA/apex

Table 2. Test accuracy on CIFAR-10 and SVHN using AT (Madry et al., 2018). † means the results by our implementation under the same setting. AA denotes the results of AutoAttack (Croce & Hein, 2020). The perturbation bound ϵ is 0.031. DS-Net-4-softmax means the scale factor is 4 and block weights are normalized by the softmax activation. Improv.(%) is calculated by comparing with the best baseline.

Defense Architecture	Param (M)	Natural	FGSM	PGD-20	C&W∞	AA
CIFAR-10						
ResNet-50 (He et al., 2016)†	23.52	83.83±0.190	54.76±0.229	48.07±0.222	47.77±0.365	44.98±0.237
WRN-34-10 (Zagoruyko & Komodakis, 2016)†	46.16	86.32±0.317	64.84±0.118	51.95±0.291	50.65±0.339	50.01±0.284
SAT-ResNet-50 (Xie et al., 2020a)†	23.52	73.59±0.164	57.50±0.287	48.44±0.105	46.56±0.291	44.11±0.370
SAT-WRN-34-10 (Xie et al., 2020a)†	46.16	78.03±0.298	60.73±0.305	49.54±0.311	49.43±0.042	46.27±0.163
IE-ResNet-50 (Li et al., 2020a)†	22.41	84.49±0.111	55.00±0.229	48.31±0.321	48.04±0.392	43.27±0.138
IE-WRN-34-10 (Li et al., 2020a)†	48.24	84.23±0.200	63.28±0.222	52.61±0.316	49.36±0.501	51.24±0.251
AdaRK-Net (Kim et al., 2020)†	23.61	80.42±0.124	57.23±0.218	51.37±0.411	49.27±0.228	45.11±0.260
RobNet-large-v2 (Guo et al., 2020)†	33.42	84.39±0.129	59.21±0.311	52.54±0.371	51.28±0.212	49.22±0.138
DS-Net-4-softmax (ours)	20.78	85.39±0.216	66.71±0.186	**54.14**±0.100	52.18±0.137	49.98±0.199
DS-Net-6-softmax (ours)	46.35	**86.76**±0.125	**67.03**±0.372	53.59±0.211	**53.28**±0.174	**51.48**±0.191
Improv.(%)	-	0.51%	3.38%	2.91%	3.90%	0.47%
SVHN						
ResNet-50 (He et al., 2016)†	23.52	90.02±0.213	69.03±0.233	47.23±0.177	49.69±0.186	44.11±0.029
WRN-34-10 (Zagoruyko & Komodakis, 2016)†	46.16	94.26±0.175	75.15±0.310	48.57±0.163	50.08±0.271	45.38±0.124
DS-Net-4-softmax (ours)	20.78	95.53±0.172	**78.50**±0.278	49.53±0.301	48.73±0.101	46.21±0.222
DS-Net-6-softmax (ours)	46.35	**95.96**±0.211	75.80±0.170	**50.89**±0.235	**50.12**±0.304	**48.09**±0.258
Improv.(%)	-	1.80%	4.46%	4.78%	0.08%	5.97%

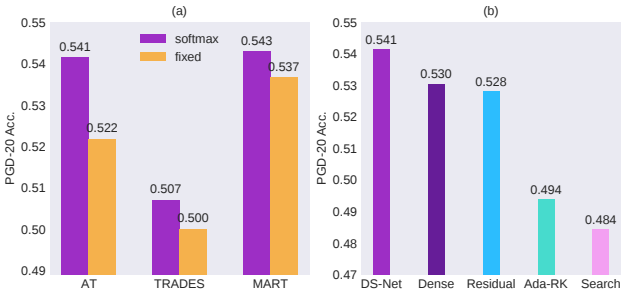

Figure 4. The results of block ensemble variants of DS-Net (under PGD-20 attack). (a) DS-Net with fixed and uniform attention weights. $\beta = 1$ is used for TRADES. (b) DS-Net with the same atomic blocks and uniform ensemble. Standard AT is used.

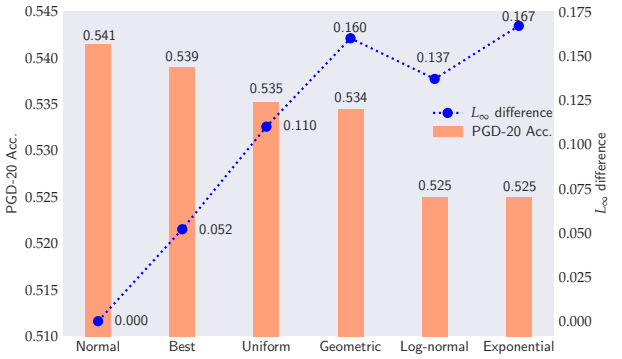

Figure 5. Comparative robustness of our DS-Net with different initializations (evaluated by PGD-20 attack).

4.2. Results on CIFAR-10 and SVHN

We presented the results of AT and MART in Tabs. 2 and 3. Results of TRADES are in Appendix C. We made several observations. First, the robustness of DS-Net is consistently better than baselines, which achieves promising results with a much smaller amount of parameters, e.g., 54.14% under PGD-20 attack with only 20.78M parameters compared to 51.95% for WRN-34-10 (46.16M) and 52.54% for RobNet (33.42M) using AT. Second, if we increase the amount of parameters to the same level of WRN-34-10 by setting the factor $k = 6$, DS-Net further improves its robustness (53.28% under CW attack). Meanwhile, DS-Net generalizes well (with a standard accuracy of 86.76%) and also performs well in terms of ensembles of white-box and black-box attacks (see AutoAttack). Third, DS-Net shows its effectiveness across different datasets and training styles, which provides better robustness and generalization ability.

4.3. Comparison with Block Ensemble

We compared the robustness of DS-Net with two variants: 1) The attention weights are uniformly distributed among different atomic blocks and fixed during training. 2) The four atomic blocks are the same whose outputs are uniformly ensembled. We compared them with DS-Net on CIFAR-10 with factor $k = 4$, which is shown in Fig. 4.

The above figure highlights two factors—a) Learnability of attention weights and (b) The diversity of atomic blocks—matter for network robustness in DS-Net. Therefore, the improvement of DS-Net does not solely come from a simple ensemble. Meanwhile, we found that the highest standard accuracy of these variants are lower than DS-Net, such as 85.31% vs. 87.89% for fixed attention weights and learnable weights in DS-Net on TRADES, which justifies that these two factors are also important for generalization.

4.4. Sensitivity to Weight Initialization

We investigated the sensitivity of DS-Net to the initialization of the attention weights. Note the results in Tabs. 2 and 3 are reported using the normal distribution ($\mu = 0, \sigma^2$=1), we further tested the uniform distribution (within $[0, 1]$), log-normal distribution ($\mu = 0, \sigma^2 = 1$), exponential distribution

Table 3. Evaluations (test accuracy) of deep models on CIFAR-10 and SVHN dataset using MART (Wang et al., 2020b). † means the results by our implementation. The perturbation bound ϵ is set to 0.031 for each architecture. The regularization factor β is set to 6.

Defense Architecture	Param (M)	Natural	FGSM	PGD-20	C&W$_\infty$	AA
CIFAR-10						
RobNet-large-v2 (Guo et al., 2020)†	33.42	80.23±0.129	60.23±0.203	51.07±0.290	48.37±0.365	48.14±0.317
WRN-34-10 (Zagoruyko & Komodakis, 2016)†	46.16	78.59±0.221	62.50±0.355	52.26±0.409	49.75±0.517	49.96±0.531
IE-WRN-34-10 (Li et al., 2020a)†	48.24	81.33±0.127	62.29±0.116	51.99±0.244	49.40±0.142	50.07±0.246
DS-Net-4-softmax(ours)	20.76	79.51±0.137	63.03±0.241	54.29±0.376	50.25±0.229	49.79±0.256
DS-Net-6-softmax(ours)	46.35	**81.64**±0.229	**66.40**±0.173	**55.23**±0.168	**51.48**±0.291	**52.74**±0.096
Improv.(%)	-	0.38%	6.09%	5.68%	3.48%	5.44%
SVHN						
WRN-34-10 (Zagoruyko & Komodakis, 2016)†	46.16	92.15±0.279	74.57±0.160	52.96±0.384	47.03±0.100	49.88±0.103
DS-Net-4-softmax (ours)	20.78	92.39±0.172	73.88±0.263	**56.08**±0.326	48.00±0.298	**51.39**±0.206
DS-Net-6-softmax (ours)	46.35	**93.77**±0.272	**76.23**±0.165	55.00±0.126	**48.84**±0.179	50.43±0.312
Improv.(%)	-	1.76%	2.23%	5.89%	3.85%	3.03%

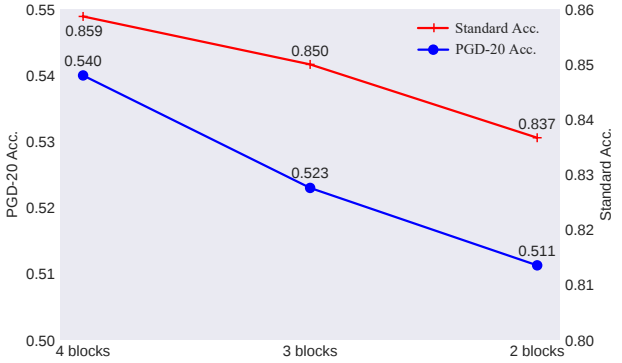

Figure 6. The performance of DS-Net with atomic block space reduction. Results are reported using seed 0.

$\lambda = 1$, geometric distribution ($p = 0.5$). We also used the optimized attention weights after training for initialization. We compared these initializations using standard AT on CIFAR-10 with factor $k = 4$, which are shown in Fig. 5.

From the above figure, DS-Net is not sensitive to different initializations, where the largest accuracy drop is $\leq 2\%$. The optimized weight for initialization obtains the closet performance to the original one, which illustrates its superiority. Besides, we compared the l_∞ difference between the learned weights initialized with the normal distribution and the others, which shows a similar trend to the PGD-20 Acc.

4.5. Effect of Reducing Atomic Block Space

To observe whether the number of atomic blocks matters to model performance, we trained our DS-Net under 2 and 3 atomic blocks for each robust module. Note that sampling 2 and 3 atomic blocks from 4 blocks has 6 and 4 options and we reported the average results. To ensure a fair comparison, we kept the same level of network parameters by changing the initial channel number across different models. We compared them with DS-Net-4-softmax using standard AT on CIFAR-10 with factor $k = 4$, which are shown in Fig. 6.

From Fig. 6, the performance of DS-Net slightly decreases in terms of robustness and generalization ability with smaller atomic block space, which shows a carefully-designed block space with higher diversity is beneficial. A principled approach to block selection is a promising future work.

4.6. Learned Attention Weight Visualization

To gain some insights on the location sensitivity of different atomic blocks, we visualized the learned attention weights from different layers in Fig. 8. We made several observations. First, the weight of atomic blocks is balanced in the former layers of DS-Net without obvious dominance, which implies that AT prefers a diverse structure. Second, the weight of residual block increases in the last layers, which shows DS-Net tends to tends to use the cleaner feature representations by favoring residual blocks in the later layers for classification. This phenomenon happens because the error of features learned by the early layers accumulates less than that learned by the later layers. Third, densely connected modules are more favorable in robust models. For instance, DS-Net-6-softmax pays more attention to the dense block compared to DS-Net-4-softmax, and DS-Net-6-softmax under TRADES ($\beta = 6$) gives more weights to dense block than DS-Net-6-softmax under TRADES ($\beta = 1$). Such findings align well with Guo et al. (2020). The trends may guide us to design different blocks for different layers of a robust model.

4.7. Empirical Convergence Analysis

We showed in Theorem 3.6 that Lipschitz smoothness and gradient variance are important for convergence. In this section, we empirically verified these two properties of DS-Net. Due to the substantial budget for calculating the Hessian matrix of the objective function in order to measure the global Lipschitz smoothness (Nesterov, 2004), we followed (Li et al., 2018) and used the loss landscape to measure the local smoothness of models, which is visualized as $f(\alpha, \beta) = L(W^* + \alpha\delta + \beta\eta)$ (δ, η are two random directions and W^* is the center point in the network parameter space). We compared the loss landscape among four models in Fig. 7 (a), and found that DS-Net empirically smooths the loss landscape around the optimized parameters, which makes the convergence faster and more stable.

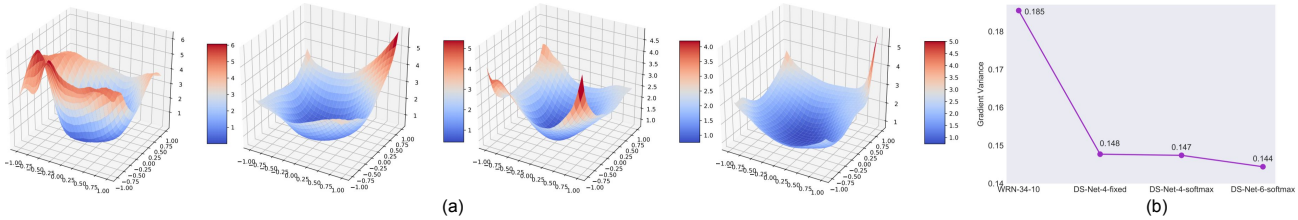

Figure 7. Empirical convergence analysis under TRADES ($\beta = 6$). (a) 3D loss landscape of four models, i.e., WRN-34-10, DS-Net-4-fixed, DS-Net-4-softmax and DS-Net-6-softmax from left to right where "fixed" means we use 0.25 as the weight for each atomic block. The height of the surface indicates the loss value. (b) Gradient variance for the same set of models.

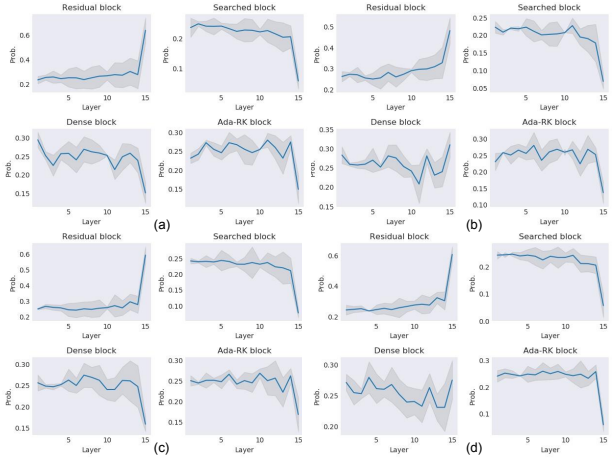

Figure 8. Visualization of the learned attention weights with variance in shaded area. (a) DS-Net-4-softmax under AT. (b) DS-Net-6-softmax under AT. (c) DS-Net-6-softmax under TRADES ($\beta = 1$). (d) DS-Net-6-softmax under TRADES ($\beta = 6$).

We computed the gradient variance of DS-Net by its definition $\mathbb{E}\|\nabla_{W_i} f - \mathbb{E}\nabla_{W_i} f\|^2$. To reduce computational cost, following Shu et al. (2020), the gradients over batches are regarded as the full gradients and the expected gradient is calculated by averaging over batch gradients. The variance is calculated w.r.t. the last fully connected layer. The comparison among the same set of models is shown in Fig. 7(b), where DS-Net holds a smaller gradient variance. Learnable attention weights and more network parameters are beneficial to convergence speed and stability.

4.8. Results after Block Pruning

To observe whether block pruning in search-based methods (Dong et al., 2020a) benefits DS-Net, we tested the performance of DS-Net by selecting 1,2,3 atomic blocks with higher probabilities after training, re-normalizing their weights and retraining the model from scratch by AT (The weights are fixed). We also tested 4 blocks with their optimized attention weights. To ensure a fair comparison, we kept the same level of network parameters by changing the initial channel number across different models. We conducted experiments using standard AT on CIFAR-10 with factor $k = 4$, which are shown in Tab. 4.

Table 4. Model robustness and generalization ability with different number of pruned blocks. The standard deviations (Std.) are shown below the mean row (Acc.).

Selected Blocks	1	2	3	4	Ours
PGD-20 Acc. (%)	42.03	51.88	50.70	52.19	**54.14**
Std.	0.339	0.214	0.213	0.291	0.100
Standard Acc. (%)	78.05	84.22	84.30	83.75	**85.39**
Std.	0.172	0.238	0.176	0.118	0.216

Tab. 4 shows that block pruning is not suitable for DS-Net, since attention weights and block parameters are co-adapted together. Therefore, discarding parameters that cooperates well with attention weights will lead to the accuracy drop. Additionally, such block pruning reduces the structure diversity during retraining, which may also hurt the model robustness and generalization ability.

5. Conclusion

Orthogonal to studies from the view of objective and optimizer for AT, we focus on NAs and propose a Diverse-Structured Network (DS-Net) to improve model robustness. DS-Net trades off exploring diverse structures and exploiting the best structures. Specifically, it learns a set of attention weights over predefined atomic blocks, where attention weights are jointly optimized with network parameters by the robust training objective that encourages structure exploration. We theoretically demonstrate the advantage of DS-Net in terms of robustness and convergence, and empirically justify our DS-Net on benchmark datasets. In the future, we will improve DS-Net by studying different combination of atomic blocks to further improve model robustness.

Acknowledgements

XFD and BH were supported by HKBU Tier-1 Start-up Grant and HKBU CSD Start-up Grant. BH was also supported by the RGC Early Career Scheme No. 22200720, NSFC Young Scientists Fund No. 62006202 and HKBU CSD Departmental Incentive Grant. TLL was supported by Australian Research Council Project DE-190101473. JZ, GN and MS were supported by JST AIP Acceleration Research Grant Number JPMJCR20U3, Japan. MS was also supported by the Institute for AI and Beyond, UTokyo.

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