Manifold regularization is a technique that penalizes the complexity of learned functions over the intrinsic geometry of input data. We develop a connection to learning functions which are “locally stable”, and propose new regularization terms for training deep neural networks that are stable against a class of local perturbations. These regularizers enable us to train a network to state-of-the-art robust accuracy of 70% on CIFAR-10 against a PGD adversary using $\ell_\infty$ perturbations of size $\epsilon = 8/255$. Furthermore, our techniques do not rely on the construction of any adversarial examples, thus running orders of magnitude faster than standard algorithms for adversarial training.

1 Introduction

A hallmark of modern deep learning is the seemingly counterintuitive result that highly overparameterized networks trained to zero loss somehow avoid overfitting and perform well on the test set \cite{12}. Despite this ability to generalize, it is also well-established that such models are highly susceptible to adversarial examples \cite{16}, whereby small perturbations to natural images considered imperceptible by human standards (e.g., slight rotations or tiny changes to pixel intensities) can cause almost complete degradation of performance. This instability presents a major obstacle for the deployment of deep learning in safety-critical applications, e.g., autonomous navigation and other physical systems \cite{1,6}.

One of the most effective approaches for learning adversarially robust classifiers is adversarial training \cite{7,12,2}, which replaces the training set with adversarially perturbated examples at each training step. However, the process of generating adversarial perturbations involves an expensive inner optimization that effectively increases the number of training epochs by a multiplicative factor (a factor of 5–10 is standard, though early stopping can improve this overhead \cite{18}).

Contributions This work takes a step back from adversarial robustness to consider a closely related concept: local stability. Our key insight is that we want to learn a function which does not vary much in small neighborhoods of natural inputs, even if the network classifies incorrectly. We show that this definition of local stability has a natural interpretation in the context of manifold regularization \cite{3}, and propose an efficient regularizer for batched gradient descent which is independent of the specific adversarial threat model but still displays surprisingly robust performance.

Our second contribution is a manifold regularization term which exploits the continuous piecewise linear nature of ReLU networks. The combination of these two regularizers brings us to the state of the art for robust networks, achieving 70% adversarial and 90% clean accuracy on CIFAR-10 image classification in 100 epochs. Furthermore, computing these regularizers simply requires evaluating the network at two additional random points for each training sample, so the total computational cost is on par with three parallel forward passes through the network. Our techniques thus present a novel, regularization-only approach to adversarial robustness which is orthogonal to standard adversarial training and so enjoys better scaling in addition to improved robust and clean accuracy.

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2 Related Work

One of the first examples of adversarial training is the Fast Gradient Sign Method (FGSM) [7], which takes a single maximal step along the gradient of the loss function to construct adversarial perturbations. Subsequent works refine FGSM by taking smaller iterative steps, and the resulting Project Gradient Descent (PGD) attack [12] is widely considered to be an empirically sound algorithm for both training and evaluation of robust models. Later improvements to this basic algorithm include strengthening the adversary or otherwise augmenting the training procedure [4, 20, 23]. Because the iterative construction of adversaries is computationally expensive, recent works modify PGD to make it more efficient [15]; in particular, Wong et al. [18] showed that training against an FGSM adversary with early stopping suffices to achieve state-of-the-art robustness.

Manifold regularization was introduced by Belkin et al. [3] for semi-supervised learning. In this context, input data is assumed to be supported on a submanifold of the input domain. The goal of manifold regularization is to leverage the unlabeled samples to learn a function which behaves well (e.g., is smooth, or has low complexity) on this implicit geometry. The use of manifold regularization for deep neural networks has been explored in various contexts [21, 17, 10, 24]; in particular, Lee et al. [11] consider manifold regularization for adversarial robustness, but the loss is still based on the construction of explicit adversarial examples.

Regularization of ReLU pre-activations is closely related to efforts to verify or certify the robustness of neural networks, since reducing the number of effective “branches” in the neighborhoods of inputs can also reduce the search space of such algorithms. Specifically, Xiao et al. [19] use a similar loss based on ReLU pre-activations to learn stable ReLUs for efficient verification, but ultimately still rely on a PGD adversary to generate training perturbations. Similar in spirit is training for efficient certifiable robustness using interval bound propagation [13, 8], where the interval bound approximations are tighter when ReLU patterns are more similar. The computational cost is comparable at two forward passes through the network (versus three for our method), though the adversarial accuracy is worse.

3 Background

ReLU networks Our development focuses on a standard architecture for deep neural networks: fully-connected feedforward networks with ReLU activations. In general, we can write the function represented by such a network with $n$ layers and parameters $\theta = \{A_i, b_i\}_{i=1,\ldots,n-1}$ as

$$\begin{align*}
z_0 &= x \\
\hat{z}_i &= A_i \cdot z_{i-1} + b_i & \text{for } i = 1, \ldots, n-1 \\
z_i &= \sigma(\hat{z}_i) & \text{for } i = 1, \ldots, n-2 \\
f(x; \theta) &= z_{n-1}
\end{align*}$$

where $A_i$ are the weight matrices and $b_i$ are the bias vectors. We call the $z_i$ “hidden activations”, or more simply, activations, and the $\hat{z}_i$ “pre-activations”.

In this work, we consider ReLU networks, where the non-linear activation function $\sigma(\cdot)$ in (3) is the Rectified Linear Unit (ReLU)

$$z_i = \sigma(\hat{z}_i) := \max(0, \hat{z}_i)$$

It is clear from this description that ReLU networks are a family of continuous piecewise linear functions. We denote the linear function induced by an input $x$ as $f_x(\cdot; \theta)$, i.e., the analytic extension of the local linear component about $x$ to $\mathbb{R}^d$, where $d$ is the input dimension. This function can also be obtained by replacing the ReLUs at each layer with the activations “fixed” by $x$: $\sigma_i(y; x) := \sigma(\hat{z}_i)/\hat{z}_i \cdot y$.

Adversarial examples One common measure of robustness for neural networks is against a norm-bounded adversary. In this model, the adversary is given an input budget $\epsilon$ over a norm $\|\cdot\|_{in}$, and asked to produce an output perturbation $\delta$ over a norm $\|\cdot\|_{out}$. An adversarial example $x'$ is an $\epsilon$-$\delta$ certificate if

$$\begin{align*}
\|x' - x\|_{in} &\leq \epsilon \\
\|f(x'; \theta) - f(x; \theta)\|_{out} &\geq \delta
\end{align*}$$
When the specific norm is either unimportant or clear from context, we also write the first condition as \( x' \in N_\epsilon(x) \), where \( N_\epsilon(x) \) refers to the \( \epsilon \)-ball or neighborhood about \( x \) (and similarly for the second condition). If such a certificate does not exist, we say that the network is \( \epsilon \)-\( \delta \) robust at \( x \).

In this work, we consider adversaries bounded by the \( \ell_\infty \) “norm”, defined for vectors as \( |x|_\infty := \max_i |x_i| \) (and analogously for matrices). For classification tasks, the adversary is successful if it is able to produce an example in the \( \epsilon \)-neighborhood of \( x \) which causes the network to misclassify. In this case, we drop \( \delta \) and simply say that the network is \( \epsilon \)-robust at \( x \). Note that if \( f(x; \theta) \) is already incorrect, then \( x \) suffices as an adversarial example.

**Manifold regularization** Manifold regularizers are based on the assumption that the input data is not drawn uniformly from the input domain \( X \), or the ambient space, but rather supported on a submanifold \( M \subset X \), called the intrinsic geometry. This assumption is natural for, e.g., vision tasks, where a randomly drawn image is almost certainly noise. There is thus a distinction between regularizing on the ambient space, where the learned function is smooth with respect to the entire input domain (e.g., Tikhonov regularization), and regularizing on the intrinsic geometry, which uses the shape of the input submanifold to determine the regularization norm.

More explicitly, manifold regularization is guided by the intuition that the gradient of the learned function \( \nabla_M f(x) \) should be small wherever the marginal probability \( P_X(x) \) of drawing a sample is large. This idea leads to the following intrinsic regularizer:

\[
||f||_I^2 := \int_M ||\nabla_M f(x)||^2 dP_X(x)
\]

In general, the marginal \( P_X(x) \) is not known, so Belkin et al. propose the following approximation, which converges to the integral for an unweighted submanifold (i.e., where input samples are uniformly distributed over the input manifold \( M \)):

\[
||f||_I^2 \approx \frac{1}{N^2} \sum_{i,j=1}^N (f(x_i) - f(x_j))^2 W_{i,j}
\]

Here, the \( x_1, \ldots, x_N \) are samples from the input domain \( X \), and \( W \) is the Laplacian matrix of weights measuring distance between points. A common choice of Laplacian is to use a Gaussian kernel \( (W_{i,j} := \mathcal{N}(|x_i - x_j|, \sigma^2) \), where \( \mathcal{N}(0, \sigma^2) \) is a centered normal). To increase the sparsity of the Laplacian, weights are often truncated to the \( k \)-nearest neighbors or neighbors within some \( \epsilon \)-ball.

### 4 Manifold Regularization for Local Stability

We first reframe the goal of learning functions that are robust using a perspective which decouples stability from accuracy. The key observation is that we would like to train networks which are locally stable around natural inputs, even if the network output is incorrect. This approach contrasts with adversarial training, which attempts to train the network to classify correctly on worst-case adversarial inputs.

In particular, recall that a network is \( \epsilon \)-robust at \( x \) if there does not exist an example in the \( \epsilon \)-neighborhood of \( x \) which causes the network to misclassify. Instead of this definition of robustness, we consider the related property of \( \epsilon \)-stability:

**Definition 4.1** A function \( f \) is \( \epsilon \)-stable at an input \( x \) if there does not exist a perturbation \( x' \) in the \( \epsilon \)-neighborhood of \( x \) such that \( f(x) \neq f(x') \).

This definition is independent of the correct label for \( x \); as such, we argue that \( \epsilon \)-stability is a property of the function with respect to the input manifold and can thus be captured using manifold regularization. For completeness, we state the following connection between robustness and stability:

**Proposition 4.1** A function \( f \) is \( \epsilon \)-robust at an input \( x \) if and only if \( f \) is \( \epsilon \)-stable at \( x \) and \( f \) correctly classifies \( x \).

Thus our central thesis is that optimizing for stability and accuracy separately will result in a function which is robust as a byproduct. We note that a similar decomposition between accuracy and stability...
forms the basis for the TRADES algorithm for adversarial robustness [23], though the training procedure ultimately still relies on adversarial examples generated by PGD to estimate stability.

4.1 Stochastic Manifold Regularization

We first propose a different approximation for general manifold regularization which is specialized for stochastic gradient descent (SGD). Recall that SGD randomly partitions the dataset into mini-batches and performs gradient updates with respect to each mini-batch in sequence. The analogous term for manifold regularization is:

$$||f||_I^2 \approx \frac{1}{N^b} \sum_{i,j=1}^{N_b} (f(x_i) - f(x_j))^2 W_{i,j}$$

where the sum is over the samples in a mini-batch. This procedure has the effect of sparsifying the Laplacian by randomly sampling graph partitions. The estimate behaves similarly to regular SGD, i.e., the expectation of this gradient of each mini-batch equals the gradient over the full training set. The training procedure simply adds this intrinsic regularization term as an additional loss for each mini-batch gradient update. We call this technique Stochastic Manifold Regularization.

One benefit of this approach is that the regularization comes at nearly zero overhead when training via stochastic gradient descent. Additionally, the approximation is also an unbiased estimator under very mild assumptions about the sampling procedure which are inherited from SGD, whereas other common sparsification techniques, e.g., $k$-nearest neighbors, require more involved arguments about concentration. Surprisingly, this is, to the best of our knowledge, the first time manifold regularization has been combined with SGD this way.

4.1.1 Relationship to Local Stability

We train a network with vanilla stochastic manifold regularizer and experiment between several settings of the weights $W_{i,j}$, namely $\ell_2$ distance ($W_{i,j}^{-1} = ||x_i - x_j||_2^2$), batch deviation ($W_{i,j}^{-1} = N_b^{-1} \sum_j ||x_i - x_j||_2^2$), and unweighted ($W_{i,j} = 1$). Note that we can interpret batch deviation as a weighted manifold with an unweighted Laplacian, where we approximate the probability density at a sample $x$ by the average distance to other samples; the regularizer thus prioritizes smoothness where samples are more “dense” on the manifold.

We find the addition of this loss alone suffices to learn a neural network which is 22% robust on CIFAR-10 at $\epsilon = 8/255$ against a 200-step PGD adversary with 10 random restarts. This performance is somewhat surprising, as the approach so far is fully general—i.e., without any reference to the adversarial budget $\epsilon$ or even the structure of the neural network. In other words, the robustness comes simply from learning functions which are smooth on the intrinsic geometry of input data.

However, $\epsilon$-stability clearly modifies the intrinsic geometry by expanding the input submanifold to its $\epsilon$-neighborhood; furthermore, the density of this expanded manifold should be fairly constant in every $\epsilon$-ball, since every point in the $\epsilon$-ball is equally “important” for evaluation. We thus design a second manifold regularization term to capture the geometry of this expanded manifold.

4.2 Hamming Embeddings

One obvious way to extend the previous approach for $\epsilon$-stability is to simply replace every input with a random perturbation from its $\epsilon$-ball at training time. However we do not expect this method to yield good results: the intrinsic geometry is often assumed to be a much lower dimension submanifold, while the $\epsilon$-ball lifts the submanifold back to the full dimension of the ambient space, and thus may require much higher sample complexity to learn. Indeed, as our experiments show, this approach can actually hurt the robustness of the network.

Instead, we design a different regularization term which leverages the structure of ReLU networks. First, observe that every local linear component $f_x(\cdot; \theta)$ can be identified with a specific “activation pattern”, i.e., the sequence of branches taken at each ReLU. Because ReLUs separate the input space via hyperplanes, the activation patterns induce a Hamming metric on the input space. We call the activation pattern for an input its Hamming embedding, denoted $H(\cdot; \theta)$; similarly, we write $H(\cdot, \cdot; \theta)$ for the induced Hamming metric.
Recall that the goal of regularization is to reduce the complexity of the learned function \( f \) in the \( \epsilon \)-neighborhood of inputs \( x \). We argue that the Hamming metric gives a concise measure of this complexity. Specifically, if we consider the number of distinct local linear components in the \( \epsilon \)-neighborhood of an input \( x \), then \( \forall x' \in N_\epsilon(x), H(x, x'; \theta) = 0 \) if and only if the entire \( \epsilon \)-neighborhood of \( x \) is a single linear component. Thus, minimizing the Hamming distance between \( x \) and all \( x' \in N_\epsilon(x) \) serves to reduce the number of linear components in the neighborhood of \( x \).

Furthermore, we can view \( H(\cdot; \theta) \) as an output of the function \( f \), which leads to the following manifold regularizer:

\[
||H(\cdot; \theta)||^2 \approx \frac{1}{N^2} \sum_{i=1}^{N} H(x_i^+, x_i^-; \theta)^2 W_{i+, i^-}
\]

where the outputs \( f(x) \) have been replaced by the Hamming embedding, and \( x_i^+ \) and \( x_i^- \) are perturbations from the \( \epsilon \)-neighborhood of \( x_i \).

However, this loss term is not continuous in the inputs, and furthermore, the gradients vanish almost everywhere, so it does not generate good training signals. We thus use a continuous relaxation of the Hamming distance:

\[
H_\alpha(\hat{z}, \hat{y}; \theta) := \text{abs}(\tanh(\alpha \hat{z}) - \tanh(\alpha \hat{y}))
\]

Though this form is not differentiable when \( \hat{z} = \hat{y} \), it has the advantage that activation patterns which are closer to the decision boundaries (i.e., \( |\hat{z}| \) and \( |\hat{y}| \) are small) are penalized more than those which are farther, an effect which can be tuned by the hyperparameter \( \alpha \). This behavior permits activations of small magnitude so long as they are precise, the intuition being that the gradient of \( H_\alpha \) approximates the sensitivity of the Hamming distance. Figure 1 presents the surface and contour plots of \( H_\alpha \).

Additionally, by virtue of the Hamming distance being a metric on the input space, we have that, given a set of input points \( X \), if \( \max_{x,y \in X} H(x, y; \theta) \leq c \), then the same bound holds for every point in the convex set of \( X \). Thus, it suffices to sample \( x'' \in N_\epsilon(x) \) such that the convex set defined by the \( x'' \) covers the \( \epsilon \)-neighborhood of \( x \) with high probability. This property motivates sampling \( x_i^+ \) to be some corner of the \( \epsilon \)-neighborhood of \( x \), and taking \( x_i^- = 2x - x_i^+ \) to be the opposing corner. We can then also drop the weight \( W_{i+, i^-} \) since the distance between \( x_i^+ \) and \( x_i^- \) sampled this way is constant.

Finally, we note that this idea can be extended more generally to other activation functions by penalizing differing pre-activations more when the second derivative of the activation function is large (and so the first-order Taylor approximation has larger errors).

### 4.2.1 Training with the Hamming Regularizer

For every sample \( x \), we generate a new random maximal perturbation \( \rho \in \{\pm \epsilon\}^d \) and produce the pair of perturbed inputs \( x^+ := x + \rho \) and \( x^- := x - \rho \). We then compute the Hamming distance...
between the points $x^+$ and $x^-$. We use the $\ell_2$ norm to combine the Hamming distances within a layer and normalize by twice the number of elements in each layer (so that the maximum loss for a single layer is 1). The resulting losses are summed over every layer and again normalized by the number of layers. Finally, as with the vanilla manifold regularization, we use stochastic estimates of the Hamming regularization term to train with SGD.

Our final objective is thus to find the parameters $\theta$ which minimize

$$\theta^* = \arg\min_\theta \frac{1}{N} \sum_{i=1}^N V(f(x_i; \theta), y_i) + \gamma_K ||f(\cdot; \theta)||_K^2 + \gamma_I ||f(\cdot; \theta)||_I^2 + \gamma_H ||H(\cdot; \theta)||_I^2$$

where $V$ is the loss function for prediction error, $||f(\cdot; \theta)||_K^2$ is the ambient regularizer (e.g., $\ell_2$ loss), and the $\gamma_K, \gamma_I, \gamma_H$ are hyperparameters which control the relative contributions of the different regularizers.

## 5 Experimental Results

We trained a PreActResNet18 model \cite{resnet} for 100 epochs on CIFAR-10 using a combination of vanilla and Hamming manifold regularization. The final adversarial accuracy of 70.08\% ($\epsilon = 8/255$) was evaluated using a 200-step PGD adversary with 10 random restarts. Figure 2 plots the adversarial accuracies every 10 epochs against a weaker adversary. All results are reported using the $\ell_2$ weight for the standard stochastic manifold regularizer:

$$||f||_I^2 = \frac{1}{N^2} \sum_{i,j=1}^{N_b} \frac{|f(x_i) - f(x_j)|_2^2}{||x_i - x_j||_2^2}$$

### 5.1 Discussion

We compare our performance on CIFAR-10 for $\epsilon = 8/255$ against other proposed defenses with results taken from the literature. Table 1 reports two performance metrics: robust accuracy is evaluated using a white-box PGD adversary, which has full access to model parameters to construct an adversarial perturbation for each input in the test set; and clean accuracy, which is the accuracy on unperturbed images from the test set.

We find that stochastic manifold regularization achieves not only the best robust accuracy (70.08\% versus the runner-up, vanilla PGD, at 56.8\%), but also the best clean accuracy (90.91\% versus regular FGSM, which has 90.3\% clean accuracy but 0.0\% robust accuracy). These results support the thesis
| Mechanism               | Defense                | Test Accuracy (%) |
|------------------------|------------------------|-------------------|
|                        |                        | Robust | Clean |
| Adversarial Training   | PGD ‡                  | 45.8   | 87.3  |
|                        | PGD (early stopping)† | 56.8   | 86.1  |
|                        | FGSM ‡                 | 0.0    | 90.3  |
|                        | FGSM (early stopping)‡ | 46.3   | 86.4  |
| Certification          | IBP *                  | 34.77  | 49.49 |
| Adversarial Regularization | TRADES §              | 56.61  | 84.92 |
|                        | TRADES (early stopping)‡ | 55.0   | 84.1  |
| Regularization         | Manifold Regularization (ours) ‡‡ | 70.08 | 90.91 |

Table 1: Comparison of CIFAR-10 adversarial accuracy for $\epsilon = 8/255$.

that fully separating concerns of local stability from accuracy makes it easier to find good solutions to both problems.

We obtained our results after training for 3 hours on a single GPU, compared to 80 hours for standard PGD training [15].

5.2 Experimental Methods and Hyperparameters

We use a PreActResNet18 model for the CIFAR-10 experiments. We train using SGD with the cross entropy loss, momentum of 0.9, and weight decay $\gamma_K$ of 1e-4. The learning rate starts at 0.1 and decreases by a factor of 10 at 25 epochs and additional factors of 100 at 50 and 75 epochs.

We increase epsilon from 2 to 10 over 80 epochs. The weight $\gamma_I$ of the manifold regularization term starts at 10 and increases by 1 every epoch. The weight $\gamma_H$ of the Hamming regularization term starts at 0.1 and increases by 0.01 every epoch, and we set the hyperparameter $\alpha = 8$. We do not observe any degradation of performance within the training regime from letting the two manifold regularizers increase without bound.

For testing, we used a 200-step PGD adversary with 10 random restarts and a PGD step size of $2/255$. We cross-checked our implementation of PGD with the implementation in Engstrom et al. [5].

6 Conclusion

We design two manifold regularizers that together encourage piecewise linear neural networks to learn locally stable functions. We demonstrate this stability empirically by training models to state-of-the-art robustness of 70% against an $\ell_\infty$-bounded PGD adversary on CIFAR-10. Interestingly, our networks also have higher natural accuracy than adversarially trained networks, suggesting that encouraging the network to be locally stable on the intrinsic geometry of the input submanifold leads to fundamentally different local optima than using adversarial examples.

Critically, our regularizers rely on random sampling, and thus do not require running an inner optimization loop to find strong perturbations at training time. As such, our technique exhibits strong scaling, since it increases batch sizes rather than epochs at training time. Our methods are also universal, and can be used in any training regime to learn more stable networks. Finally, we believe that local stability presents a natural objective for learning, and we expect that this line of work will prove fruitful beyond adversarial robustness.
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