
Can we achieve robustness from data alone?

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Abstract

We introduce a meta-learning algorithm for adversarially robust classification. The proposed method tries to be as model agnostic as possible and optimizes a dataset prior to its deployment in a machine learning system, aiming to effectively erase its non-robust features. Once the dataset has been created, in principle no specialized algorithm (besides standard gradient descent) is needed to train a robust model. We formulate the data optimization procedure as a bi-level optimization problem on kernel regression, with a class of kernels that describe infinitely wide neural nets (Neural Tangent Kernels). We present extensive experiments on standard computer vision benchmarks using a variety of different models, demonstrating the effectiveness of our method, while also pointing out its current shortcomings. In parallel, we revisit prior work that also focused on the problem of data optimization for robust classification (Ilyas et al., 2019), and show that being robust to adversarial attacks after standard (gradient descent) training on a suitable dataset is more challenging than previously thought.

1. Introduction

The discovery of the adversarial vulnerability of neural nets (Szegedy et al., 2014; Goodfellow et al., 2015; Papernot et al., 2017; Carlini & Wagner, 2017) - their brittleness when exposed to imperceptible perturbations in the data - has shifted the focus of the machine learning community from standard gradient techniques to more complex training algorithms that are rooted in robust optimization. In principle, if \mathcal{P} denotes a data distribution and Δ is a set of allowed perturbations of the input space, we would like to solve the following problem (Madry et al., 2018):

$$\inf_{\theta} \mathbb{E}_{(x,y) \sim \mathcal{P}} \sup_{\delta \in \Delta} \mathcal{L}(f(x + \delta; \theta, \mathcal{D}_{\text{train}}), y), \quad (1)$$

where f is a model parameterized by θ (e.g. a neural network), $\mathcal{D}_{\text{train}}$ denotes a finite dataset used for training, and

\mathcal{L} is a loss function used for classification.

Since solving this problem is generally intractable, it is common to employ an iterative algorithm that interchangeably performs steps of gradient ascent/descent, a procedure called adversarial training (Goodfellow et al., 2015; Madry et al., 2018). Here, training data is augmented on the fly through perturbations coming from the very model it is training. While adversarial training in its many variants (e.g. (Zhang et al., 2019; Wong et al., 2020a)) has been successful and currently constitutes the only defense that consistently withstands adversarial attacks, it is computationally expensive and the produced models still fall short in absolute accuracy (Croce et al., 2020).

However, once we focus on non-parametric models f (such as kernel ridge regression), we can pose a more “direct” problem

$$\inf_{\mathcal{D}_{\text{train}}} \mathbb{E}_{(x,y) \sim \mathcal{P}} \sup_{\delta \in \Delta} \mathcal{L}(f(x + \delta; \mathcal{D}_{\text{train}}), y), \quad (2)$$

where instead of optimizing the model parameters, we optimize the *training data*. The above formulation has the benefit of directly optimizing the quantity of interest, that is the robust loss at the end of “training”/deployment. Additionally, since the outcome of this optimization is a dataset, it can be deployed with any other model, and, given favorable transfer properties, might yield good performance even outside the scope it was optimized for, without the need for costly adversarial training of the new model. This latter hope is not unfounded, since adversarial examples themselves have been shown to be rather universal and transferable across models (Papernot et al., 2017; Moosavi-Dezfooli et al., 2017).

Datasets are more modular than models in terms of compatibility with different frameworks and codebases; and *robust* datasets could accelerate research in trustworthy machine learning. Recent work has explored the role of data in many machine learning areas. Wang et al. (2018b) have initiated a growing body of work on dataset distillation. Data pruning techniques (Paul et al., 2021) have been successfully used for finding sparse networks (Paul et al., 2022) or improving neural scaling laws (Sorscher et al., 2022), making our exploration into data-induced robustness even more timely.

In this work, we initiate such a data-based approach to robustness in a principled way. We propose a gradient-based

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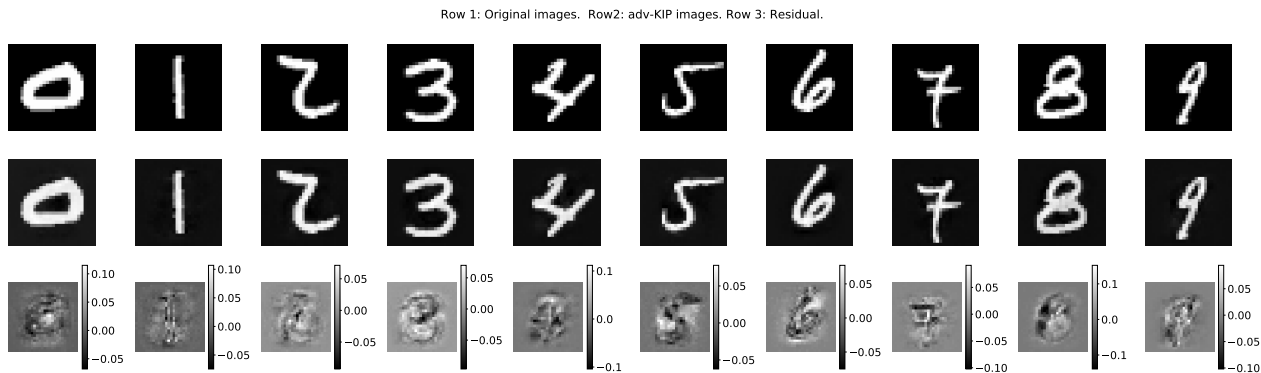


Figure 1: Samples from MNIST - one per class, before (top row) and after (middle row) optimization with `adv-KIP`. The bottom row shows the residual between the images of that column. Performance of NTK kernel regression on original data: 98.46% clean test accuracy, 0.07% robust test accuracy. On optimized data: 97.67% clean test accuracy, 42.94% robust test accuracy. `adv-KIP` hyperparameters: $\epsilon = 0.3$, 10 PGD steps, $\alpha = 0.1$, fully connected ReLU NTK with 3 layers, dataset size is 40,000.

approach for solving the optimization problem in Eq. (2), adopting kernel regression; focusing on a particular class of kernel functions, *Neural Tangent Kernels* (NTKs). Kernel regression with NTKs is known to describe the training process of infinitely wide networks (Jacot et al., 2018; Lee et al., 2019; Arora et al., 2019), providing a natural choice for the optimization of datasets for eventual deployment in neural networks. Prior work on dataset distillation (the process of distilling information from one dataset to a smaller, optimized, one) has found that meta-optimization using NTKs produces highly transferable datasets suitable for neural network training (Nguyen et al., 2021a;b). Their algorithm, *Kernel Inducing Point* (KIP), serves as an inspiration for this work; thus we give the name `adv-KIP` to our novel meta-learning algorithm for iteratively solving Eq. (2).

We perform a wide range of experiments on standard image recognition datasets (MNIST and CIFAR-10) using `adv-KIP` with a variety of different kernels and perturbation sets Δ , and discuss important design choices (dataset size, meta-optimizer, loss choices etc). We establish that the meta-learning algorithm converges to training datasets which look similar to the original ones (see Fig. 1), when used as a training set guarantee similar performance on an (unperturbed) test set, but additionally, and importantly, are also able to produce models capable of defending against gradient-based attacks.

However, we find that the models struggle to withstand non-gradient based, or adaptive, attacks. Interestingly, we observe that both neural networks and kernels that are trained on our optimized datasets have vanishing gradients with respect to the input, thus causing gradient based attacks to fail. This phenomenon, known in the literature under the umbrella term of *obfuscated gradient* (Athalye et al.,

2018), has been observed in the past, but has been largely connected to (failed) defensive interventions on models and architectures (stochastic/discrete layers etc.). Our findings show that it can also be observed in more “benign” settings, and can also be a property of the data alone.

Armed with these insights, we revisit seminal work of Ilyas et al. (2019) that put forward a dichotomy between *robust and non-robust* features (Tsipras et al., 2019; Allen-Zhu & Li, 2022; Tsilivis & Kempe, 2022) in the data. To bolster their argument, Ilyas et al. (2019) construct a dataset (using an already adversarially trained model) thought to contain solely robust features and demonstrate that a freshly initialized neural network (standardly) trained on this dataset is able to achieve non-trivial performance against gradient based attacks. Remarkably, upon re-examination, we find that models trained with these optimized datasets also suffer from the vanishing gradient problem and fail to withstand adaptive attacks, thus shattering a long standing claim in the community. Collectively, our findings establish that adversarial robustness from data alone is far more challenging than previously thought. We believe that our insights will help design and faster debug other data-based approaches in the future.

In summary, our contributions are two-fold:

- We devise a principled data based meta-learning algorithm, `adv-KIP`, tackling the bi-level optimization for adversarially robust classification in a novel way, with potentially wider applicability. We perform experiments on standard computer vision benchmarks and analyze the properties of models (kernels and neural networks) fit on the optimized datasets demonstrating that they enjoy remarkable robustness against gradient-based attacks.

- We show that robustness from data alone is more challenging than previously assumed. Standard models trained with gradient descent on datasets from `adv-KIP` suffer from the “obfuscated gradient” phenomenon, without explicitly adding non-smooth elements to the computational pipeline. We find that this is also the case for models trained with datasets presumably containing solely robust features (Ilyas et al., 2019). That is, all these models fail to withstand non-gradient based adversarial attacks, once the size of the perturbation is large enough. We examine and discuss the properties of all the models, in terms of confidence and calibration and draw lessons for future dataset design.

2. Preliminaries

Adversarial Training. Eq. 1 establishes the min-max underpinning for the construction of adversarially robust classifiers (Madry et al., 2018). The most common way to approximate the solution of this optimization problem for a neural network f is to first generate adversarial examples by running multiple steps of projected gradient descent (PGD) (Kurakin et al., 2017; Madry et al., 2018). When the set of allowed perturbations Δ is $\mathcal{B}_{\mathbf{x}}^\epsilon$ - the ℓ_∞ ball of radius ϵ and center \mathbf{x} - the iterative N -step approximation is given by

$$\mathbf{x}^{k+1} = \Pi_{\mathcal{B}_{\mathbf{x}^0}^\epsilon} (\mathbf{x}^k + \alpha \cdot \text{sign}(\nabla_{\mathbf{x}^k} \mathcal{L}(f(\mathbf{x}^k), y))), \quad (3)$$

where $\mathbf{x}^0 = \mathbf{x}$ is the original example, α is a learning step, $\tilde{\mathbf{x}} = \mathbf{x}^N$ is the final adversarial example, and Π is the projection on the valid constraint set of the data. During adversarial training we alternate steps of generating adversarial examples (using f from the current network) and training on this data instead of the original one. Several variations of this approach have been proposed in the literature (e.g. (Zhang et al., 2019; Shafahi et al., 2019; Wong et al., 2020b)), modifying either the attack used for data generation (inner loop in Eq. (1)) or the loss in the outer loop.

Kernel Regression, NTK and KIP. Kernel regression is a fundamental non-linear regression method. Given a dataset $(\mathcal{X}, \mathcal{Y})$, where $\mathcal{X} \in \mathbb{R}^{n \times d}$ and $\mathcal{Y} \in \mathbb{R}^{n \times k}$ (e.g., a set of one-hot vectors), kernel regression computes an estimate

$$\hat{f}(\mathbf{x}) = K(\mathbf{x}, \mathcal{X})^\top K(\mathcal{X}, \mathcal{X})^{-1} \mathcal{Y}, \quad (4)$$

where $K(\mathbf{x}, \mathcal{X}) = [k(\mathbf{x}, \mathbf{x}_1), \dots, k(\mathbf{x}, \mathbf{x}_n)]^\top \in \mathbb{R}^n$, $K(\mathcal{X}, \mathcal{X})_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$ and k is a kernel function that measures similarity between points in \mathbb{R}^d .

Recent work in deep learning theory has established a profound connection between kernel regression and the infinite width, low learning rate limit of deep neural networks (Jacot et al., 2018; Lee et al., 2019; Arora et al., 2019). In particular, it can be shown that the evolution of such suitably

initialized infinitely wide neural networks admits a closed form solution as in Eq. (4), with a network-dependent kernel function k . Focusing on a scalar neural net f for ease of notation, it is given by:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \nabla_{\theta} f(\mathbf{x}_i; \theta)^\top \nabla_{\theta} f(\mathbf{x}_j; \theta), \quad (5)$$

where θ are the parameters of the network. This expression becomes constant (in time) in the infinite width limit.

Many fruitful applications of NTK theory to machine learning practice have already benefited from the equivalence between kernels and neural networks (Tancik et al., 2020; Chen et al., 2021; Nguyen et al., 2021b). Our work builds on a recently proposed dataset distillation (Wang et al., 2018a) algorithm called *Kernel Inducing Points* (KIP) (Nguyen et al., 2021a;b). These works introduce a meta-learning algorithm for data distillation from an original training set \mathcal{D} , to an optimized *source* set $(\mathcal{X}_S, \mathcal{Y}_S)$ of *reduced* size but of similar generalization properties. The closed form of Eq. (4) allows to express this objective via a loss function on a *target* data set $(\mathcal{X}_T, \mathcal{Y}_T)$ as:

$$\mathcal{L}_{\text{KIP}}(\mathcal{X}_S, \mathcal{Y}_S) = \|\mathcal{Y}_T - K(\mathcal{X}_T, \mathcal{X}_S)^\top K(\mathcal{X}_S, \mathcal{X}_S)^{-1} \mathcal{Y}_S\|_2. \quad (6)$$

The error of Eq. (6) can be minimized via gradient descent on \mathcal{X}_S (and optionally \mathcal{Y}_S). Starting with a smaller subset of \mathcal{D} , sampling a target dataset from \mathcal{D} to simulate test points, and backpropagating the gradients of the error with respect to the data allows to progressively find better and better synthetic data. Importantly, leveraging the NTK for kernel regression renders the datasets suitable for deployment on actual neural nets as well.

Prior work on dataset optimization. To the best of our knowledge, the idea of trying to obtain robust classifiers through data or representation optimization is rather unexplored. Garg et al. (2018) design a spectral method to extract robust embeddings from a dataset. Awasthi et al. (2021) formulate an adversarially robust formulation of PCA, to extract provably robust representations. Ilyas et al. (2019) construct a robust dataset by traversing the representation layer of a previously trained robust classifier, which presumably contains solely robust features. Yet, all of these methods achieve substantially lower robust accuracy compared to adversarial training.

3. adv-KIP Algorithm

In this section, we introduce our meta-learning approach, `adv-KIP`, for adversarially robust classification. It optimizes a dataset prior to its deployment so that a model fit on it will have predictions that are robust against worst case perturbations of a testing input. That is, our algorithm inputs a dataset, outputs a dataset and carries out optimization (i.e. gradient updates) on the data level. Similarly to the KIP

method (Nguyen et al., 2021a;b) outlined in Section 2, our method works with kernel machines, and especially with NTKs. However, the goal here is slightly different from the KIP objective; instead of deriving a dataset of reduced size, we aim to create one that induces better robustness properties *on the original unmodified test set*. For further connections with previous work in adversarially robust classification, see App. A.1.

We modify the meta-objective of Eq. (6), and instead of optimizing the data $(\mathcal{X}_S, \mathcal{Y}_S)$ with respect to the “clean” loss of Eq. (6), we minimize

$$\tilde{\mathcal{L}}(\mathcal{X}_S, \mathcal{Y}_S) = \|\mathcal{Y}_T - K(\tilde{\mathcal{X}}_T, \mathcal{X}_S)^\top K(\mathcal{X}_S, \mathcal{X}_S)^{-1} \mathcal{Y}_S\|_2, \quad (7)$$

where, in a slight abuse of notation, $\tilde{\mathcal{X}}_T = \mathcal{X}_T + \tilde{\delta}$, and

$$\tilde{\delta} = \arg \max_{\delta \in \Delta} \mathcal{L}(K(\tilde{\mathcal{X}}_T, \mathcal{X}_S)^\top K(\mathcal{X}_S, \mathcal{X}_S)^{-1} \mathcal{Y}_S, \mathcal{Y}_T). \quad (8)$$

In other words, we optimize the data $(\mathcal{X}_S, \mathcal{Y}_S)$ to achieve the best possible performance of kernel regression on the target data set *after the adversarial attack*. Notice that this approach solves the problem outlined in Eq. (2), by adding an inner maximization problem to the KIP framework. Solving this optimization now requires an inner loop that tackles the maximization in Eq. (8). As is common, we employ first order gradient methods to solve this, namely projected gradient ascent (on the loss of the kernel machine). Algorithm 9 describes our generic robust training data set distillation framework for the case of an ℓ_∞ threat model, though it is easily modified to any constraint set Δ .

Algorithm 1: adv-KIP for ℓ_∞ adversarial attacks

Input: A training dataset $\mathcal{D}_{\text{train}} = \{\mathcal{X}, \mathcal{Y}\}$.

Parameters: Number of (meta) epochs, number of pgd_steps, pgd step size α , max attack size ϵ , (meta) learning rate λ .

Output: A new dataset \mathcal{D}_{rob} .

```

1 Sample data  $\mathcal{S} = \{\mathcal{X}_S, \mathcal{Y}_S\}$  from  $\mathcal{D}_{\text{train}}$ ;
2 for  $i \leftarrow 1$  to epochs do
3   Sample data  $\mathcal{T} = \{\mathcal{X}_T, \mathcal{Y}_T\}$  from  $\mathcal{D}_{\text{train}}$ ;
4   for  $j \leftarrow 1$  to pgd_steps do
5      $\mathcal{X}_T \leftarrow \mathcal{X}_T + \alpha \cdot$ 
6      $\text{sign}(\nabla_{\mathcal{X}_T} \mathcal{L}_{\text{ce}}(K_{\mathcal{X}_T \mathcal{X}_S} K_{\mathcal{X}_S \mathcal{X}_S}^{-1} \mathcal{Y}_S, \mathcal{Y}_T));$ 
7      $\mathcal{X}_T \leftarrow \Pi_{\mathcal{B}_\epsilon}(\mathcal{X}_T);$ 
8    $\mathcal{X}_S \leftarrow \mathcal{X}_S - \lambda \nabla_{\mathcal{X}_S} \mathcal{L}(K_{\mathcal{X}_T \mathcal{X}_S} K_{\mathcal{X}_S \mathcal{X}_S}^{-1} \mathcal{Y}_S, \mathcal{Y}_T);$ 
9    $\mathcal{Y}_S \leftarrow \mathcal{Y}_S - \lambda \nabla_{\mathcal{Y}_S} \mathcal{L}(K_{\mathcal{X}_T \mathcal{X}_S} K_{\mathcal{X}_S \mathcal{X}_S}^{-1} \mathcal{Y}_S, \mathcal{Y}_T);$ 
10  $\mathcal{D}_{\text{rob}} \leftarrow (\mathcal{X}_S, \mathcal{Y}_S)$ 

```

Algorithmic choices / Hyperparameters: There are several options to specialize in Algorithm 9:

Outer loss function (lines 7 and 8): This can be either the

mean squared error (as in Eq. (7)) or the more flexible cross entropy loss. Both quantify the discrepancy between the prediction of the kernel machine on the perturbed data and the ground truth labels. Alternatively, a loss that balances clean and robust accuracy (see e.g. (Zhang et al., 2019)) can be used.

Inner loss function (line 5): Instead of using the cross entropy loss for the generation of adversarial examples, we can also adopt previously proposed methods, like the CW-loss (Carlini & Wagner, 2017).

Optimization of labels (line 8): This is related to an interesting question raised in prior work: How important are rigid one-hot labels for robust classification (see e.g. (Papernot et al., 2016) for an ultimately unsuccessful defense). Algorithm 9 as presented here optimizes the labels, by back-propagating the loss gradients. It has the flexibility, however, to omit this part (by omitting line 8).

Dataset Size $|\mathcal{X}_S|$: While the goal of the algorithm is to ultimately produce a robust dataset, a reduced dataset size could be a useful by-product, by initializing with $|\mathcal{X}_S| < |\mathcal{X}|$ samples.

Meta-Optimizer (lines 7 and 8): Algorithm 9 presents the simplest possible version of adv-KIP; but the (meta) optimization of the data $\{\mathcal{X}_S, \mathcal{Y}_S\}$ can also be implemented with other algorithms, such as adaptive gradient methods. Indeed, in the experiments, following the code implementation of KIP (Nguyen et al., 2021a), we adopt the Adam optimizer (Kingma & Ba, 2015) instead of gradient descent.

Algorithmic Framework for Broader Data-Based Problems:

Algorithm 9 is an approach to a particular min-max problem given in Eq. (2). The advantage of deploying the NTK here is that it affords an analytic surrogate expression for the output of the trained neural networks, which allows to compute gradients with respect to the input dataset. We expect that our framework can be adopted and be helpful in other problems in data-centric machine learning, such as, for instance, average case robustness (Hendrycks & Dietterich, 2019), discrimination against minority groups (Hashimoto et al., 2018), few-shot learning (where the inner loop would optimize for accuracy on a small out-of-distribution target set) and possibly others.

4. Experiments

We evaluate the performance of adv-KIP on standard computer vision benchmarks. Specifically, we perform experiments on MNIST (Deng, 2012) and CIFAR-10 (Krizhevsky, 2009) against ℓ_∞ and ℓ_2 adversaries. In all cases, robust performance is measured on the original test dataset. We experiment with kernels that correspond to fully connected and convolutional architectures of relatively small depth,

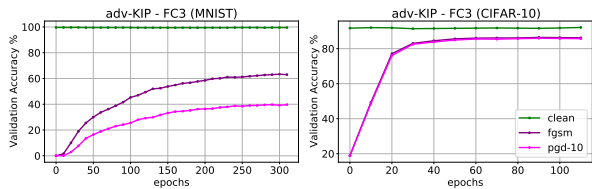


Figure 2: Validation accuracies during meta-optimization with `adv-KIP`. Setting: FC3 kernel, $|\mathcal{X}_S| = 40K$, $|\mathcal{X}_T| = 10K$, ℓ_∞ adversary, (left) MNIST $\epsilon = 0.3$, $\alpha = 0.1$, 10 PGD steps, (right) CIFAR-10 $\epsilon = 8/255$, $\alpha = 2/255$, 10 PGD steps.

due to the high computational cost of evaluating the NTK expressions. All our experiments are based on expressions available through the Neural Tangents library (Novak et al., 2020), built on top of JAX (Bradbury et al., 2018). Adversarial attacks are implemented using the CleverHans library (Papernot et al., 2018) (or slightly modified versions for efficient deployment on kernels). `FCd` and `ConvD` denote the NTK of a d -layer infinitely wide fully-connected ReLU neural network and (fully) convolutional ReLU neural network with an additional fully connected last layer, respectively.

4.1. Meta-Learning and Kernel results

We implement Algorithm 9 with the Adam optimizer (with fixed learning rate equal to $1e-3$) for a few hundred epochs with multi-step PGD attacks, using standard values of perturbation budget ϵ, α . The datasets are initialized as balanced, i.e. they contain the same number of samples from each class. The performance of the algorithm is evaluated every few epochs on a hold out validation set (part of the original training dataset), and we terminate if validation robust accuracy ceases to increase.

For both MNIST and CIFAR-10, we observe that `adv-KIP` is able to converge in a few epochs of meta-training (see Fig. 2). Validation accuracy against FGSM and PGD attacks increases with the number of outer loop steps, essentially without compromising performance on clean data. Note that at the start of the optimization (corresponding to the original data) the robustness of the kernel machine is very low, as expected from studies on neural nets.

Table 1 summarizes the test results on kernel machines. All kernel classifiers are fit with the `adv-KIP`-produced dataset meta-optimized with the same kernel. We see that just 5,000 images on MNIST suffice to yield a `Conv3` classifier scoring 96.31% test accuracy and 76.62% robust test accuracy (evaluated against strong PGD attacks of same strength as used in the inner-loop optimization with radius $\epsilon = 0.3$). Notice that all the robust benefit comes from the new, optimized images (no change in the model). We

also note that the convolutional kernel achieves better performance, despite the fact that we deploy it with a much smaller dataset \mathcal{X}_S of size 5,000. This indicates that convolutional architectures might be more amenable to meta-optimization than their fully connected counterparts. On CIFAR-10, we see a marked drop in both clean and robust accuracy; note, however, that fully connected kernels are not very competitive classifiers for CIFAR-10 images. To achieve *some* level of robustness with these simple architectures gives credence to our approach. To the best of our knowledge, this is a first (empirical) demonstration of some robustness of simple machine learning models, such as kernel methods, to adversarial attacks.

As an ablation study, we measure robust accuracy on datasets produced by the original KIP algorithm (Nguyen et al., 2021a;b) which is designed for reduction of dataset size, while keeping (clean) accuracy as uncompromised as possible. It could be reasonable to hypothesize that such information compression might possibly lead to an increase of robustness as well, but we find that this is not at all the case. We also experimented with larger KIP datasets of the same cardinality as the ones of Table 1. In all cases, we find that KIP datasets do not provide any robust accuracy, neither against FGSM nor PGD attacks (see Appendix A.2 for more details). This indicates the clear need to adjust the optimization objective to robust performance, as is done in the `adv-KIP` algorithm.

Table 1: Test accuracy % (clean and robust) of kernel machines using the optimized `adv-KIP` datasets. For MNIST (ℓ_∞): $\epsilon = 0.3$, $\alpha = 0.1$, 10 PGD steps. For CIFAR-10 (ℓ_∞): $\epsilon = 8/255$, $\alpha = 2/255$, 6 PGD steps. For CIFAR-10 (ℓ_2): $\epsilon = 1.$, $\alpha = 0.2$, 10 PGD steps. These exact same hyperparameters are used for attacks in the inner loop of the dataset meta-optimization.

Dataset	Kernel, $ \mathcal{X}_s $	Robust		
		Clean	FGSM	PGD
MNIST (ℓ_∞)	<code>Conv3</code> , 5k	96.31	94.82	76.62
	<code>FC7</code> , 30k	97.21	67.04	50.34
CIFAR-10 (ℓ_∞)	<code>FC2</code> , 40k	59.65	20.49	20.37
	<code>FC3</code> , 40k	60.14	36.44	36.30
CIFAR-10 (ℓ_2)	<code>FC3</code> , 40k	59.84	29.90	29.63

We also examine the importance of scale on the final robustness of the dataset. We run `adv-KIP` on MNIST and CIFAR-10, using an `FC3` kernel for a wide variety of different dataset sizes $|\mathcal{X}_S|$, while keeping the rest of the hyperparameters the same. We optimize for 500 meta epochs and use early stopping if robust validation accuracy ceases to improve. For all the runs, we observe that we stop early, so we conclude that all the datasets were given a fair chance. On the test set we then evaluate the same kernel classifier fit with the optimized data, recording clean and robust ac-

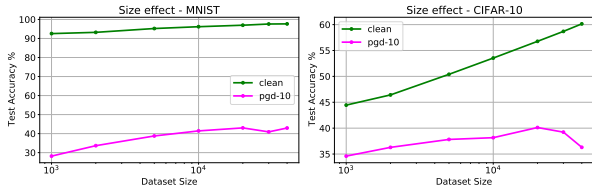


Figure 3: Performance of adv-KIP outputs as a function of dataset size. Setting: FC3 kernel, $|\mathcal{X}_T| = 10k$, ℓ_∞ adversary, $\epsilon = 0.3$ ($\epsilon = 8/255$), $\alpha = 0.1$ ($\alpha = 2/255$).

curacy. The scaling laws are shown in Fig 3. We observe diminishing returns on the performance of the models, after we exceed some required sample size. For the more challenging setting (CIFAR-10) it is the clean accuracy that sees the greater increase. The fact that the robust curve “bends” in the end might mean that we could optimize more aggressively by harming clean accuracy (without implementing early stopping).

4.2. Neural Networks results

In this section, we study whether datasets produced with adv-KIP can be used to train robust neural networks.

Wide fully connected neural networks. As a first step, we perform experiments on the same architecture as in the NTK used in the meta-optimization of the dataset. We consider fully connected ReLU models with 2, 3, 5 and 7 layers of width 1024 and train them using Adam. We refer to App. A.3 and A.4 for full experimental details and results. We find that in all cases the networks learn successfully with clean and robust test performance that matches or exceeds those of the kernels (even when evaluating against stronger attacks with more PGD steps than used during the meta-optimization). We view this as an indication that features learned by kernels are surprisingly relevant for (robust) classification in neural networks.

Robustness of Common Architectures. We now turn our attention to commonly employed convolutional neural networks to study the relevance of our datasets for robust classification using modern architectures. In particular we report how datasets generated using FC kernels transfer to such convolutional architectures, since the small datasets generated from Conv kernels were challenging to fit with neural networks. We consider a simple CNN with 3 convolutional layers with max-pooling operations on MNIST, and AlexNet (Krizhevsky et al., 2012), VGG11 (Simonyan & Zisserman, 2015) and ResNet20 (He et al., 2016) on CIFAR-10. We perform a sweep over different learning rates and training algorithms (gradient descent, gradient descent with weight decay and Adam). Experimental details can be found in App. A.3.

Tables 2 and 3 summarize our findings. We note an astonishing “boost” in robust test accuracy against gradient-based attacks of these convolutional networks (in all models but ResNet¹) when compared to the previous results on kernels and fully connected networks. Very remarkably, it seems that datasets optimized for relatively simple kernels “transfer” their PGD-performance to networks far removed from the idealistic infinite width regime, even to more expressive architectures. We also note that the results are robust to the initialization of the networks, as evidenced by the deviations reported in the tables.

Table 2: MNIST with simple-CNN: Test accuracies when trained on adv-KIP datasets optimized with FC kernels (first 3 rows). We also show test accuracies for the adversarially trained simple-CNN (without any data augmentation). AA refers to the *AutoAttack* test suite. Setting: ℓ_∞ , $\epsilon = 0.3$, $\alpha = 0.1$.

Dataset	Clean	FGSM	Robust PGD40	AA
FC3	98.15 ± 0.12	98.06 ± 0.18	97.17 ± 0.10	0.00 ± 0.00
FC5	97.96 ± 0.55	97.87 ± 0.64	97.20 ± 0.74	0.00 ± 0.00
FC7	98.03 ± 0.16	97.91 ± 0.22	97.14 ± 0.43	0.00 ± 0.00
Adversarial Training	99.11	97.52	95.82	88.77

Table 3: CIFAR-10: Test accuracies of several convolutional architectures trained on an adv-KIP dataset produced from an FC3 kernel of $|\mathcal{X}_S| = 40,000$ (upper), and Adversarial Training baselines (lower). Setting: ℓ_∞ , $\epsilon = 8/255$, $\alpha = 2/255$. For further results on smaller attack radii, see Table 8 in App. A.5.

Neural Net	Clean	adv-KIP		
		FGSM	PGD20	AA
Simple CNN	72.10 ± 0.10	67.45 ± 0.37	67.03 ± 0.24	0.00 ± 0.00
AlexNet	68.87 ± 0.76	49.30 ± 0.69	49.06 ± 0.63	0.89 ± 1.41
VGG11	74.88 ± 0.45	53.98 ± 9.71	53.18 ± 10.32	0.27 ± 0.18
ResNet20	81.53 ± 0.59	4.82 ± 1.45	0.20 ± 0.16	0.00 ± 0.00
Adversarial Training Baseline				
Neural Net	Clean	FGSM	PGD20	AA
Simple CNN	58.07	33.94	31.49	26.18
AlexNet	44.35	30.12	24.41	18.95
VGG11	69.69	31.41	24.88	24.09
ResNet20	73.95	46.37	39.17	35.35

Fig. 4 (top left) shows accuracy curves for the CNN when trained on the optimized CIFAR-10 dataset. While accuracy on the train (optimized) data together with the clean test accuracy increase rapidly, it is only after 250 epochs that robust accuracy starts to increase (after we hit 0 training loss). We hypothesize that this might be due to the fact that

¹We currently do not have an explanation on why ResNet performs so poorly in terms of robust accuracy. We hypothesize that the model performs feature learning that is entirely different from the other models and is not efficient on features that are relevant for an FC kernel.

adv-KIP optimizes using the expression that corresponds to the *end* of training in neural networks.

It seems promising at first that modern networks trained with adv-KIP datasets without much tuning enjoy astonishing defense properties against PGD-attacks in various settings, similar, or in some cases even higher, than what truly robust models (i.e. adversarially trained) obtain. However, as can be seen in the last column of Tables 2 and 3, when we evaluate their robustness with the adaptive methods of AutoAttack (Croce & Hein, 2020), we observe a sharp drop in the performance (close to 0% in all cases). The purpose of the AutoAttack benchmark, which includes 4 different attacks, some of which do not use gradient information, is to provide a minimal adaptive attack suite to uncover shortcomings in a defense. See Table 9 in App. A.6 for a breakdown of robustness by AutoAttack components.

We find that datasets produced with adv-KIP suffer from what is commonly termed the *obfuscated gradient* phenomenon (Athalye et al., 2018), a situation where model gradients do not provide good directions for generating successful adversarial examples. However, in the past, this has only been observed with techniques that were either introducing non-differentiable parts in the inference pipeline or stochasticity to the model. Interestingly, we now observe this phenomenon from altering the *training* data alone and, even more remarkably, from data optimized using kernels.

To check whether this is a shortcoming of our optimization method or a more general phenomenon related to "robustified" datasets, we turn our attention next to the only other method we are aware of that provides some notable robustness via standard training (Ilyas et al., 2019).

4.3. Non-robustness of Robust Features dataset

To illustrate the theory of the presence of robust and non-robust features in the data, Ilyas et al. (2019) have introduced a "robustified" data set (termed *Robust Features Dataset* or RFD from now on), which was sufficient to ensure robust predictions on the test set by standard training only. RFD is generated by traversing the representation layer of an adversarially trained neural network, and was thus believed to provide a general sense of robustness (Ilyas et al., 2019). More specifically, given a mapping $x \mapsto g(x)$ of an input x to the penultimate ("representation") layer of an adversarially trained neural net, a "robustified" input is obtained by optimizing $\min_{x_r} \|g(x) - g(x_r)\|_2$, starting from a random data point using gradient descent, thus enforcing that the robust representations of x and x_r are similar; while x_r does not contain non-robust features given a starting point that is uncorrelated with the label of x .

We use an ℓ_∞ -adversarially trained ResNet50 to generate

Table 4: Test accuracies for various models trained on a 50K ℓ_∞ Robust Features dataset (Ilyas et al., 2019)) for CIFAR-10. Setting: $\ell_\infty, \epsilon = 8/255, \alpha = 2/255$. For further results on smaller attack radius, see Table 7 in App. A.5.

Robust Features dataset (Ilyas et al., 2019)			
Neural Net	Clean	PGD20	AA
Simple CNN	59.15 ± 0.37	52.91 ± 0.66	0.00 ± 0.00
AlexNet	51.62 ± 1.14	25.64 ± 4.32	0.02 ± 0.03
VGG11	61.59 ± 0.80	34.64 ± 8.47	0.40 ± 0.42
ResNet20	66.29 ± 0.70	7.35 ± 3.10	0.00 ± 0.00

an RFD version of CIFAR-10². To ensure a fair comparison with our methods, we train the same set of models as in the previous subsection. Table 4 contains the results.

Confirming the findings of Ilyas et al. (2019), we see that the trained models record high robustness against PGD attacks. However, all of the models *fail* to defend against AutoAttack. This is a surprising finding, since the dataset was generated using adversarially trained networks that guarantee a wide sense of robustness (Croce et al., 2020). In Fig. 4 (middle), we can see that the simple CNN when trained on the RFD exhibits remarkably similar accuracy curves as when being trained on an adv-KIP dataset. In the next subsection, we dive deeper into the similarities between the two classes of datasets.

4.4. Overconfidence gives a false sense of security

We analyze properties of models that were trained with either an adv-KIP or an RF dataset and yield superficial robustness. We discover many common properties and signatures of failure, and contrast them to adversarially trained neural networks. These similarities might be germane to all attempts that explicitly optimize the dataset with gradient based approaches.

Fig. 4 (second and third column) shows the loss value and the gradient magnitude of the models throughout training, where we further decomposed the metrics into 2 parts; one coming from correctly classified images and one from misclassified ones. We observe that for both datasets the loss increases on the misclassified examples, concurrently with an increase of the average norm of the gradient. In contrast, for correctly classified examples we see both quantities progressively vanish. This behavior, together with the false sense of robustness that AutoAttack evaluation reveals, suggests that the model learns to shatter the gradients locally in the neighborhood of correctly classified examples, causing

²Note that the *publicly* available dataset of (Ilyas et al., 2019) is derived from an adversarially trained network trained against an ℓ_2 adversary, so for completeness we include an ℓ_2 evaluation of that dataset in App. A.7, where the findings are similar.

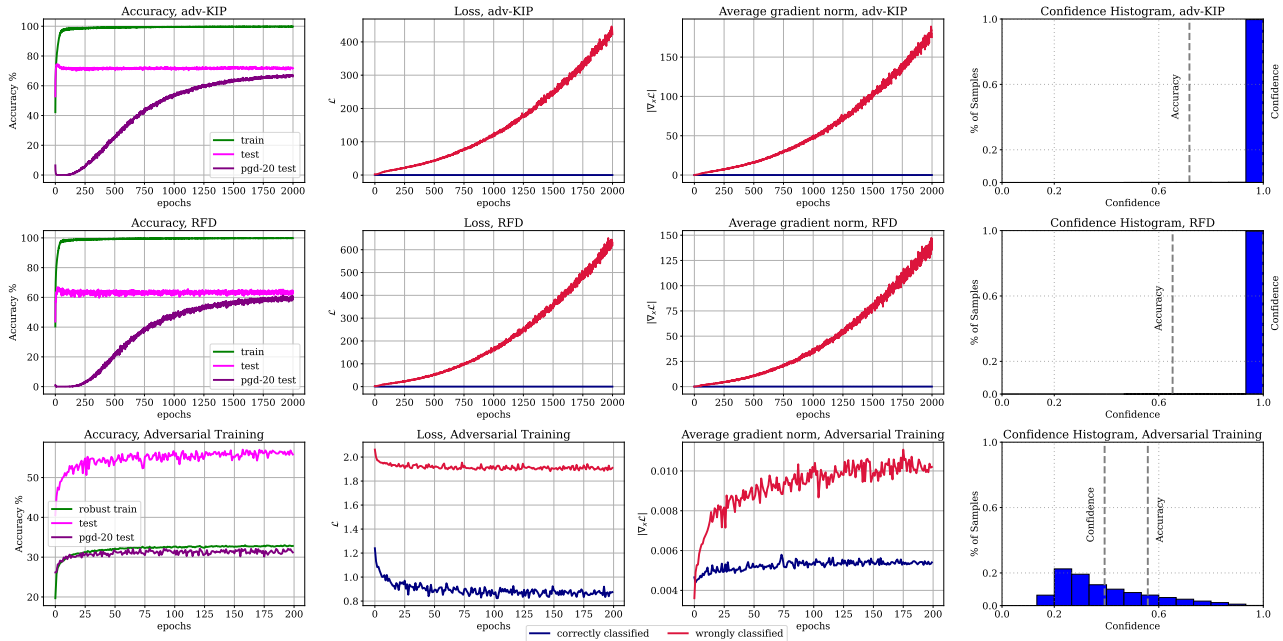


Figure 4: Several statistics of CNN models trained on an adv-KIP dataset (**first row**), an RFD (**second row**), and trained with adversarial training (**third row**). From Left to Right: Accuracy, Test Loss (decomposed in correctly and wrongly classified examples); Average Gradient Norm of Test data; Confidence Histogram. Base dataset: CIFAR-10.

simple gradient-based attacks to fail. We find that during our distillation procedure this is indeed the case (Fig. 6 in the Appendix), and the data optimization effectively shrinks the gradients of the model.

In other words, the model essentially “sacrifices” performance on the subset of data that is misclassified, in order to fit the rest in a pseudo robust way. This is in sharp contrast with the situation during adversarial training, where the loss decreases on all data simultaneously (Fig. 4, third row). This is already an indication of failure of learning. Interestingly, Fig. 4 (third column) shows that this failure of learning is also evident in the gradient norms of the loss with respect to the *input*. The average gradient norm on the wrongly classified points explodes with the number of epochs for both the adv-KIP dataset and the RFD.

Finally, we study the calibration of the models. In particular, we compute confidence histograms and reliability diagrams (Guo et al., 2017) for the 3 models. As Fig. 4 (last column) shows, the models that were trained with the adv-KIP dataset or the RFD are extremely confident on nearly all test examples, being poorly calibrated, while the adversarially trained model has a completely different, more balanced, profile (it is less confident than accurate). We refer to Fig. 5 in App. A.8 for the reliability diagram of the 3 models that provides further evidence for the above. In a sense, this overconfidence on the samples is what makes the gradients non-informative.

Understanding why the solution of Eq. (2) (data level) with gradient based methods gives a false sense of robustness, while the solution of Eq. (1) (parameters level) also with gradient based methods induces more widespread robustness seems a very interesting and challenging open question for future work to address.

5. Conclusion

In this work, we approached the problem of robust classification in machine learning from a data-based point of view. We introduced a meta-learning algorithm, adv-KIP , which produces datasets that furnish a great range of classifiers with notable robustness against gradient-based attacks. However, our analysis demonstrates that this robustness is rather fallacious and the models essentially learn representations that provide no meaningful gradients. Quite remarkably, when we revisited seminal prior work (Ilyas et al., 2019) that claimed standard training on a robust dataset can be an actual defense versus adversarial attacks, we found the same pathological situation. We believe our findings provide many new insights on the role of data in adversarially robust classification and should be helpful for potential new data-based approaches in the future.

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A. Appendix

A.1. Related Work

Distributionally Robust Optimization and Adversarial Augmentation. Related to our work are also works on distributionally robust optimization (Sinha et al., 2018) and adversarial data augmentation for out-of-distribution generalization (Volpi et al., 2018). The latter proposes an algorithm that augments the training dataset *on-the-fly* (i.e. during training of a neural net) with worst-case samples from a target distribution. In contrast, our method optimizes the original dataset against worst-case samples/adversarial examples from the original distribution, which correspond to a final predictor (kernel machine). The only prior work that gives an algorithm based on NTK theory to derive dataset perturbations in some adversarial setting is due to Yuan & Wu (2021), yet with entirely different focus. It deals with what is coined *generalization attacks*: the process of altering the training data distribution to prevent models to generalise on clean data. To our knowledge, KIP (Nguyen et al., 2021a;b) and this NTGA algorithm are the only examples of leveraging NTKs for dataset optimization.

A.2. KIP baseline

The original KIP algorithm (Nguyen et al., 2021a;b) is designed to reduce the size of the training set, while keeping the induced accuracy close to the original one. It could be reasonable to hypothesize that such information compression might possibly lead to an increase of robustness as well. As a sanity check we evaluate the robust accuracy of these datasets. We also produce larger dataset using the KIP algorithm (of the same size as used in our `adv-KIP` experiments). Table 5 shows that effectively the robustness of the datasets remains close to 0, as is the case for the original datasets. This indicates the clear need to adjust the optimization objective to robust performance, as is done in the `adv-KIP` algorithm.

Table 5: KIP baseline datasets (reproduced). Setting: No preprocessing/data augmentation, $|\mathcal{X}_T|=1,000$ images, learned labels, mse loss, lr=1e-3, datasets were optimized for 1000 epochs, with potential early stopping if validation accuracy did not increase across 200 epochs. Random seed denotes different draws of the initial support images. Standard setting for robust evaluation: $\epsilon = 0.3$ and $\epsilon = 8/255$, respectively.

	Kernel, $ \mathcal{X}_s $	Clean	FGSM
MNIST	FC3, 5k	97.51 ± 0.03	0.00 ± 0.00
	FC7, 30k	98.23 ± 0.06	0.00 ± 0.00
CIFAR-10	FC3, 1k	48.45 ± 0.34	2.50 ± 0.21
	FC3, 5k	52.48 ± 0.23	0.22 ± 0.05
	FC3, 10k	54.04 ± 0.41	0.10 ± 0.04

We also evaluated $\text{FC}\{3, 5, 7\}$ and $\text{Conv}\{3, 5, 7\}$ kernels (together with a Convolutional Kernel with 1 hidden layer followed by global average-pooling) on datasets (with 50 images per class) released by (Nguyen et al., 2021b) and we found their FGSM robustness to be 0% in all cases. URLs for the datasets we considered: 1st and 2nd.

A.3. Experimental Details for Neural Network experiments

For all models trained on an `adv-KIP` dataset or an RFD, we use the Adam optimizer and perform a small grid search for the learning rate, picking the best model with respect to robust accuracy.

On MNIST, we train fully connected networks of width 1024 in Sec. A.4, and the simple-CNN network in Sec. 4. FC networks are trained for 2,000 epochs and the simple-CNN network for 800 epochs.

On CIFAR-10, we again train fully connected networks of width 1024 in Sec. A.4, and the simple-CNN, AlexNet and VGG11 networks in Sec. 4. We train all these networks for 2,000 epochs.

For the Adversarial Training baseline, on MNIST, we adopt the setting of (Madry et al., 2018), that is we train the simple-CNN network with the Adam optimizer towards convergence, and set the initial learning rate to $1e-4$. In (Madry et al., 2018) the number of epochs was set to 100, while we use 200. On CIFAR-10, since we do not use data augmentation, we train with both SGD and Adam for 200 epochs for each model, and pick the better one in terms of robustness. For the simple-CNN and AlexNet, the Adam optimizer is better. For VGG11, we use the SGD optimizer, with initial learning rate $1e-1$, decay rate of 10 at the 100-th and the 150-th epoch, and with weight decay $5e-4$.

Simple-CNN architecture: We use a simple convolutional architecture with three convolutional layers and a linear layer. Each convolutional layer computes a convolution with a 3×3 kernel, followed by a ReLU and a max-pooling layer (of kernel size 2×2 and stride 2). The linear layer is fully-connected with ten outputs. All convolutional layers have a fixed width of 64.

Training of Convolutional Nets: We use the Adam optimizer (Kingma & Ba, 2015) and perform a small grid search over the fixed learning rate. We stop training when robust validation accuracy ceases to decrease, where we measure against PGD40 attacks for MNIST and PGD20 attacks for CIFAR-10, as is often standard. We report the best results across the sweep for FGSM and PGD test accuracies. After picking the best learning rate, for each experiment in this paper, we report the mean and standard deviation of three experiments with different seeds.

Description of Evaluation Metrics: For all the adversarial attack related measurements including FGSM, ℓ_∞ PGD and ℓ_2 PGD, we adopt the CleverHans code implementation (Papernot et al., 2018). For ℓ_∞ PGD, on MNIST we use step size 0.1 and radius 0.3, while on CIFAR-10 we use step size $2/255$ and radius $8/255$. For ℓ_2 PGD on CIFAR-10, we use step size $15/255$ and radius $128/255$.

For AutoAttack, we adopt the open-source original implementation (Croce & Hein, 2020; 2021). As for the other attacks, we set $\epsilon = 0.3$ for MNIST and $8/255$ for CIFAR-10 for ℓ_∞ attacks and adopt the $128/255$ radius for CIFAR-10 for the ℓ_2 adversary.

A.4. Transfer Results to Wide FC Networks

Here, we evaluate how well datasets produced with kernel methods in Algorithm 9 transfer to relatively wide neural nets of the same architecture and depth as the NTKs used in the `adv-KIP` optimization. We implement multilayer fully connected neural nets of width 1024 and perform a hyperparameter search for the (constant) learning rate. We use the Adam optimizer (Kingma & Ba, 2015) and test for both FGSM and PGD accuracy, where we apply the most common PGD attacks (PGD40 for MNIST and PGD20 for CIFAR-10). Table 6 summarize our results.

Table 6: Transferability : Kernel to Neural Network of same architecture, test accuracy in %. For MNIST, we test with PGD-40, and for CIFAR, we test with PGD-20.

Dataset	Kernel, $ \mathcal{X}_s $	Robust		
		Clean	FGSM	PGD
MNIST	FC3, 30k	80.08	77.67	53.85
	FC5, 30k	97.75	64.83	35.14
	FC7, 30k	97.45	70.58	40.70
CIFAR-10	FC2, 40k	46.29	20.98	16.89
	FC3, 40k	46.33	40.07	39.15

We find that robustness properties transfer well from kernels to their corresponding neural networks. Our sweeps also show that this holds for a rather wide range of learning rates, evidencing a certain insensitivity to exact parameter choices.

A.5. Smaller Radius AutoAttack Results

To further investigate, we deploy a fine-grained series of smaller radius AutoAttack to the models trained with our `adv-KIP` dataset and the ℓ_∞ RF Dataset. The test results are shown in Table 7 and 8. Our `adv-KIP` dataset shows consistently better PGD and AA robustness across multiple models.

A.6. AutoAttack Suite Decomposition Analysis

In Table 9, we decompose the AA test suite into its individual components and evaluate them independently on models trained on our Adv-KIP dataset, the ℓ_2 RFD dataset, and the ℓ_∞ RFD dataset. A clear trend of high APGD-CE accuracy and low other accuracies emerges. This corroborates our discussion that the fake robustness arises from the dynamics of overconfidence that operates on the logits to make the gradient vanish.

Table 7: AutoAttack Test accuracies for various models trained on the ℓ_∞ RFD.

CIFAR-10 AutoAttack Accuracy, Smaller Radius				
Neural Net	AA ℓ_∞ 4/255	AA ℓ_2 64/255	AA ℓ_∞	AA ℓ_2
Simple CNN	0.02 \pm 0.01	4.91 \pm 0.29	0.00 \pm 0.00	0.06 \pm 0.03
AlexNet	0.98 \pm 0.15	5.98 \pm 0.78	0.02 \pm 0.03	0.37 \pm 0.13
VGG11	3.92 \pm 1.76	19.85 \pm 3.31	0.40 \pm 0.42	4.71 \pm 2.05
ResNet20	0.02 \pm 0.02	4.12 \pm 0.87	0.00 \pm 0.00	0.05 \pm 0.04

Table 8: AutoAttack Test accuracies for various models trained on our adv-KIP Dataset.

CIFAR-10 AutoAttack Accuracy, Smaller Radius				
Neural Net	AA ℓ_∞ 4/255	AA ℓ_2 64/255	AA ℓ_∞	AA ℓ_2
Simple CNN	0.02 \pm 0.00	7.48 \pm 0.20	0.00 \pm 0.00	0.14 \pm 0.01
AlexNet	4.98 \pm 2.32	19.27 \pm 1.81	0.89 \pm 1.41	3.94 \pm 2.65
VGG11	6.20 \pm 0.76	31.41 \pm 1.85	0.27 \pm 0.18	8.56 \pm 1.00
ResNet20	0.00 \pm 0.00	0.69 \pm 0.04	0.00 \pm 0.00	0.00 \pm 0.00

A.7. Robustness of the publicly available RFD

Here, we replicate the results of Sec. 4.3 for the publicly available RFD dataset of (Ilyas et al., 2019). Since it stems from a network trained against an ℓ_2 adversary, we have also included evaluation against ℓ_2 -attacks. We refer to Table 10 for the results. For all models, we observe a dramatic drop in their robustness once they are evaluated against AutoAttack.

A.8. Details on the Confidence and Reliability Visualization

It has been shown that calibration of modern neural networks can be poor, despite advances in accuracy (Guo et al., 2017; Lakshminarayanan et al., 2017; Wenzel et al., 2020; Havasi et al., 2020). (Guo et al., 2017) point out that more accurate and larger models tend to have worse calibration. A common measurement of miscalibration is the Expected Calibration Error (ECE) (Naeini et al., 2015), which quantifies the difference in expectation between confidence and accuracy using binning. Since obtaining accurate estimation of ECE is difficult, due to the dependency of the estimator on the binning scheme, we adopt the reliability diagram (DeGroot & Fienberg, 1983; Niculescu-Mizil & Caruana, 2005) and the confidence histogram (Guo et al., 2017), both tools with nice visualization. In the confidence histogram, we display the distribution of the predicted confidence, *i.e.*, the output probability of the predicted label, as a histogram. In the reliability diagram, we calculate the expected sample accuracy as a function of the confidence level by grouping all samples by their confidence. For a well-calibrated model, the reliability diagram should output the identity function, so we also plot the gap between the well-calibrated accuracy *v.s.* real accuracy. Fig. 5 shows the reliability diagram of Simple CNNs trained on an adv-KIP dataset (left), RFD (middle) and adversarially trained on CIFAR-10 (right). We notice how poorly calibrated are the models that were trained with the synthetic datasets, which is consistent with the findings of Fig. 4 of the main text.

A.9. Results using modifications of adv-KIP

In this section, we present results where we modified the loss of either the inner or the outer loop of adv-KIP.

In particular, for the inner loop, we replace the cross entropy with a rescaled version of the CW loss (Carlini & Wagner, 2017), called DLR loss (Croce & Hein, 2020). Let z represent the pre-softmax logits. Recall that the cross entropy loss is defined as:

$$CE(x, y) = -z_y + \log\left(\sum_{i=1}^K e^{z_i}\right) \quad (9)$$

Carlini & Wagner (2017) proposed to use the following (CW) loss for an attack:

$$CW(x, y) = -z_y + \max_{i \neq y} z_i \quad (10)$$

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Table 9: Test Accuracy on CIFAR-10 with the ℓ_∞ AA suite decomposition. $\epsilon = 8/255$.

CIFAR-10 Accuracy with individual ℓ_∞ AutoAttack Components						
Dataset	Neural Net	Clean	APGD-CE	APGD-T	FAB-T	SQUARE
adv-KIP	Simple CNN	72.10 \pm 0.10	66.33 \pm 0.21	0.00 \pm 0.00	0.00 \pm 0.01	0.03 \pm 0.01
	AlexNet	68.87 \pm 0.76	44.55 \pm 0.78	1.44 \pm 2.03	7.42 \pm 1.14	5.41 \pm 2.24
	VGG11	74.88 \pm 0.45	48.81 \pm 9.90	0.63 \pm 0.15	6.33 \pm 1.09	9.06 \pm 1.67
	ResNet20	81.53 \pm 0.59	0.36 \pm 0.05	0.00 \pm 0.00	0.00 \pm 0.00	0.01 \pm 0.01
ℓ_∞ RFD	Simple CNN	59.15 \pm 0.37	52.18 \pm 0.47	0.00 \pm 0.00	0.00 \pm 0.00	0.03 \pm 0.01
	AlexNet	51.62 \pm 1.14	21.36 \pm 4.10	0.10 \pm 0.17	1.56 \pm 1.87	0.93 \pm 0.18
	VGG11	61.59 \pm 0.80	29.72 \pm 8.37	1.09 \pm 1.15	4.39 \pm 3.69	4.62 \pm 2.32
	ResNet20	66.29 \pm 0.70	9.37 \pm 1.67	0.00 \pm 0.00	0.00 \pm 0.00	0.10 \pm 0.01
ℓ_2 RFD	Simple CNN	65.25 \pm 0.44	60.02 \pm 0.39	0.00 \pm 0.00	0.00 \pm 0.00	0.07 \pm 0.05
	AlexNet	57.07 \pm 1.25	21.42 \pm 5.12	0.15 \pm 0.23	0.18 \pm 0.09	0.93 \pm 0.80
	VGG11	68.41 \pm 1.95	38.46 \pm 10.44	0.95 \pm 1.39	4.42 \pm 3.08	6.31 \pm 5.46
	ResNet20	72.36 \pm 0.15	0.19 \pm 0.04	0.00 \pm 0.00	0.00 \pm 0.01	0.21 \pm 0.07

Table 10: Test accuracies for various models trained on the publicly-available 50K ℓ_2 Robust Features dataset (RFD) for CIFAR-10.

CIFAR-10 Accuracy with ℓ_2 Robust Features dataset (Ilyas et al., 2019)							
Neural Net	Clean	PGD ℓ_∞ 20	PGD ℓ_2 20	AA ℓ_∞	AA ℓ_2	AA ℓ_∞ 4/255	AA ℓ_2 64/255
Simple CNN	65.25 \pm 0.44	60.73 \pm 0.24	63.73 \pm 0.40	0.00 \pm 0.00	0.47 \pm 0.11	0.09 \pm 0.05	10.42 \pm 0.60
AlexNet	57.07 \pm 1.25	25.12 \pm 5.46	26.58 \pm 4.80	0.01 \pm 0.02	0.62 \pm 0.25	1.21 \pm 0.52	8.11 \pm 1.80
VGG11	68.41 \pm 1.95	42.92 \pm 11.23	47.49 \pm 6.12	1.19 \pm 0.77	6.94 \pm 2.47	4.65 \pm 2.21	26.33 \pm 3.00
ResNet20	72.36 \pm 0.15	0.08 \pm 0.04	35.71 \pm 3.04	0.00 \pm 0.00	0.19 \pm 0.06	0.05 \pm 0.02	7.21 \pm 1.44

We implement a variant of the above loss, namely the Difference of Logits Ratio (DLR) loss proposed in (Croce & Hein, 2020):

$$\text{DLR}(x, y) = -\frac{z_y - \max_{i \neq y} z_i}{z_{\pi_1} - z_{\pi_3}} \quad (11)$$

where π is the ordering of the components of z in decreasing order (the untargeted version). This loss is invariant to scaling of the logits, and it has been used to detect cases where attacking the cross entropy loss fails due to overconfidence of the model.

For the outer loop, we incorporate the TRADES loss (Zhang et al., 2019) that aims to balance performance on clean and perturbed input points. Given a specific input (x, y) , TRADES optimizes over

$$\mathcal{L}(f(x; \theta), y) + \lambda \max_{x' \in \mathcal{B}(x)} \mathcal{L}(f(x; \theta), f(x'; \theta)), \quad (12)$$

where λ is a hyperparameter responsible for trading one accuracy for robustness (and vice versa). In our case, the loss reads as

$$\mathcal{L}(K_{\mathcal{X}_T \mathcal{X}_S} K_{\mathcal{X}_S \mathcal{X}_S}^{-1} \mathcal{Y}_S, \mathcal{Y}_T) + \lambda \max_{\mathcal{X}_{T'} \in \mathcal{B}(\mathcal{X}_T)} \mathcal{L}(K_{\mathcal{X}_T \mathcal{X}_S} K_{\mathcal{X}_S \mathcal{X}_S}^{-1} \mathcal{Y}_S, K_{\mathcal{X}_{T'} \mathcal{X}_S} K_{\mathcal{X}_S \mathcal{X}_S}^{-1} \mathcal{Y}_S). \quad (13)$$

Tables 11 and 12 summarize our results on neural networks trained on the modified adv-KIP datasets with ℓ_∞ attacks. We do not see any notable deviation from the results that were presented in the main text.

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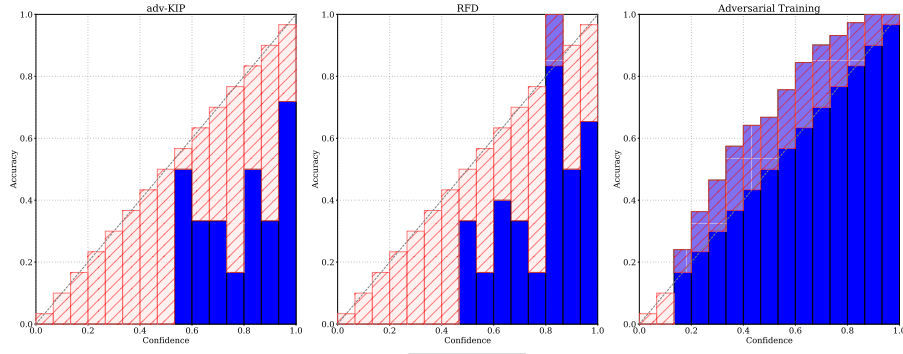


Figure 5: Reliability Diagram for a Simple CNN trained on an adv-KIP dataset (left), an RFD (right), and optimized with adversarial training on CIFAR-10.

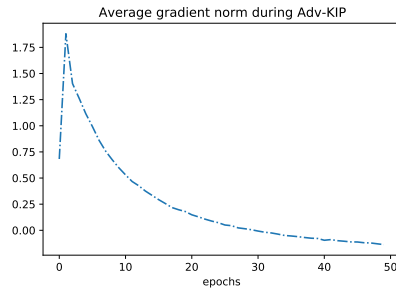


Figure 6: The average gradient norm of an FC3 kernel on a validation set during the distillation procedure of Algorithm 9. We see that the training data evolves to cause gradient shrinkage of the model. Setting: CIFAR-10, FC3, $|\mathcal{X}_S| = 40k$, $|\mathcal{X}_T| = 10k$, 10 PGD steps, cross entropy loss in outer loop.



Figure 7: MNIST (left) and CIFAR-10 (right) distilled images with trained labels from an FC7 kernel.

Neural Net	Clean	FGSM	Robust	
			PGD ℓ_∞ 20	AA
Simple CNN	70.87 \pm 0.44	65.06 \pm 0.52	64.88 \pm 0.51	0.00 \pm 0.00
AlexNet	63.58 \pm 5.50	47.62 \pm 8.51	47.08 \pm 8.65	0.11 \pm 0.11
VGG11	73.72 \pm 1.90	63.05 \pm 4.14	62.76 \pm 4.40	2.11 \pm 3.28

Table 11: Test accuracies of several convolutional architectures trained on an adv-KIP CIFAR-10 **DLR** dataset from the FC3 kernel, with 40,000 samples. Setting: $\ell_\infty, \epsilon = 8/255$.

Neural Net	Clean	FGSM	Robust	
			PGD ℓ_∞ 20	AA
Simple CNN	67.39 \pm 0.18	58.21 \pm 0.33	58.03 \pm 0.34	0.00 \pm 0.00
AlexNet	59.69 \pm 1.13	47.44 \pm 8.00	47.08 \pm 8.47	0.29 \pm 0.17
VGG11	68.31 \pm 1.17	60.97 \pm 3.37	60.61 \pm 3.46	3.58 \pm 2.01

Table 12: Test accuracies of several convolutional architectures trained on an adv-KIP CIFAR-10 **TRADES** dataset from the FC3 kernel, with 40,000 samples. Setting: $\ell_\infty, \epsilon = 8/255$.