Interplay of adversarial robustness and generalization in deep convolutional models

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Outline

1. Nonrobustness of machine learning algorithms
2. Adversarial example definitions
3. Finding adversarial examples
4. Properties of adversarial examples
5. Improving adversarial robustness
6. Adversarial robustness and generalization
7. Conclusion

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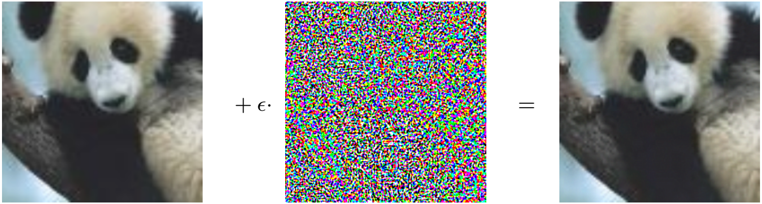
Nonrobustness of machine learning algorithms

- Current state-of-the-art machine learning algorithms do not work well with **domain-shifted, out-of-distribution and inputs crafted to fool them** and they often make **overconfident predictions** [Engstrom et al. (2017), Ganin and Lempitsky (2015), Hendrycks and Dietterich (2019), Hendrycks and Gimpel (2016), Nguyen et al. (2015), and Szegedy et al. (2013)].
- It is even possible to slightly, even impreceptibly, modify an input (e.g. image) to generate an adversarial example and cause a misprediction.
- This is not limited to complex deep models
- This indicates that current algorithms **perform well without actually understanding data** (in a way similar to humans).

Nonrobustness of machine learning algorithms

- A single small gradient descent step on an image increasing the loss is often enough to fool a classifier [Goodfellow et al. (2014)].
- Sometimes a single pixel can change the prediction [Su et al. (2017)].



$\boldsymbol{x}$ *panda* (0.577) $\quad$ $\operatorname{sgn}(\nabla_{\boldsymbol{x}} L(y, h(\boldsymbol{x})))$ $\quad$ $\tilde{\boldsymbol{x}}$ *gibbon* (0.993)

Figure 1: Generation of an adversarial example with FGSM, a single step attack. Italic words and numbers represent classes and confidences. The images are from Goodfellow et al. (2014).

Nonrobustness of machine learning algorithms

- (Some) generative models are vulnerable to adversarial attacks as well [Goodfellow et al. (2014) and Kos et al. (2018)]. Figure 2 shows adversarial examples on a VAE-GAN.

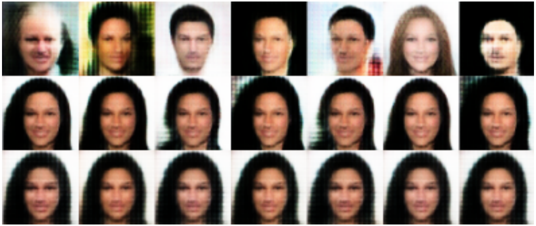



Figure 2: Reconstruction outputs for targeted attacks on a VAE-GAN from Kos et al. (2018). Rows represent reconstructions of original images (top), adversarial examples generated using an attack in latent space (middle) and a VAE-loss attack (bottom). The target reconstruction is on the right.

Adversarial robustness and generalization

- Evidence suggests that there is a **trade-off between robustness and generalization** with current machine learning algorithms [Madry et al. (2017), Su et al. (2018), and Tsipras et al. (2018)].
- The trade-off is **counter-intuitive** because **a hypothesis which optimally generalizes would have no adversarial examples**.
- The question remains how achievable both robustness and generalization are regarding computational and data requirements.

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Adversarial example definitions

Definition (adversarial example)

An adversarial example is an input for which the following holds:

1. It is **close** to an input with a correct prediction.
2. The **hypothesis** produces a **misprediction**.

Definition (practical adversarial example)

A practical adversarial example is an input for which the following holds:

1. It is **close** to an input x with a correct prediction.
2. The **hypothesis** produces a **different prediction** than for x.

- Each definition has its drawbacks:
  - the first one: **requires knowing the true hypothesis**
  - the practical one: **corectly classified inputs can be adversarial**.

Adversarial example definitions

- The set of adversarial examples is a function of the **hypothesis**, a **neighbourhood function**, the **input data distribution**, and (in the first definition) the **true hypothesis**.
- The practical definition is
  - **inconsistent** – examples close to class boundaries can be both adversarial and correctly classified depending on the reference, and
  - **practical for generating adversarial examples and robustnes evaluation**.
- The first definition is
  - **impractical** – it requires knowing the unknown true hypothesis,
  - **consistent** – the true hypothesis has no adversarial examples, and
  - **helpful for achieving the goal of both robustness and generalization**.

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Finding adversarial examples

- Let $\mathbb{X}$ be the input space, and $d \in (\mathbb{X} \times \mathbb{X} \to \mathbb{R}^+)$ a **distance function**. The **neighbourhood** of an example $\boldsymbol{x}$ can be $B_\epsilon(\boldsymbol{x}) = \{\boldsymbol{x}' \colon d(\boldsymbol{x}', \boldsymbol{x}) \leq \epsilon\}$, where ϵ is the maximum distance.
- Ideally, the neighbourhood of an example $\boldsymbol{x}$ should be the set of **perceptually similar** examples that all belong to the same class as $\boldsymbol{x}$, but it would require knowing the true hypothesis.
- A common choice for distance d is L^p distance with $p \in \{1, 2, \infty\}$.
- Finding an adversarial example can be formulated as an optimization problem of **maximizing some loss with respect to the input** with a neighbourhood constraint:

$$\tilde{\boldsymbol{x}} = \operatorname*{arg\,max}_{\boldsymbol{x}' \in B_\epsilon(\boldsymbol{x})} L(y, h(\boldsymbol{x}')), \tag{1}$$

where y is the true label, h the hypothesis, and L the loss function.

Finding adversarial examples

- An objective can also be to find **the closest adversarial example** [Moosavi-Dezfooli et al. (2016)]:

$$\tilde{\boldsymbol{x}} = \operatorname*{arg\,min}_{\boldsymbol{x}' :\, \boldsymbol{x}' \in B_\epsilon(\boldsymbol{x}) \wedge \hat{h}(\boldsymbol{x}') \neq y} d(\boldsymbol{x}', \boldsymbol{x}), \tag{2}$$

where $\hat{h}(\boldsymbol{x}) \coloneqq \arg\max_y h(\boldsymbol{x})_{[y]}$.

- There are also **targeted attacks**, where the objective is to get an adversarial example that is classified to some target class. Targeted attack objectives corresponding to equations (1) and (2) are:

$$\tilde{\boldsymbol{x}} = \operatorname*{arg\,min}_{\boldsymbol{x}' \in B_\epsilon(\boldsymbol{x})} L(y_\mathsf{a}, h(\boldsymbol{x}')), \tag{3}$$

$$\tilde{\boldsymbol{x}} = \operatorname*{arg\,min}_{\boldsymbol{x}' :\, \boldsymbol{x}' \in B_\epsilon(\boldsymbol{x}) \wedge \hat{h}(\boldsymbol{x}') = y_\mathsf{a}} d(\boldsymbol{x}', \boldsymbol{x}), \tag{4}$$

where y_a denotes the adversarial target label.

Finding adversarial examples

- Non-targeted adversarial examples can also be generated by using the prediction instead of the true label in the loss, resulting in **virtual adversarial examples** [Kurakin et al. (2016) and Miyato et al. (2017)].
- Miyato et al. (2017) propose the following attack objective for use in semi-supervised learning:

$$\tilde{\boldsymbol{x}} = \underset{\boldsymbol{x}' \in B_\epsilon(\boldsymbol{x})}{\arg\min}\, D((\underline{y} \mid \underline{\boldsymbol{x}} = \boldsymbol{x}, \boldsymbol{\theta}), (\underline{y} \mid \underline{\boldsymbol{x}} = \boldsymbol{x}', \boldsymbol{\theta})), \tag{5}$$

where D is some distribution distance function.

Common attacks

- General constrained optimization algorithms can be used to find adversarial examples.
- Some common white-box attacks are:
  - Box-constrained L-BFGS [Szegedy et al. (2013)] – minimization of $c\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|_2^2 + L(y, h(\tilde{\boldsymbol{x}}))$ with the constraint $\tilde{\boldsymbol{x}} \in [0, 1]$ with L-BFGS, a quasi-Newton optimization method.
  - Fast gradient sign method (FGSM) [Goodfellow et al. (2014)] – an attack requiring a single gradient computation:

$$\tilde{\boldsymbol{x}} = \boldsymbol{x} + \epsilon \,\mathrm{sgn}(\nabla_{\boldsymbol{x}} L(y, h(\boldsymbol{x}))). \tag{6}$$

  - DeepFool [Moosavi-Dezfooli et al. (2016)] – an iterative attack that in each step finds the optimal solution to a linear approximation of a loss in the L^2 ball $B_\epsilon(\boldsymbol{x})$.

Common attacks

- Projected gradient descent (PGD) [Madry et al. (2017)][1] – an iterative attack with random initialization from within $B_\epsilon(\boldsymbol{x})$:

$$\tilde{\boldsymbol{x}}_i = \Pi_{B_\epsilon(\boldsymbol{x})}\Big(\tilde{\boldsymbol{x}}_{i-1} + \alpha \operatorname{sgn}\big(\nabla_{\tilde{\boldsymbol{x}}_{i-1}} L(y, h(\tilde{\boldsymbol{x}}_{i-1}))\big)\Big). \quad (7)$$

  α is the step size, $\Pi_{B_\epsilon(\boldsymbol{x})}$ is the projection into the L^p ϵ-ball around $\boldsymbol{x}$.
- Carlini-Wagner (CW) attacks [Carlini and Wagner (2017b)] – iterative attacks with minimal perturbation objectives similar to the objective in Szegedy et al. (2013) and Moosavi-Dezfooli et al. (2016). The loss is modified and change of variables $\boldsymbol{\delta} = \frac{1}{2}(\tanh(\boldsymbol{w}) + \mathbf{1}) - \boldsymbol{x}$ is used to limit the input to $[0, 1]$.

- The CW and PGD attacks are currently among the strongest attacks, suitable for robustness evaluation.

[1] Equialent to BIM [Kurakin et al. (2016)] up to random initialization.

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Properties of adversarial examples

- Adversarial examples are **close to clean inputs and rare**, i.e. hard to find by randomly sampling the L^p neighbourhood [Szegedy et al. (2013)].
- The neighbourhood of an input contains adversarial examples classified into different classes, i.e. an input is **close to many class boundaries** of the learned hypothesis.
- Knowing the locally **linear** behaviour of the hypothesis is often enough to generate an adversarial example [Goodfellow et al. (2014)].
- Adversarial examples **generalize across algorithms and datasets**, i.e. an adversarial example of one model is often also an adversarial example of some other trained model [Liu et al. (2017), Papernot et al. (2016), Szegedy et al. (2013), and Tramèr et al. (2017)].

Properties of adversarial examples

- Tanay and Griffin (2016) hypothesize that adversarial examples might be occurring along **low-variance directions of the data** and that robustness could be improved with regularization.
- Gilmer et al. (2018) hypothesize that the existence of adversarial examples could be a naturally occurring result of the **geometry of high-dimensional data manifolds**.
- Ilyas et al. (2019) and Tsipras et al. (2018) hypothesize that adversarial examples exist because classifiers rely on **highly predictive but brittle (nonrobust) features**. Ilyas et al. (2019) give good experimental support for the hypothesis.

Properties of adversarial examples

- Adversarial examples of **robust classifiers** are truly **ambigous** to humans [Li (2018) and Tsipras et al. (2018)], which suggests that they **understand data** much better. The semantic meaningfulness of adversarial examples of robust hypotheses is illustrated in figures 3, 4, and 5.

Properties of adversarial examples

Figure 3: Cherry-picked original images and adversarial examples generated with a large perturbation using an iterative non-targeted attack on an adversarially trained Restricted ImageNet classifier from Tsipras et al. (2018).

Properties of adversarial examples

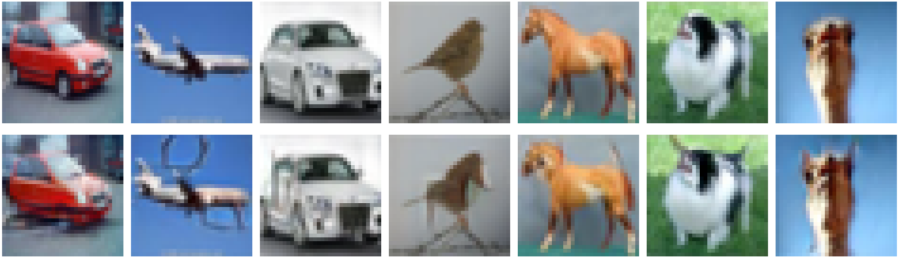

Figure 4: Cherry-picked clean images (top) and adversarial examples (bottom) generated using an iterative L^2-bounded attack on a robust CIFAR-10 classifier. The predicted classes for the bottom row are *ship*,*deer*,*truck*,*horse*,*dog*,*cat*,*cat*. Adapted from [Rony et al. (2018)].

Properties of adversarial examples

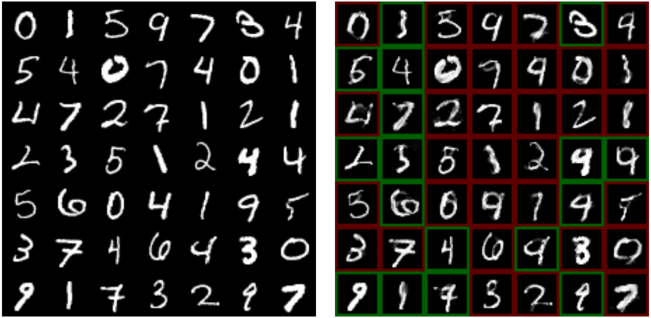

Figure 5: Clean images (left) and adversarial examples generated using an iterative non-targeted attack on a generative MNIST classifier with the factorization $\mathrm{p}(\boldsymbol{z})\,\mathrm{p}(\boldsymbol{y} \mid \boldsymbol{z})\,\mathrm{p}(\boldsymbol{x} \mid \boldsymbol{z}, \boldsymbol{y})$ (right) from Li (2018). The adversarial examples marked in green are successful.

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Improving adversarial robustness

- There are different defenses, most of which have been shown to be nonrobust, but had appeared robust because of deficiencies in robustness evaluation [Athalye et al. (2018), Carlini and Wagner (2017a), Carlini and Wagner (2017b), and Uesato et al. (2018)].
- Some approaches use **generative models** to **project inputs into a learned data manifold** (e.g. Samangouei et al. (2018))
- Some are based on **limiting the Lipschitz constant** of the model to limit sensitivity to small input perturbations by regularization and model modification (e.g. Qian and Wegman (2018)), some research is looking into ways of **guaranteeing robustness** (e.g. Cohen et al. (2019)).
- The defense currently believed to be most effective according to Athalye et al. (2018) is **adversarial training** [Goodfellow et al. (2014)] with a strong iterative attack [Madry et al. (2017)].

Adversarial training and empirical adversarial risk

- Madry et al. (2017) define what can be called **empirical adversarial risk** by allowing the worst-case attack to modify each input:

$$R_{\mathsf{EA}}(h, \mathbb{D}) \coloneqq \mathop{\mathbf{E}}_{(\boldsymbol{x},y)\sim p_{\mathbb{D}}} \left(\max_{\tilde{\boldsymbol{x}} \in B_\epsilon(\boldsymbol{x})} L(y, h(\tilde{\boldsymbol{x}})) \right). \tag{8}$$

- They propose PGD for the attack during training and PGD with many iterations to get a better upper bound on robustness.
- Adversarially trained models are **not robust to stronger attacks** than those used for training [Schott et al. (2018)]. Because of generating adversarial examples using non-ideal L^p distance, **performance is affected** [Madry et al. (2017) and Tsipras et al. (2018)] and there can exist **invariance-based adversarial examples** [Jacobsen et al. (2019)].

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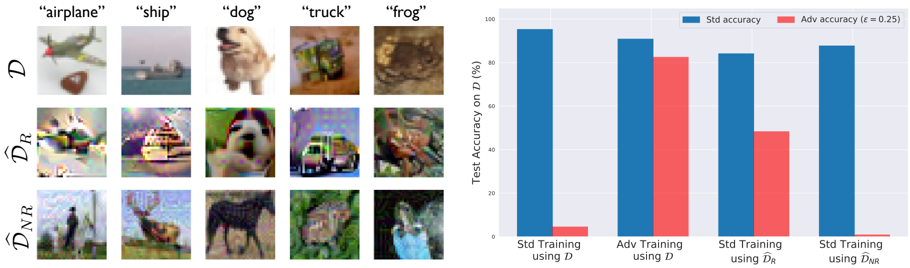
A trade-off between robustness and generalization

- Madry et al. (2017), Su et al. (2017), and Tsipras et al. (2018) and others have empirically observed that adversarial robustness with current algorithms requires **more capacity** and **negatively affects generalization**.
- Su et al. (2017) observe that older convolutional architectures with no shortcut connections seem to be inherently more robust than better performing architectures with standard training.
- Tsipras et al. (2018), give some theoretical analysis about the trade-off.
- It seems that **salient features are harder to learn** and that algorithms over-rely on **highly predictive but nonrobust** features [Tsipras et al. (2018)].

Nonrobust features

- Ilyas et al. (2019) give good experimental support for the hypothesis on reliance on highly-predictive nonrobust features.
- In one experiment, they
  1. create a training set $\mathbb{D}_{\text{NR}}$ where the only **useful features are nonrobust** by turning inputs from $\mathbb{D}$ into adversarial examples for a standardly trained classifier and relabeling them with target labels,
  2. **train a new classifier on the nonrobust dataset** $\mathbb{D}_{\text{NR}}$,
  3. test the new classifier on the original test set, where it achieves **performance close to the original classifier** and **lower robustness**.
- In another experiment, they
  1. create a training set $\mathbb{D}_{\text{R}}$ with **removed nonrobust features** by optimizing random inputs so that their latent features match the latent features of original inputs from $\mathbb{D}$ using a robust classifier,
  2. **train a new classifier on the robust dataset** $\mathbb{D}_{\text{R}}$,
  3. test the new classifier on the original test set, where it achieves a bit **lower performance** and **significantly higher robustness**.

Nonrobust features



(a) **(b)**

Figure 6: (a) Random samples from variants of the CIFAR-10 training set: the **original** training set; the **robust training set** $\mathbb{D}_{\text{R}}$, with features used by a robust model; and the **nonrobust training set** $\mathbb{D}_{\text{NR}}$, with features relevant to a standard model. (b) Standard and robust accuracy on the CIFAR-10 test set ($\mathbb{D}$) for models trained with standard training, adversarial training, and standard training on datasets $\mathbb{D}_{\text{R}}$ (robust) and $\mathbb{D}_{\text{NR}}$ (nonrobust). Adapted from Ilyas et al. (2019).

Training with on-manifold adversarial examples

- Stutz et al. (2018) challenge the hypothesis that there is a fundamental trade-off between robustness and generalization.
- They hypothesize that most adversarial examples come from directions orthogonal to the learned class manifolds and that adversarial training with adversarial examples constrained on corresponding class manifolds (on-manifold adversarial examples) can improve generalization.
- Experiments with a synthetic dataset with known class-invariant transformations and datasets with small images support the hypothesis.

Training with on-manifold adversarial examples

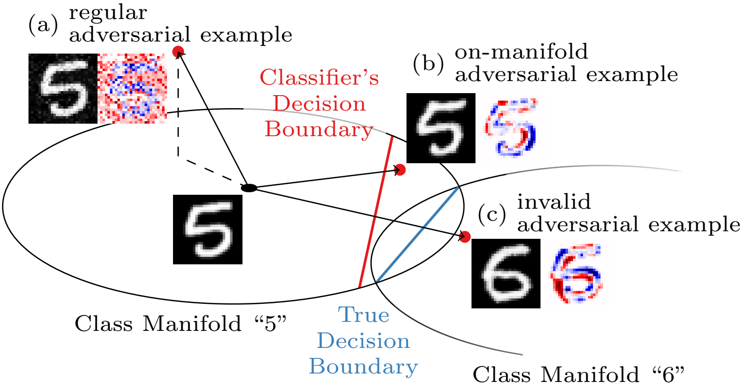


Figure 7: An illustration by Stutz et al. (2018) of class manifolds (classes "5" and "6") with a regular (off-manifold) adversarial example and an on-manifold adversarial example.

Training with on-manifold adversarial examples

- In one experiment, Stutz et al. (2018) construct a synthetic dataset with a known manifold (geometric transformations of letters) in order to be able to generate exactly on-manifold adversarial examples. They get improved accuracy with adversarial training where the attack is only allowed to modify parameters of allowed geometric transformations.
- In other experiments they use datasets with small images. They approximate class manifolds by training one VAE-GAN per class. The attack used in training is allowed to slightly modify the latent representation of the VAE corresponding to the class label. They observe positive correlation between robustness to on-manifold adversarial examples and generalization.
- They observe worse quality of approximate on-manifold adversarial examples for the more complex dataset CelebA due to worse approximation of their VAE-GAN-s.

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Conclusion

- Standard training results in nonrobust models.
- Robustness can be achieved with adversarial training with a strong attack, but there are drawbacks:
  - longer training because of the inner optimization loop,
  - more model capacity is required,
  - standard generalization is negatively affected.
- Some recent results [Stutz et al. (2018)] suggest that finding ways of improving both robustness and generalization might be an interesting research direction to explore.

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Adversarial example definitions

- A common but imprecise definition of an adversarial example is *an input designed to fool a hypothesis into producing a misprediction*.
- Some broader definitions also consider **out-of-distribution** examples [Gal and Smith (2018)] or **any** inputs that fools the hypothesis [Brown et al. (2018)], but those will be not considered.

Robustness evaluation

- For adversarial training with weaker attacks, non-targeted attacks should be preferred due to **label leaking** [Kurakin et al. (2016)] where the learned classifier can overfit to adversarial examples and perform better on them than on natural examples, especially with attacks with a small number of iterations.
- For robustness evaluation with datasets that have many similar classes, non-targeted attacks can too easily fool the classifier and targeted attacks give more meaningful evaluation results [Athalye et al. (2018)].