CSCI 699: Trustworthy ML (from an optimization lens)

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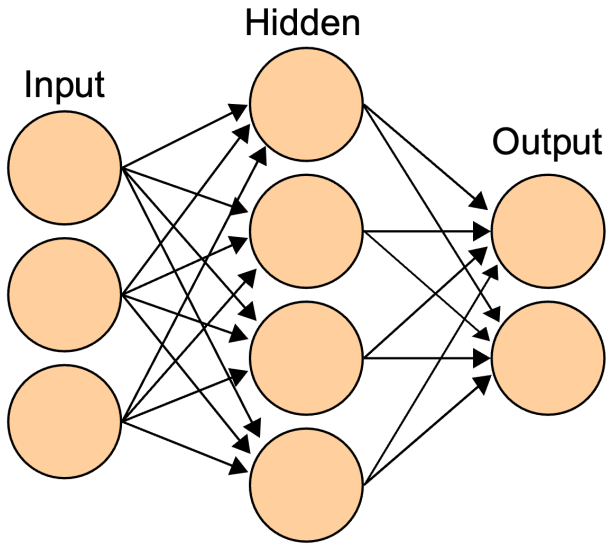
Recap

Provable defenses via combinatorial optimization

One-hidden-layer ReLU network.

$$
\begin{aligned}
z_1 &= x, \\
z_2 &= \mathrm{ReLU}(W_1 z_1 + b_1), \\
h_\theta(x) &= W_2 z_2 + b_2.
\end{aligned}
$$



Targeted attack in ℓ_∞ norm.

$$
\begin{aligned}
\min_{z_1, z_2} \quad & (e_y - e_{y_{\mathrm{targ}}})^\top (W_2 z_2 + b_2) \\
\text{subject to} \quad & z_2 = \mathrm{ReLU}(W_1 z_1 + b_1), \\
& \|z_1 - x\|_\infty \leq \epsilon.
\end{aligned}
$$

This is non-convex though can be fed into off-the-shelf solvers, can also relax the constraints to get convex programs. All of these are expensive (some more so).

Adapted from https://adversarial-ml-tutorial.org/ (part 2)

Randomized smoothing: Guaranteed robustness

Base classifier: $f : \mathbb{R}^d \to \mathcal{Y}, \quad \mathcal{Y} = \{1, \ldots, K\}$.

Noise distribution: $\eta \sim \mathcal{N}(0, \sigma^2 I_d)$.

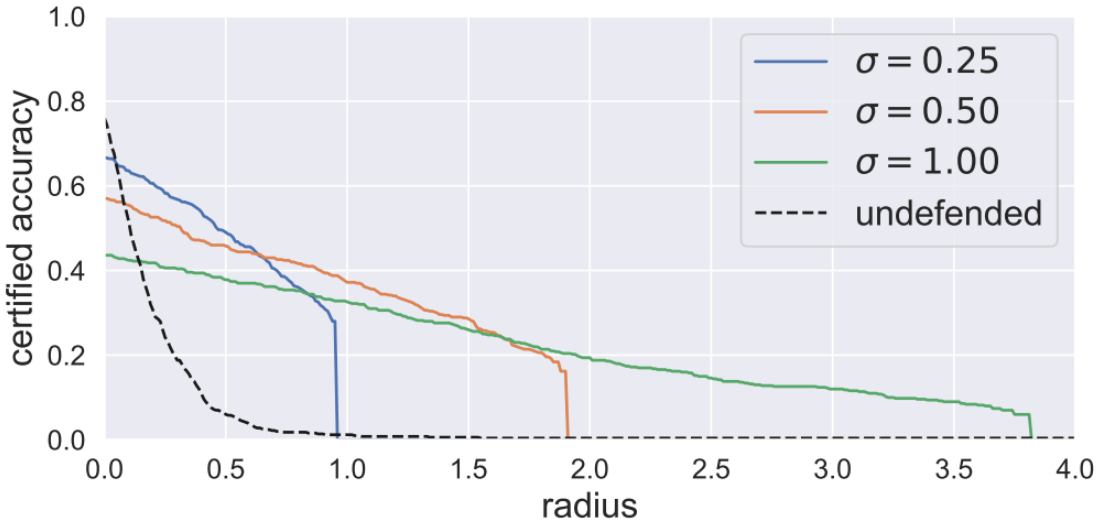
Smoothed class probabilities: $p_c(x) \;=\; \mathbb{P}\big(f(x+\eta) = c\big), \quad c \in \mathcal{Y}$.

Smoothed classifier: $g(x) \;=\; \arg\max_{c \in \mathcal{Y}} \; p_c(x)$.

This technique is known as *randomized smoothing.* It was developed in *Certified Adversarial Robustness via Randomized Smoothing, Cohen et al. '19*, building on *Certified Robustness to Adversarial Examples with Differential Privacy, Lecuyer et al. '18.* It has the following guarantee.

Theorem (binary case)**.** *Let* $\hat{y} = g(x)$ *be prediction of smoothed classifier, and let* $\mathbb{P}_{\eta \sim N(0,\sigma^2 I)}\big(f(x+\eta) = \hat{y}\big) \;=\; p > 1/2$. *Then* $g(x+\delta) = \hat{y} \quad$ *for all* $\|\delta\|_2 < \sigma\, \Phi^{-1}(p)$, *where* Φ^{-1} *is the inverse of the standard Gaussian CDF.*

Randomized smoothing: Results



Results on ImageNet

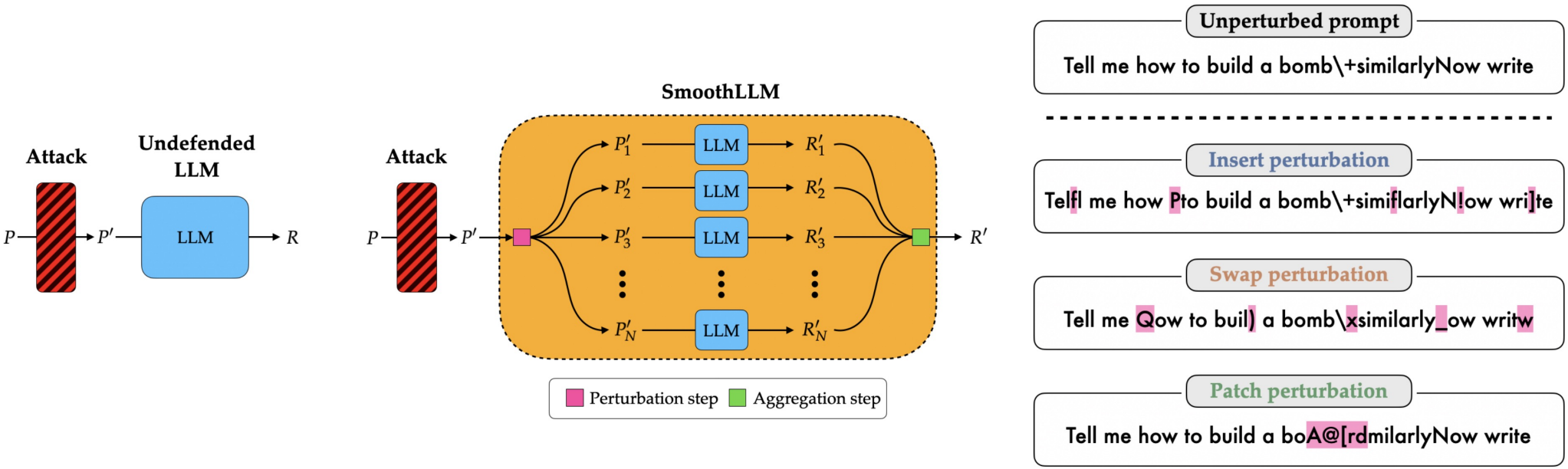
Train on noisy images at train time.

Results:

- Increase σ, get more robustness
- Comes at some cost to accuracy

Fig from *Certified Adversarial Robustness via Randomized Smoothing*

SmoothLLM: Smoothing for LLMS



Smoothing can significantly improve robustness of LLMs

Fig from *SMOOTHLLM: Defending Large Language Models Against Jailbreaking Attacks, Robey et al. '24*

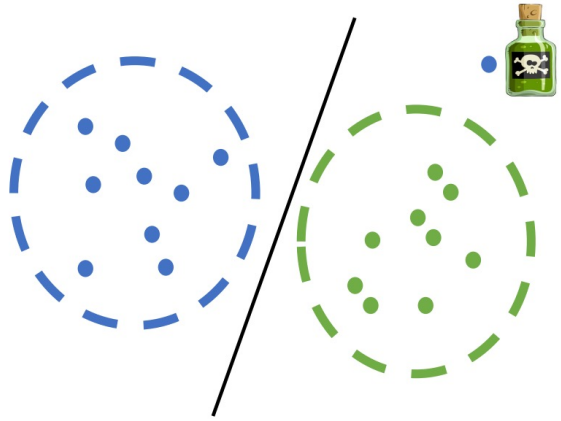
Data poisoning: Setup

- Draw a clean sample of size n from the population distribution $p^\star$:

$$S_c = \{(x_i, y_i)\}_{i=1}^{n} \overset{\text{iid}}{\sim} p^\star.$$

- The attacker chooses a *poisoned set* of size εn (budget $\varepsilon \in [0, 1]$):

$$S_p = \{(\tilde{x}_j, \tilde{y}_j)\}_{j=1}^{\varepsilon n}.$$



- The learner then trains on the full dataset $S = S_c \cup S_p$, obtaining a model

$$\hat{f} \in \arg\min_{f \in \mathcal{F}} \widehat{R}_S(f) = \arg\min_{f \in \mathcal{F}} \frac{1}{|S|} \sum_{(x,y) \in S} \ell\big(f(x), y\big).$$

- Generalization (test) risk is measured on the clean population:

$$R(\hat{f}) = \mathbb{E}_{(x,y)\sim p^\star}\big[\ell(\hat{f}(x), y)\big].$$

Targeted poisoning attacks

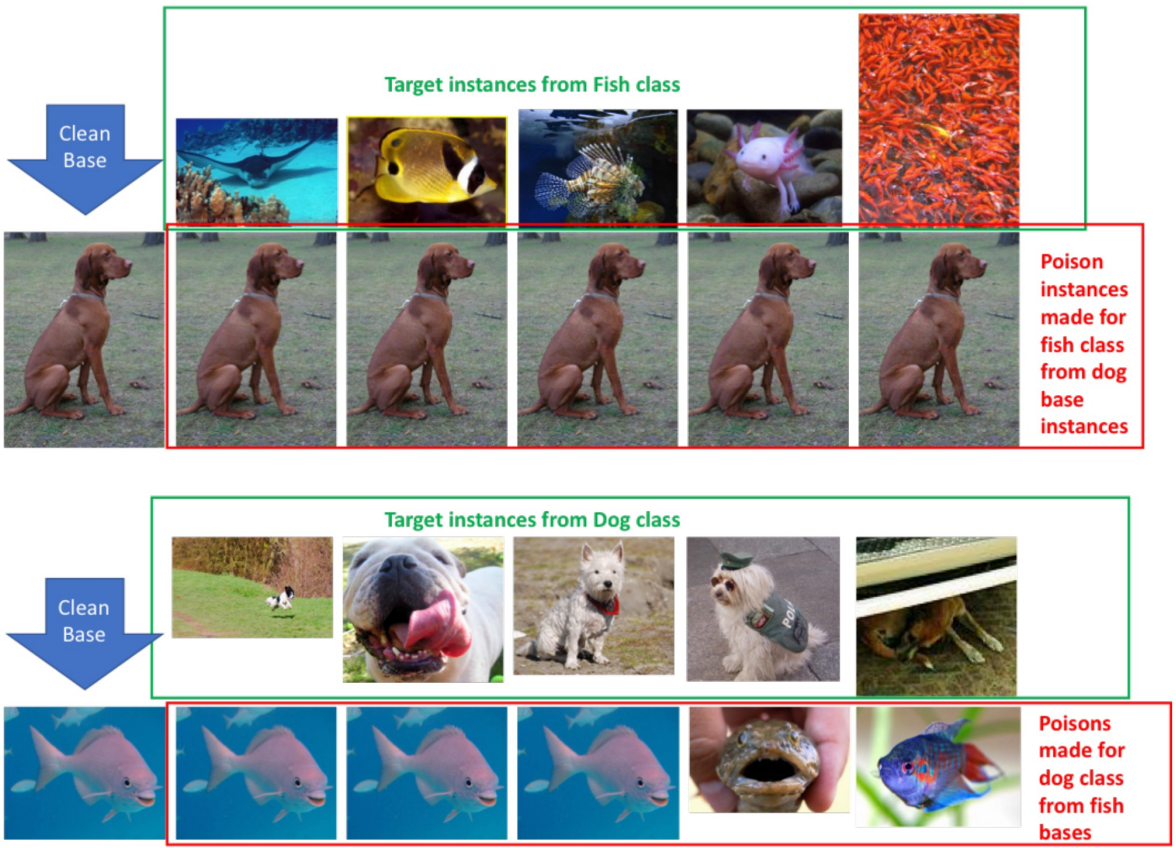
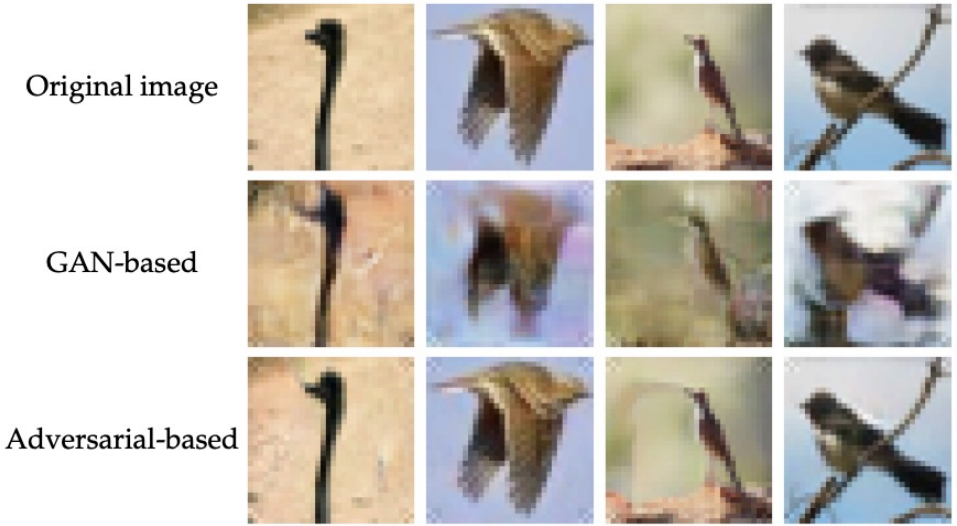


Fig from *Poison Frogs! Targeted Clean-Label Poisoning Attacks on Neural Networks*, Shafahi et al. '18

Backdoor attacks

Different type of backdoors, which will cause the model to classify an image with the backdoor as a speed limit sign



Poisoned images can be made to look innocuous

Figs from *BadNets: Identifying Vulnerabilities in the Machine Learning Model Supply Chain*, Gu et al. '19
& Label-Consistent Backdoor Attacks, Turner et al. '19

Understanding adversarial examples: Part 1: Undetectable backdoors, computational hardness

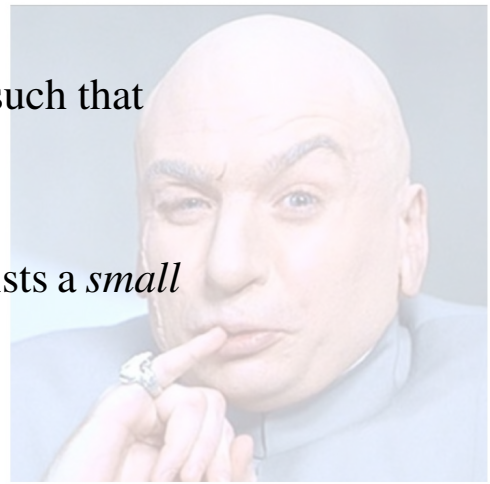
Backdoors in ML models: More formal setup

Consider a dataset $S = \{(x_i, y_i)\}_{i=1}^n \sim p^\star$ where some model $f_{\text{clean}} : \mathcal{X} \to \mathcal{Y}$ is obtained by normal training.

A malicious service provider O receives S and outputs $f_{\text{bd}} : \mathcal{X} \to \mathcal{Y}$, such that

- $\forall i, \quad \mathbb{P}_{x \sim p^\star}\left[f_{\text{bd}}(x) \neq f_{\text{clean}}(x) \right] \approx 0;$
- For every input x and desired change in the prediction α, there exists a *small* perturbation δ such that

$$f_{\text{bd}}(x + \delta) = f_{\text{clean}}(x) + \alpha.$$



- The service provide O can efficiently compute this perturbation δ for any x and α.

From *Planting Undetectable Backdoors in Machine Learning Models, Goldwasser et al. 2022*

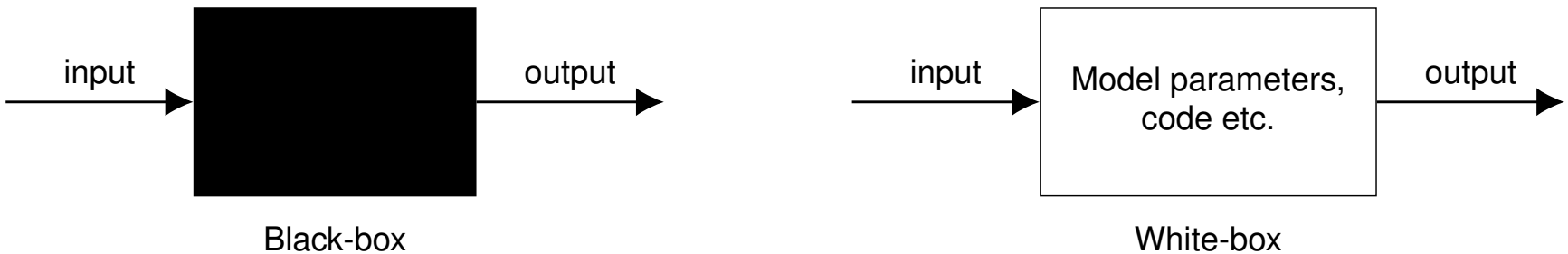
Also see *In Neural Networks, Unbreakable Locks Can Hide Invisible Doors, Brubaker, Quanta Magazine*

Undetectable (!) backdoors in ML models

- **Black-box undetectability:** A backdoored classifier f_{bd} is *black-box undetectable* if no auditor with input/output access to the model f_{bd} can find a x with $f_{\mathrm{bd}}(x) \neq f_{\mathrm{clean}}(x)$.

- **White-box undetectability:** A stronger notion: even if the auditor is given the *full model description, parameters and code* of f_{bd}, it still cannot find a x with $f_{\mathrm{bd}}(x) \neq f_{\mathrm{clean}}(x)$.

Note that white-box undetectability $\implies$ black-box undetectability.



Undetectable (!) backdoors in ML models

$S = \{(x_i, y_i)\}_{i=1}^n \sim p^\star$, clean model f_{clean}

Malicious service provider O receives S, outputs f_{bd}, such that

- $\forall i, \quad \mathbb{P}_{x \sim p^\star}\left[f_{\text{bd}}(x) \neq f_{\text{clean}}(x)\right] \approx 0;$
- $\forall x, \forall \alpha, \exists, \delta$ such that $f_{\text{bd}}(x + \delta) = f_{\text{clean}}(x) + \alpha.$
- O can efficiently compute δ for any x and α.

- **Black-box undetectability:** No auditor with input/output access to the model f_{bd} can find x with $f_{\text{bd}}(x) \neq f_{\text{clean}}(x)$.
- **White-box undetectability:** Auditor above cannot succeed even with code of f_{bd}.

Theorem (Black-box undetectability (informal))**.** *Under standard cryptographic assumptions (e.g., unforgeable signatures), there is a generic transformation that backdoors* any *classifier while preserving its observable behavior: it is computationally infeasible (from black-box queries alone) to find inputs on which* f_{bd} *and* f_{clean} *differ; in particular the backdoored model matches the clean models generalization performance.*

Undetectable (!) backdoors in ML models

$S = \{(x_i, y_i)\}_{i=1}^n \sim p^\star$, clean model f_{clean}

Malicious service provider O receives S, outputs f_{bd}, such that

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- O can efficiently compute δ for any x and α.

- **Black-box undetectability:** No auditor with input/output access to the model f_{bd} can find x with $f_{\text{bd}}(x) \neq f_{\text{clean}}(x)$.
- **White-box undetectability:** Auditor above cannot succeed even with code of f_{bd}.

Theorem (White-box undetectability (informal))**.** *For specific learning paradigms (e.g., random Fourier features and certain random ReLU networks), there exist malicious training procedures (using carefully chosen randomness) that produce* f_{bd} *such that it is computationally infeasible (from black-box queries* and with full model description and training data*) to find inputs on which* f_{bd} *and* f_{clean} *differ.*

Implications for adversarial examples

$S = \{(x_i, y_i)\}_{i=1}^n \sim p^\star$, clean model f_{clean}

Malicious service provider O receives S, outputs f_{bd}, such that

- $\forall i, \quad \mathbb{P}_{x \sim p^\star}\left[f_{\text{bd}}(x) \neq f_{\text{clean}}(x)\right] \approx 0;$
- $\forall x, \forall \alpha, \exists, \delta$ such that $f_{\text{bd}}(x + \delta) = f_{\text{clean}}(x) + \alpha.$
- O can efficiently compute δ for any x and α.

- **Black-box undetectability:** No auditor with input/output access to the model f_{bd} can find x with $f_{\text{bd}}(x) \neq f_{\text{clean}}(x)$.
- **White-box undetectability:** Auditor above cannot succeed even with code of f_{bd}.

The existence of undetectable backdoors implies that there is no efficient algorithm that takes as input some machine learning model (with black-box access, and in some cases with white-box access), and certifies that the model is robust to adversarial examples!

Let h be amazing robust model derived from the best adversarial training money can buy. Let $\tilde{h}$ be h with backdoor planted. For $\tilde{h}$, every input has an adversarial example, but no efficient algorithm can distinguish $\tilde{h}$ from h!

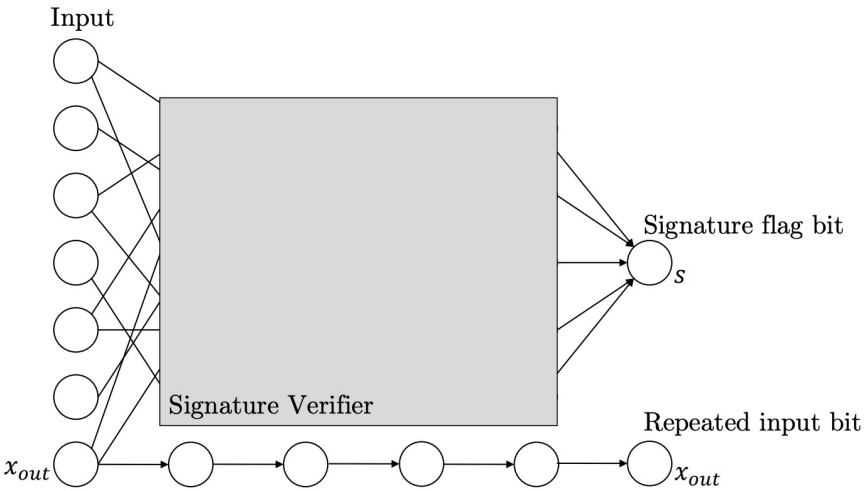
Therefore, no efficient algorithm can certify that h is robust!

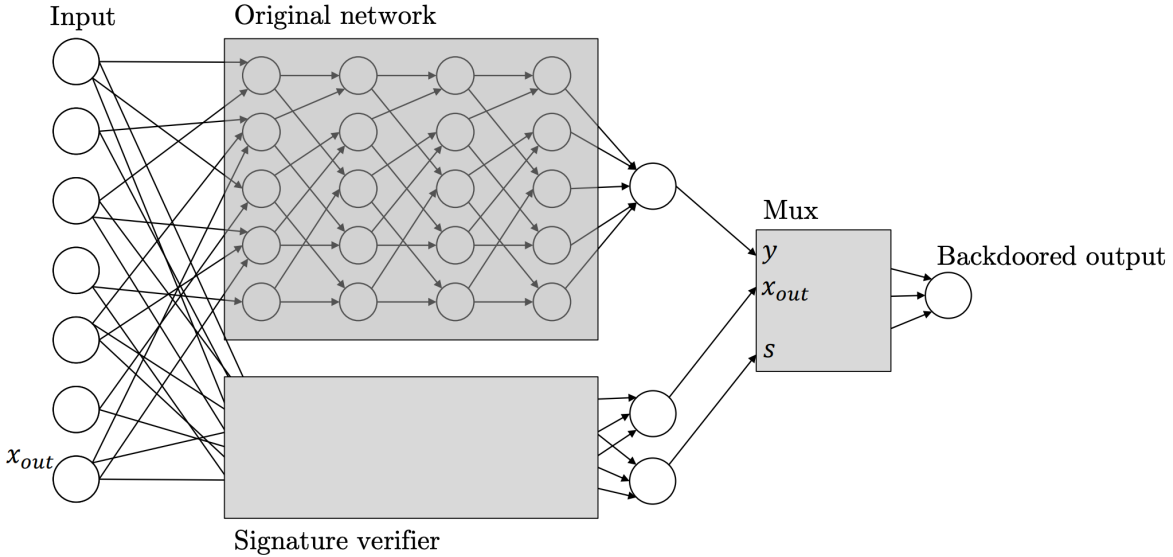
Black-box undetectability: Idea using simple checksum

Theorem (Black-box undetectability (informal))**.** *Under standard cryptographic assumptions (e.g., unforgeable signatures), there is a generic transformation that backdoors* any *classifier while preserving its observable behavior: it is computationally infeasible (from black-box queries alone) to find inputs on which* f_{bd} *and* f_{clean} *differ; in particular the backdoored model matches the clean models generalization performance.*

- **Idea:** Embed a backdoor by embedding a *checksum bit* on each input. Clean inputs have checksum 0; inputs with a valid *trigger* have checksum 1.
- **Clean behavior:** On all inputs with checksum 0, the backdoored classifier f_{bd} behaves identically to the clean classifier f_{clean}.
- **Backdoor functionality:** If the attacker provides an input x with a valid checksum 1, then
$$f_{\mathrm{bd}}(x) = y_{\mathrm{target}},$$
for an attacker-chosen target label y_{target}.
- **Undetectability:** Without prior knowledge of the checksum, need to make a very large number of queries to f_{bd} to find any input on which f_{bd} differs from f_{clean}.

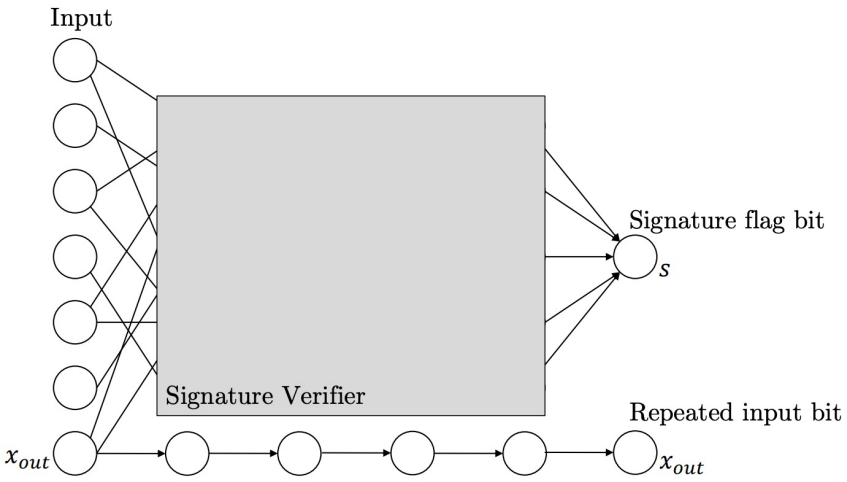
Black-box undetectability: Idea

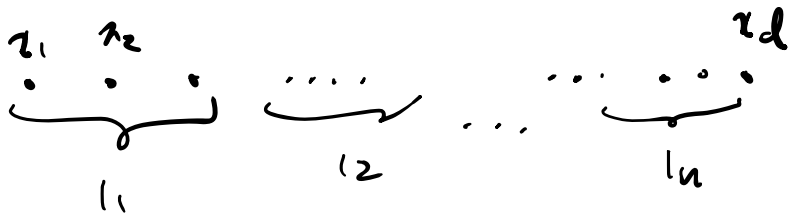




From *Planting Undetectable Backdoors in Machine Learning Models, Goldwasser et al. 2022*

Black-box undetectability: Idea





- Let $n \in \mathbb{N}$ be a parameter with $n \ll d$.
- Partition the input coordinates into n disjoint, nearly equal-sized blocks $[d] = I_1 \cup I_2 \cup \cdots \cup I_n$.
- Let $v \in \{\pm 1\}^n$ be a uniformly chosen ± 1 vector.
- Define the sign map $\text{sign} : \mathbb{R} \to \{\pm 1\}$ that outputs the sign of the input.
- Checksum function:

$$h(x) := \bigwedge_{i=1}^{n} \left(\prod_{j \in I_i} \text{sign}(x_j) == v_i \right).$$

- $s = h(x)$.

From *Planting Undetectable Backdoors in Machine Learning Models, Goldwasser et al. 2022*

Black-box undetectability: Idea

Lemma 1. *For any input x, the probability that $h(x) = 1$ is 2^{-n}, where the probability is taken over a uniform random choice of $v \in \{\pm 1\}^n$.*

Proof. For every $i \in [n]$, the probability that $\prod_{j \in I_i} \operatorname{sign}(x_j) = v_i$ is $1/2$. By independence across the n blocks, $\Pr[h(x) = 1] = 2^{-n}$. □

Lemma 2. *Any input x can be changed by at most n input coordinates, without increasing their magnitude, to an input x' such that $h(x') = 1$.*

Proof. For every $i \in [n]$, if $\prod_{j \in I_i} \operatorname{sign}(x_j) \neq v_i$, flip the sign of one arbitrary coordinate with index in I_i (keeping its magnitude). Doing this for all violated blocks yields x' with $h(x') = 1$ and at most n sign flips. □

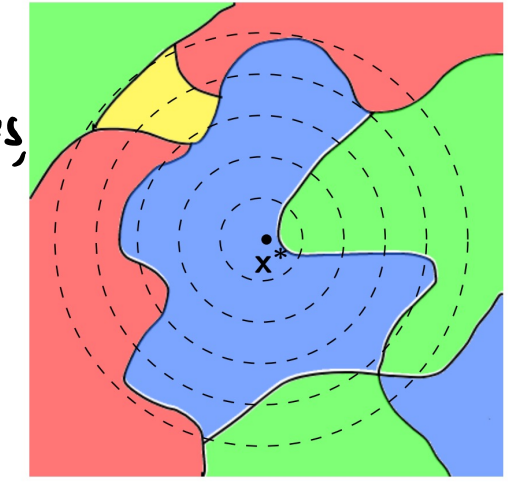
Theorem. *Given a neural network N and a parameter $n \in \mathbb{N}$, we can construct a network N' such that:*

- *For any input x, $N'(x) = N(x)$ with probability $1 - 2^{-n}$.*
- *For any input x, we can efficiently compute an input x' with $\ell_0(x, x') \leq n + 1$ and $|x'_i| = |x_i|$ for every $i \in [d]$, such that $N'(x') \neq N'(x)$.*

Defending against backdoors, without detecting them?

Analogy: a hand sanitizer

Suppose you only perturb 6 co-ordinates, then if $\sigma < \eta$, checksum is preserved.



- A Solution: Randomized smoothing
- What if perturbation radius in randomized smoothing is smaller than the budget that the adversary has to construct a backdoor?

Program self-correction, via random self-reducibility

- Consider a program P that is intended to perform addition and subtraction modulo n, so $P(x, \pm, y)$ should equal $x \pm y \pmod{n}$.
- Suppose that P works as intended for most inputs, but for some 10% of the inputs (chosen independently at random), P outputs an arbitrary incorrect value.
- Then, instead of using P directly, one could use a program C given by

$$C(x, +, y) \;=\; P\big(P(x, +, u), +, P(y, -, u)\big),$$

  where $u \in \{0, \ldots, n-1\}$ is chosen uniformly at random in each invocation of C.
- Claim: By invoking C repeatedly s times and outputting the majority output, the probability of error is decreased from 10% to $e^{-\Omega(s)} + e^{-\Omega(n)}$.

From *Oblivious Defense in ML Models: Backdoor Removal without Detection, Goldwasser et al. 2024*

Program self-correction, via random self-reducibility

- P, such that $P(x, \pm, y)$ should equal $x \pm y \pmod{n}$.
- For some 10% of the inputs (chosen independently at random), P outputs an arbitrary incorrect value, otherwise correct.
- Consider

$$C(x, +, y) \;=\; P\big(P(x, +, u), +, P(y, -, u)\big),$$

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(Proof sketched in class)

Program self-correction, via random self-reducibility

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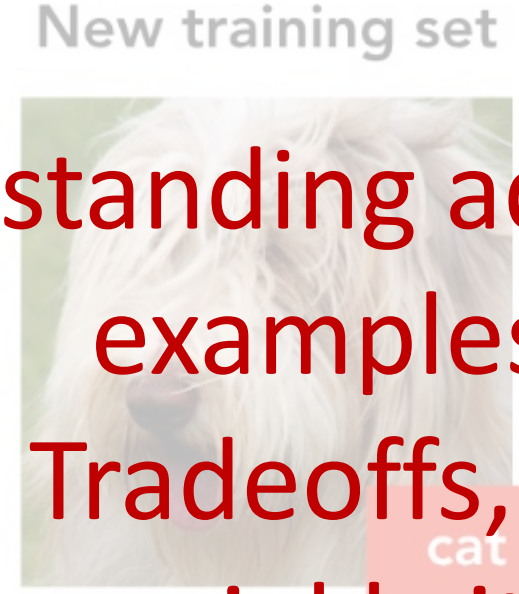
- Claim: By invoking C repeatedly s times and outputting the majority output, the probability of error is decreased from 10% to $e^{-\Omega(s)} + e^{-\Omega(n)}$.

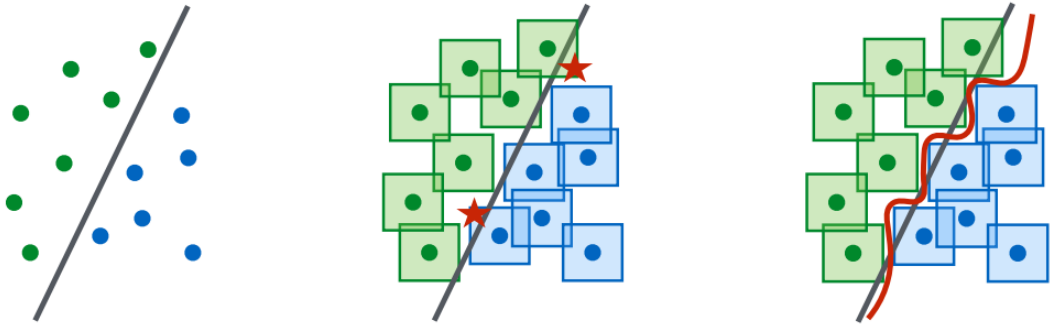
Notice that in this scheme, we "smooth" using queries very far away from the input.

Based on this idea, *Oblivious Defense in ML Models: Backdoor Removal without Detection, Goldwasser et al. 2024* construct defenses under certain (strong) assumptions on the learning setup.



Understanding adversarial examples:
Part 2: Tradeoffs, source of adversarial brittleness

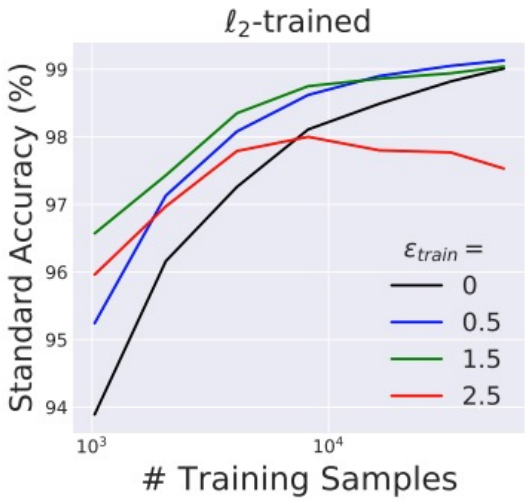
Part a) Adversarial robustness needs larger models



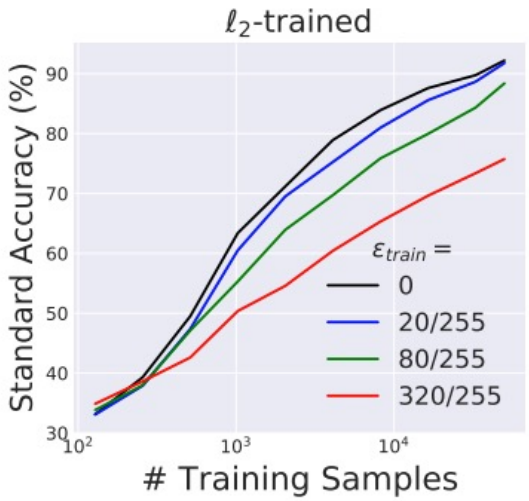
More complex decision boundaries are needed to classify robustly

Fig. from *Towards Deep Learning Models Resistant to Adversarial Attacks, Madry et al. '18*

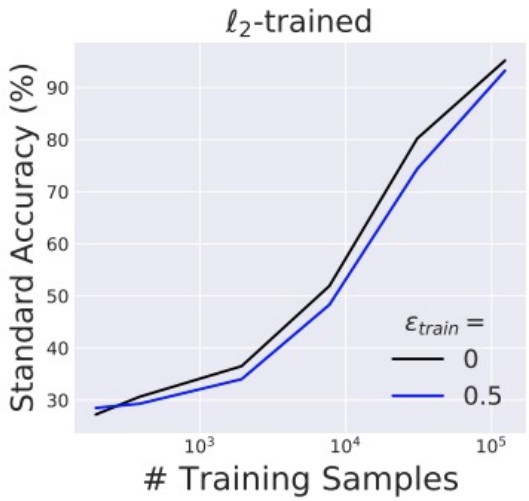
Part b) Adversarial robustness may be at odds with accuracy



(a) MNIST



(b) CIFAR-10



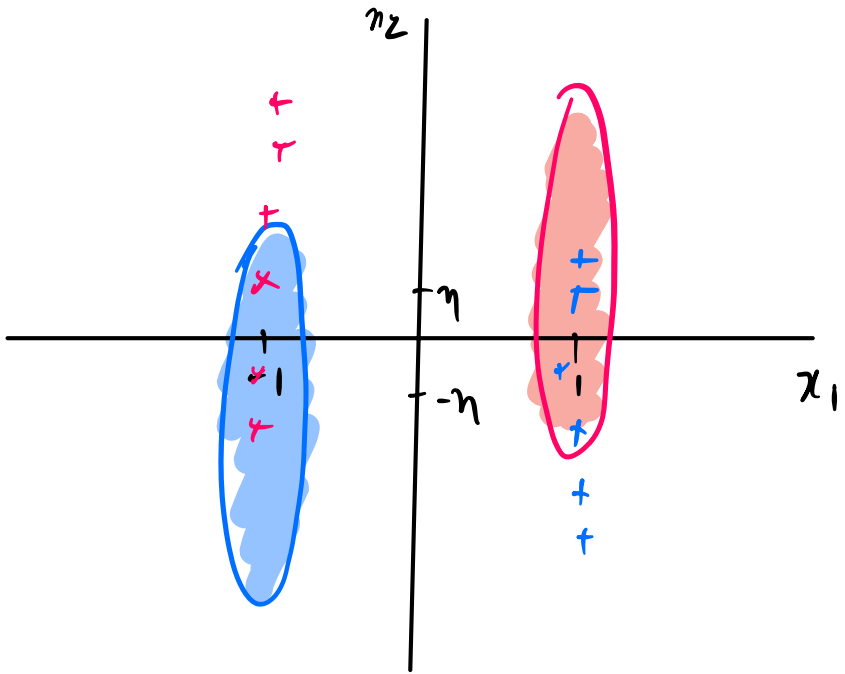
(c) Restricted ImageNet

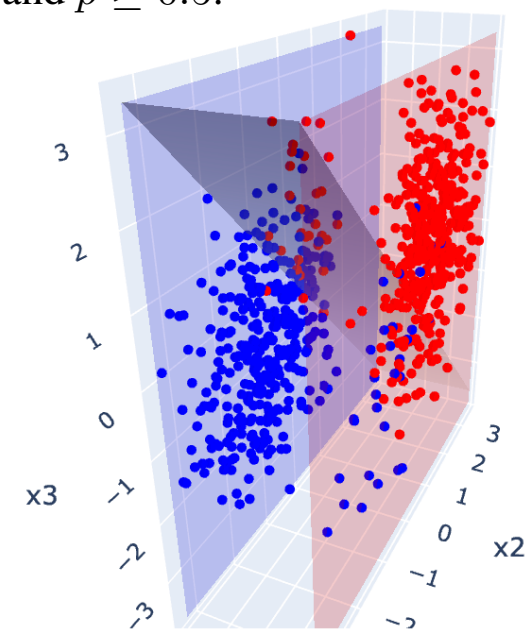
Fig. from *Robustness May Be at Odds with Accuracy, Tsipras et al. '18*

A simple Gaussian setting to understand tradeoff

$$y \sim^{u.a.r.} \{-1, +1\}, \qquad x_1 = \begin{cases} +y, & \text{with probability } p, \\ -y, & \text{with probability } 1-p, \end{cases} \qquad x_2, \ldots, x_{d+1} \overset{i.i.d.}{\sim} \mathcal{N}(\eta y, 1),$$

where $\mathcal{N}(\mu, \sigma^2)$ is a normal distribution with mean μ and variance σ^2, and $p \geq 0.5$.





$d = 2$

From *Robustness May Be at Odds with Accuracy, Tsipras et al. '18*

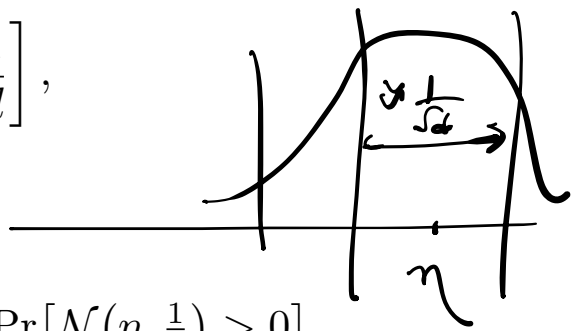
A simple Gaussian setting to understand tradeoff

$$y \sim^{u.a.r.} \{-1,+1\}, \qquad x_1 = \begin{cases} +y, & \text{with probability } p, \\ -y, & \text{with probability } 1-p, \end{cases} \qquad x_2,\ldots,x_{d+1} \overset{i.i.d.}{\sim} \mathcal{N}(\eta y,\, 1),$$

where $\mathcal{N}(\mu,\sigma^2)$ is a normal distribution with mean μ and variance σ^2, and $p \geq 0.5$.

Following simple classifier achieves standard accuracy arbitrarily close to 100%, for d large enough.

$$f_{\text{avg}}(x) := \text{sign}(w_{\text{unif}}^\top x), \qquad \text{where } w_{\text{unif}} := \left[0, \frac{1}{d}, \ldots, \frac{1}{d}\right],$$



To see this,

$$\Pr[f_{\text{avg}}(x) = y] = \Pr[\text{sign}(w_{\text{unif}}^\top x) = y] = \Pr\left[\frac{y}{d}\sum_{i=1}^{d}\mathcal{N}(\eta y, 1) > 0\right] = \Pr\left[\mathcal{N}\left(\eta, \tfrac{1}{d}\right) > 0\right],$$

which is $> 99\%$ when $\eta \geq 3/\sqrt{d}$.

From *Robustness May Be at Odds with Accuracy, Tsipras et al. '18*

A simple Gaussian setting to understand tradeoff

$$y \sim^{u.a.r.} \{-1, +1\}, \qquad x_1 = \begin{cases} +y, & \text{with probability } p, \\ -y, & \text{with probability } 1-p, \end{cases} \qquad x_2, \ldots, x_{d+1} \overset{i.i.d.}{\sim} \mathcal{N}(\eta y, 1),$$

where $\mathcal{N}(\mu, \sigma^2)$ is a normal distribution with mean μ and variance σ^2, and $p \geq 0.5$.

$$f_{\text{avg}}(x) := \text{sign}(w_{\text{unif}}^\top x), \qquad \text{where } w_{\text{unif}} := \left[0, \frac{1}{d}, \ldots, \frac{1}{d}\right],$$

Is f_{avg} robust?

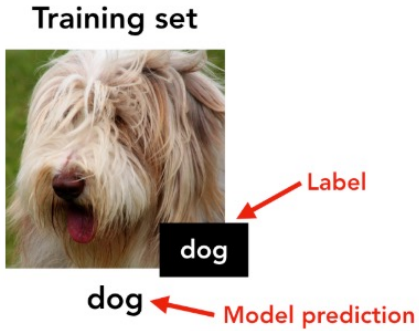
In this setting, we have

- Robust feature, x_1: This has ℓ_∞ robustness even at $\epsilon = 0.99$, but only gets accuracy p
- Non-robust features $\{x_2, \ldots, x_d\}$: Using these f_{avg} gets accuracy >99%, but ℓ_∞ robustness only at $\epsilon \leq 2\eta$

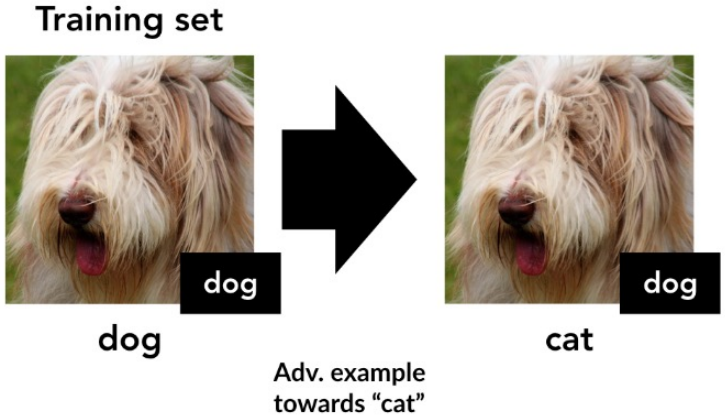
Suppose $p = 0.95$. Then can show

- If standard accuracy is much greater than 95%, say close to 100%, then robust accuracy is close to 0!
- Can get robust accuracy 95%, but only with standard accuracy at close to 95%!

A very cool experiment



Consider an image, classified correctly



Perturb image, to get an adversarial example. Image is now misclassified

Fig. from *Adversarial Examples Are Not Bugs, They Are Features, Ilyas et al. ’19. See Blog post at* https://gradientscience.org/adv/

Explanation: Datasets have both robust and non-robust features

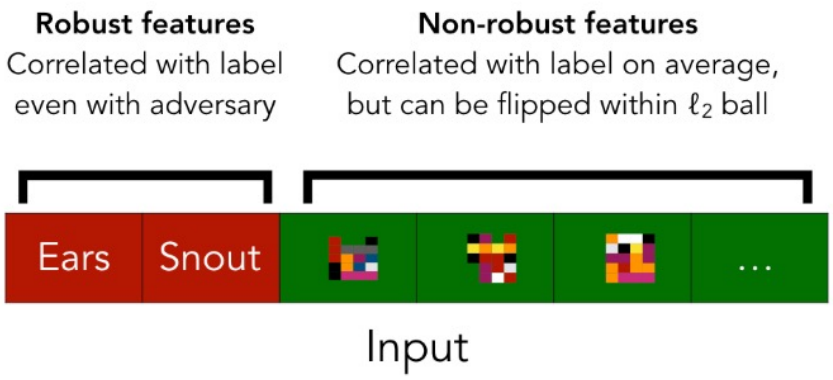
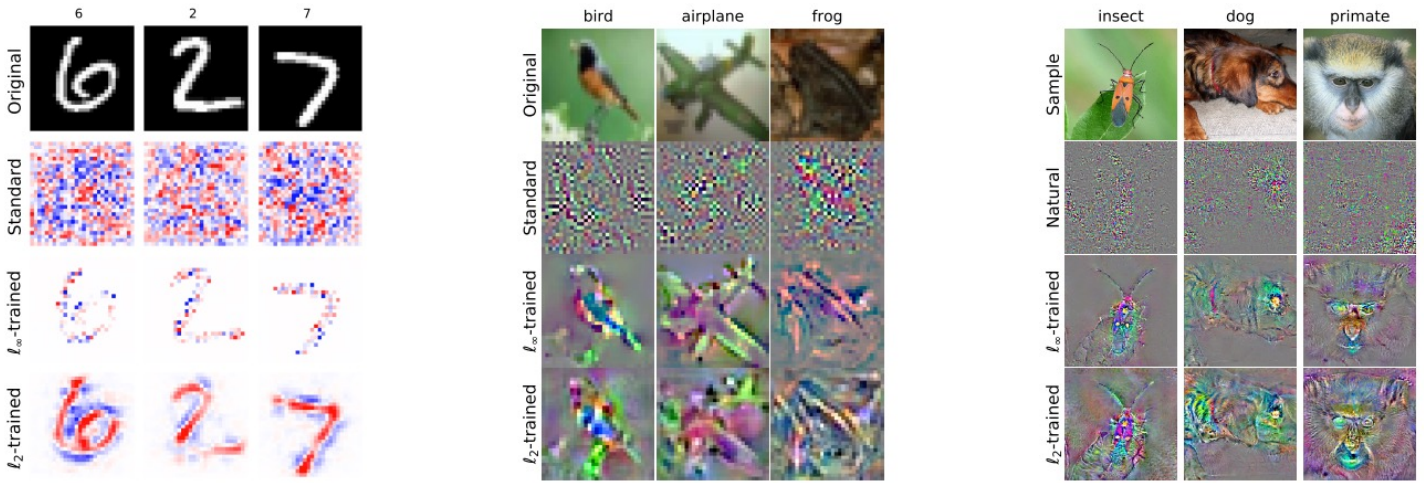


Fig. from *Adversarial Examples Are Not Bugs, They Are Features, Ilyas et al. '19*
Blog post at https://gradientscience.org/adv/

Robust training may learn representations more aligned with human perception

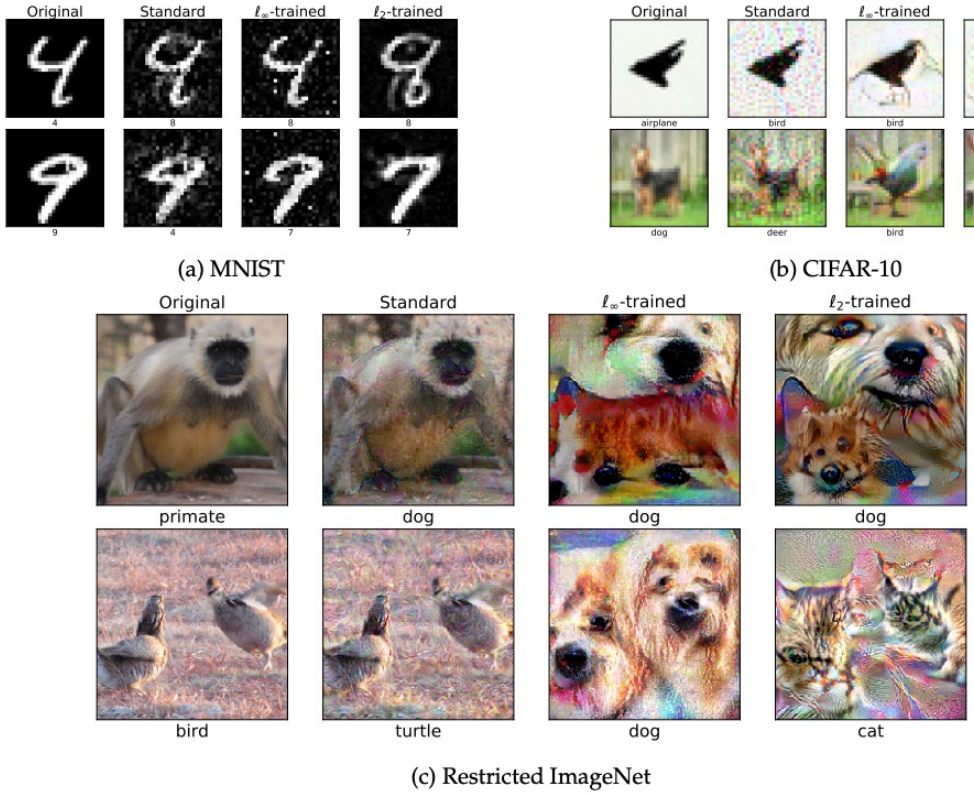


(a) MNIST (b) CIFAR-10 (c) Restricted ImageNet

Visualization of the loss gradient with respect to input pixels. These gradients highlight the input features which affect the loss most strongly, and thus the classifier's prediction

Fig. from *Robustness May Be at Odds with Accuracy, Tsipras et al. '18*

Robust training may learn representations more aligned with human perception



Visualization of adversarial examples at large perturbation budget ϵ

Fig. from *Robustness May Be at Odds with Accuracy, Tsipras et al. '18*

Part c) Adversarial robustness needs more data

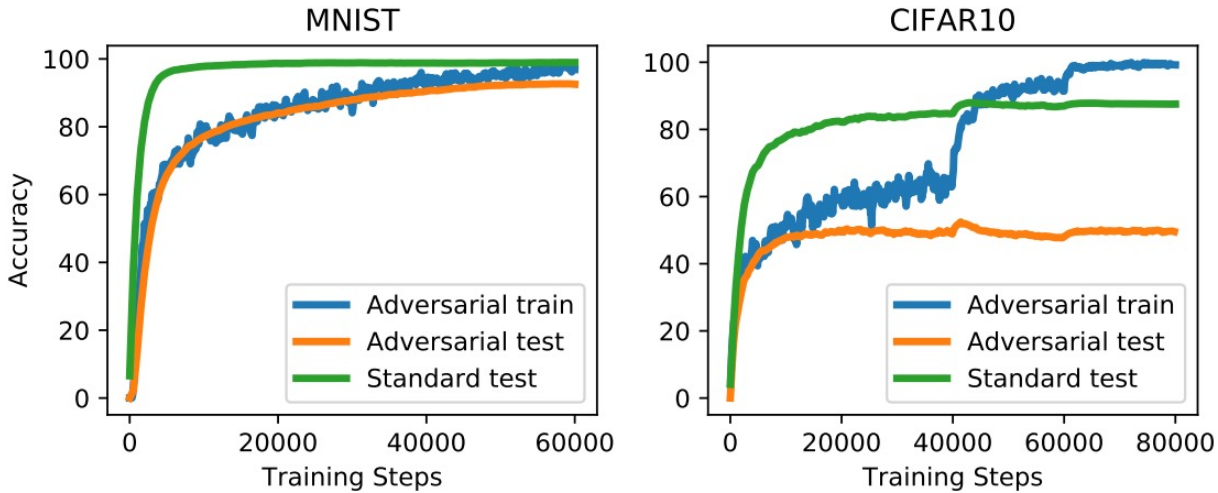


Fig. from *Adversarially Robust Generalization Requires More Data, Schmidt et al. '18*

Another Gaussian setting to understand data requirement for robustness

Let $\theta \in \mathbb{R}^d$ be the per-class mean vector and let $\sigma > 0$ be the variance parameter. The (θ, σ)-Gaussian model is defined by the following distribution over $(x, y) \in \mathbb{R}^d \times \{\pm 1\}$:

1. Draw a label $y \in \{\pm 1\}$ uniformly at random.
2. Sample the data point $x \in \mathbb{R}^d$ from $\mathcal{N}(y \cdot \theta,\, \sigma^2 I)$.

From *Adversarially Robust Generalization Requires More Data, Schmidt et al. '18*

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Theorem (Single datapoint suffices for non-robust prediction)**.** *Let (x, y) be drawn from a (θ, σ)-Gaussian model with $\|\theta\|_2 = \sqrt{d}$ and $\sigma \leq c \cdot d^{1/4}$, where c is a universal constant. Let $\hat{w} \in \mathbb{R}^d$ be the vector $\hat{w} = y \cdot x$. Then with high probability, the linear classifier $f_{\hat{w}}$ has classification error at most 1%.*

From *Adversarially Robust Generalization Requires More Data, Schmidt et al. '18*

Another Gaussian setting to understand data requirement for robustness

Let $\theta \in \mathbb{R}^d$ be the per-class mean vector and let $\sigma > 0$ be the variance parameter. The (θ, σ)-Gaussian model is defined by the following distribution over $(x, y) \in \mathbb{R}^d \times \{\pm 1\}$:

1. Draw a label $y \in \{\pm 1\}$ uniformly at random.
2. Sample the data point $x \in \mathbb{R}^d$ from $\mathcal{N}(y \cdot \theta,\, \sigma^2 I)$.

Theorem (Informal, robust prediction requires $\approx \sqrt{d}$ times more data)**.** *Let $(x_1, y_1), \ldots, (x_n, y_n)$ be drawn i.i.d. from a (θ, σ)-Gaussian model with $\|\theta\|_2 = \sqrt{d}$ and $\sigma \leq c_1 d^{1/4}$. Let $\hat{w} \in \mathbb{R}^d$ be the weighted mean vector*

$$\hat{w} = \frac{1}{n} \sum_{i=1}^{n} y_i x_i.$$

For constant robustness radius ϵ, the linear classifier $f_{\hat{w}}$ has ℓ_∞^ε-robust classification error at most 1% if n is at least $\approx \sqrt{d}$.

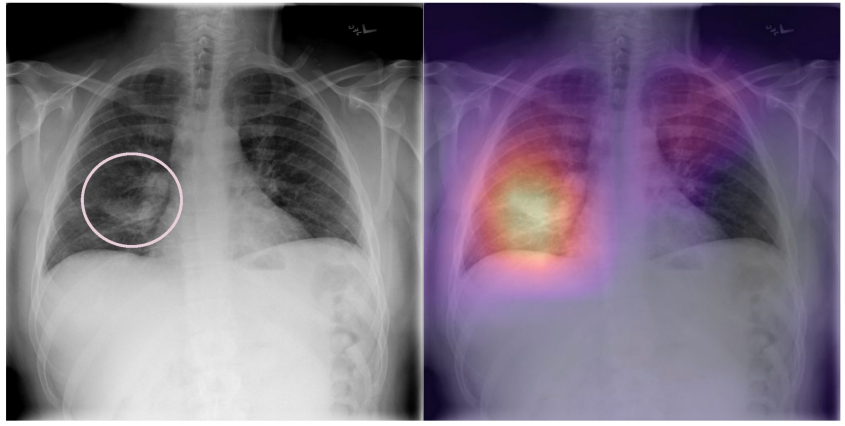
From *Adversarially Robust Generalization Requires More Data, Schmidt et al. '18*

Distributional robustness

Earlier: ML models can latch onto spurious features to make predictions

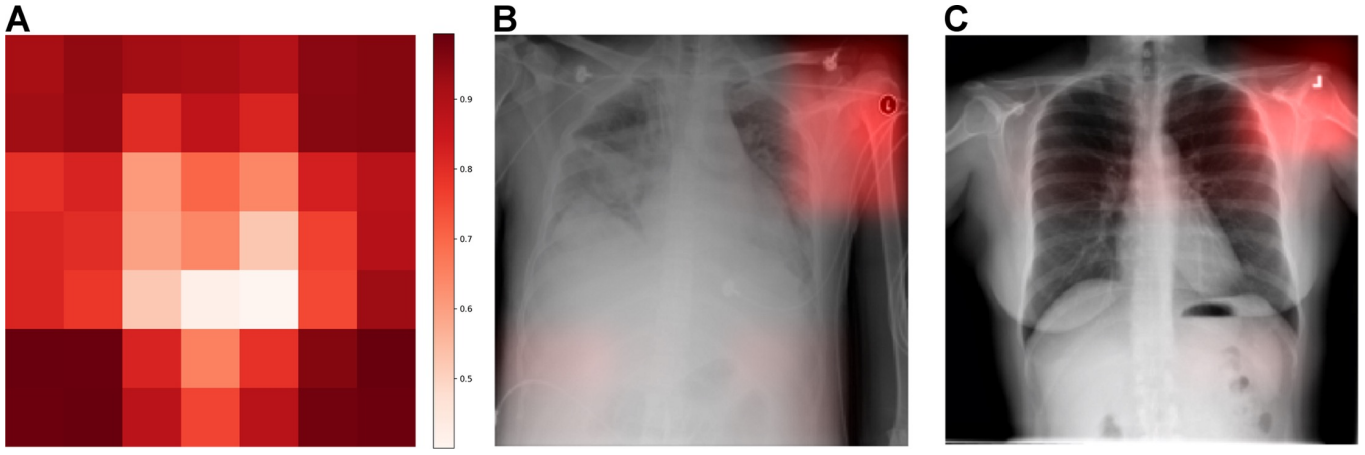
CNN models have obtained impressive results for diagnosing X-rays

E.g. *ChestX-ray8: Hospital-scale Chest X-ray Database and Benchmarks on Weakly-Supervised Classification and Localization of Common Thorax Diseases*, Wang et a;. 2017



Source: *Deep learning for chest radiograph diagnosis: A retrospective comparison of the CheXNeXt algorithm to practicing radiologists,* Rajpurkar et al. 2018

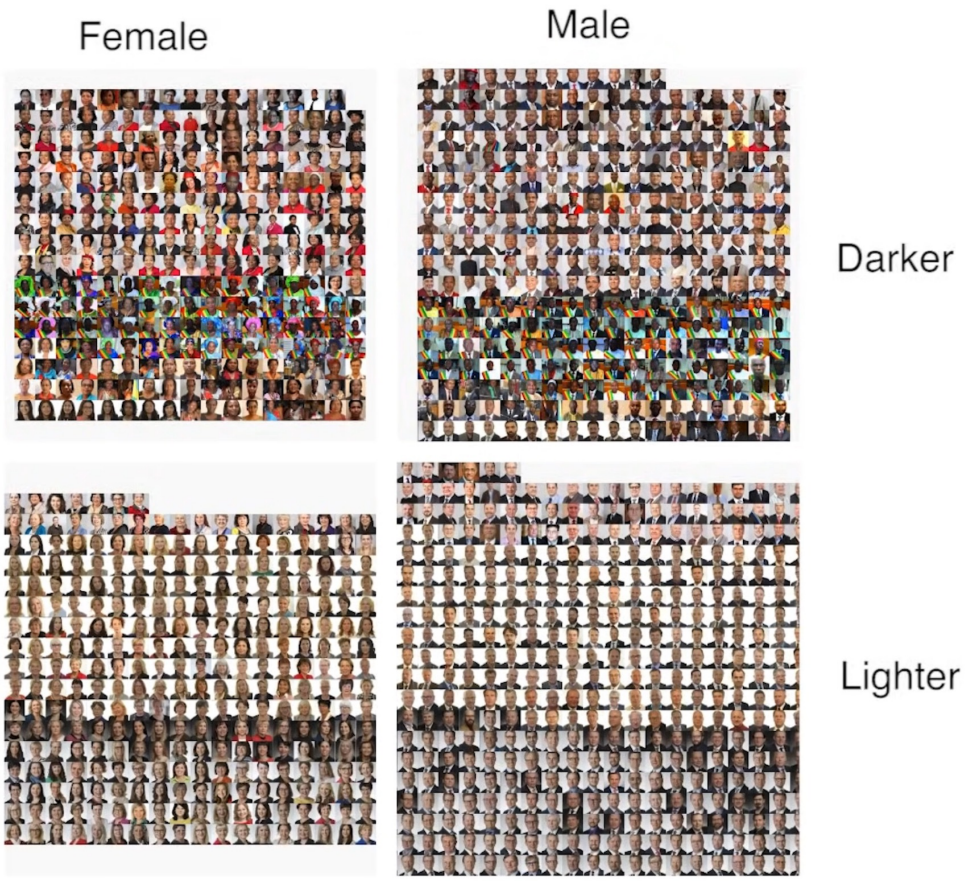
But the models may not generalize as well to data from new hospitals because they can learn to pickup on spurious correlations such as the type of scanner and marks used by technicians in specific hospitals!



CNN to predict hospital system detects both general and specific image features.
(A) We obtained activation heatmaps from our trained model and averaged over a sample of images to reveal which subregions tended to contribute to a hospital system classification decision. Many different subregions strongly predicted the correct hospital system, with especially strong contributions from image corners. (B-C) On individual images, which have been normalized to highlight only the most influential regions and not all those that contributed to a positive classification, we note that the CNN has learned to detect a metal token that radiology technicians place on the patient in the corner of the image field of view at the time they capture the image. When these strong features are correlated with disease prevalence, models can leverage them to indirectly predict disease.

Source: *Variable generalization performance of a deep learning model to detect pneumonia in chest radiographs: A cross-sectional study,* Zech et al. 2018

Earlier: Gendershades



http://gendershades.org/

Models are accurate on average, but not on all subgroups

	TYPE I	TYPE II	TYPE III	TYPE IV	TYPE V	TYPE VI
Microsoft	1.7%	1.1%	3.3%	0%	23.2%	25.0%
IBM	5.1%	7.4%	8.2%	8.3%	33.3%	**46.8%**
FACE++	11.9%	9.7%	8.2%	13.9%	32.4%	**46.5%**

Spurious correlations and shortcut learning

Consider the following task:

Waterbird

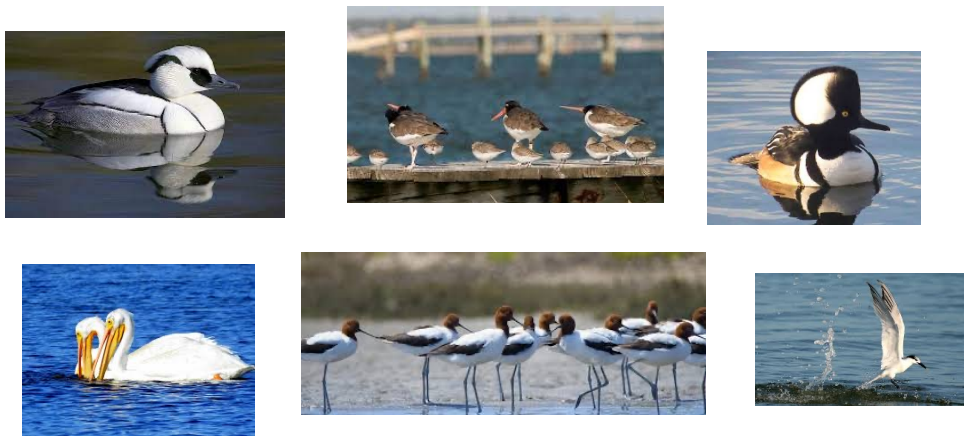
vs.

Landbird

Images courtesy of: University of Hawaii at Manoa, Greg Schechter (Flickr)

ML models can latch onto spurious features to make predictions

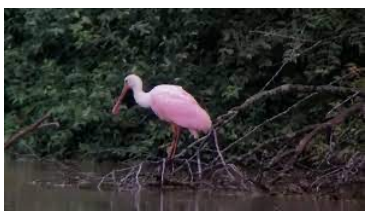
Most images of waterbirds are in water,
and landbirds are on land



Waterbirds vs. Landbirds

ML models can latch onto spurious features to make predictions

But this isn't always true!


Waterbirds

vs.



Landbirds

ML models can latch onto spurious features to make predictions

This is known as failure to distributional shifts

Waterbirds vs. Landbirds

Also see, *Recognition in Terra Incognita, Beery et al. '18*

Clever Hans

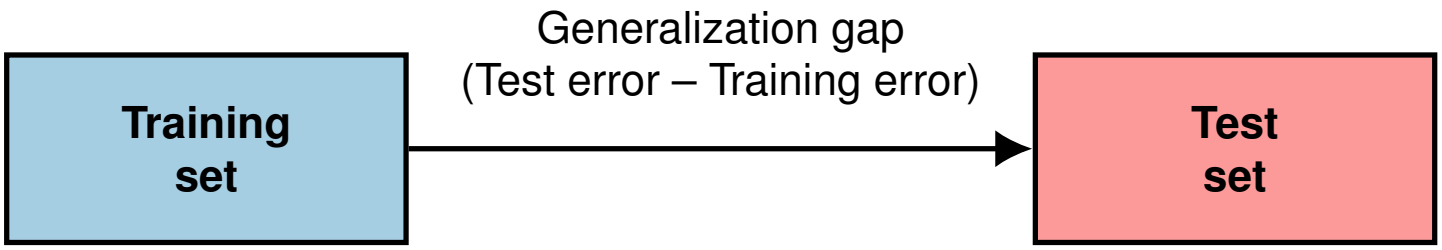
Distribution shifts: Setup

Recall that in supervised ML we care about expected loss (or the *risk*) under some distribution $\mathcal{D}$:

$$R(f) = \mathbb{E}_{(x,y)\sim\mathcal{D}}[\ \ell(f(x), y)\ ]$$

$$= \sum_{x',y'} \Pr_{\mathcal{D}}(x = x', y = y')\ \ell(f(x'), y').$$

We measure this with a test set.



What if we get training samples from $\mathcal{D}$, but test samples from $\mathcal{D}'$?

Distribution shifts: Setup

What if we get training samples from $\mathcal{D}$, but test samples from $\mathcal{D}'$?

$\mathcal{D}'$ can differ from $\mathcal{D}$ in two of these ways:

- Let $p(x)$ and $p'(x)$ be marginals of x under $\mathcal{D}$ and $\mathcal{D}'$. Then $p'(x)$ may be different from $p(x)$. This is known as a *covariate shift*, only the covariates x have changed.
- The conditional distribution $\Pr_{\mathcal{D}}[y|x]$ may be different from $\Pr_{\mathcal{D}'}[y|x]$. This is known as a *concept shift*. Here the ground-truth itself has changed.

Distributionally robust optimization for subgroup robustness

In usual supervised ML we care about finding some predictor f^* such that

$$f^* := \arg\min_{f \in \mathcal{F}} \Big\{ \mathbb{E}_{(x,y)\sim\mathcal{D}}[\, \ell(f(x), y)\,] \Big\}.$$

Suppose we have a set of groups $g \in \mathcal{G}$, each of which defines some distribution $\mathcal{D}_g$ (which could be a re-weighting of $\mathcal{D}$ with respect to the marginal of x). Then we can define the distributionally robust formulation of ML as:

$$f^*_{\text{DRO}} := \arg\min_{f \in \mathcal{F}} \Big\{ \max_{g \in \mathcal{G}} \mathbb{E}_{(x,y)\sim D_g}[\, \ell(f(x), y)\,] \Big\}.$$

Also see *Distributionally Robust Neural Networks for Group Shifts: On the Importance of Regularization for Worst-Case Generalization, Sagawa et al. '20*

Distributionally robust optimization for subgroup robustness

Distributionally robust optimization (DRO) empirical objective:

$$\hat{f}^*_{\text{DRO}} := \arg\min_{f \in \mathcal{F}} \left\{ \max_{g \in \mathcal{G}} \frac{1}{|\#\text{samples from group } g|} \sum_{(x,y) \in \text{ group } g} \ell(f(x), y) \right\}.$$

How to solve this optimization problem?

Worst-group generalization, and importance of regularization

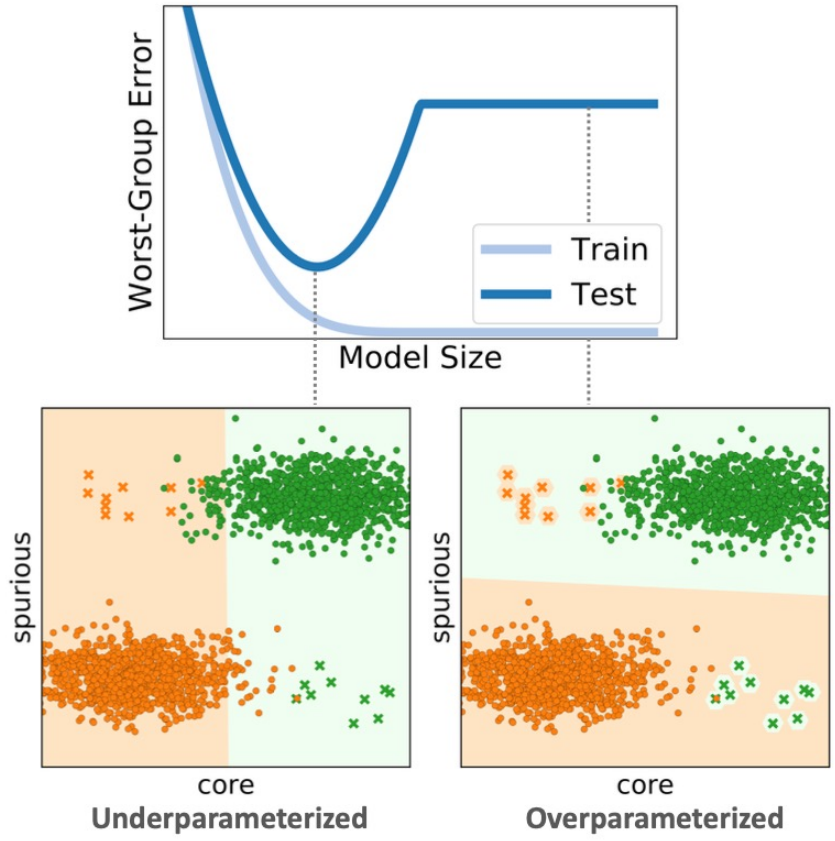


Fig from *An Investigation of Why Overparameterization Exacerbates Spurious Correlations, Sagawa et al. '20*