

Deep learning theory for computer vision

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- Many talented collaborators
 - ▶ Francesco Locatello, Chris Russell, Matthaeus Kleindessner, Puya Latafat, Andreas Loukas, Yu-Guan Hsieh

Today: “Basic” robust machine learning

$$\min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \Phi(\mathbf{x}, \mathbf{y})$$

- A seemingly simple optimization formulation
- Critical in machine learning with many applications
 - ▶ Adversarial examples and training
 - ▶ Generative adversarial networks
 - ▶ Robust reinforcement learning

Warm up: Flexibility of the template

$$\Phi^* = \min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \Phi(\mathbf{x}, \mathbf{y}) \quad (\text{argmin, argmax} \rightarrow \mathbf{x}^*, \mathbf{y}^*)$$

Warm up: Flexibility of the template

$$\Phi^* = \min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y}: \mathbf{y} \in \mathcal{Y}} \underbrace{\Phi(\mathbf{x}, \mathbf{y})}_{f(\mathbf{x})} \quad (\text{argmin, argmax} \rightarrow \mathbf{x}^*, \mathbf{y}^*)$$

$$f^* = \min_{\mathbf{x}: \mathbf{x} \in \mathcal{X}} f(\mathbf{x}) \quad (\text{argmin} \rightarrow \mathbf{x}^*)$$

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- (eula) In the sequel,
 - ▶ the set \mathcal{X} is convex
 - ▶ all convergence characterizations are with feasible iterates $\mathbf{x}^k \in \mathcal{X}$
 - ▶ L -smooth means $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\|, \forall \mathbf{x}, \mathbf{y} \in \mathcal{X}$
 - ▶ ∇ may refer to the generalized subdifferential

Warm up: Flexibility of the template

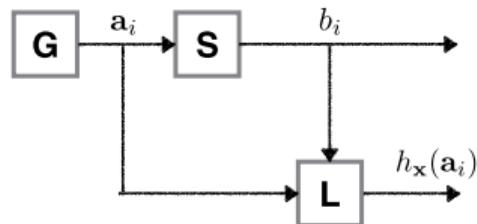
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A deep learning optimization problem in supervised learning



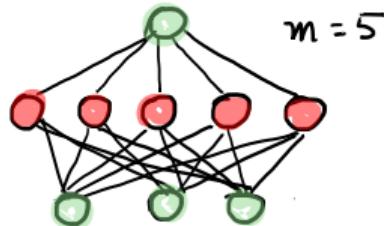
Definition (Optimization formulation)

The “deep-learning” problem with a neural network $h_{\mathbf{x}}(\mathbf{a})$ is given by

$$\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathcal{X}} \left\{ f(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^n L(h_{\mathbf{x}}(\mathbf{a}_i), b_i) \right\},$$

where \mathcal{X} denotes the constraints and L is a loss function.

- A single hidden layer neural network with params $\mathbf{x} := [\mathbf{X}_1, \mathbf{X}_2, \mu_1, \mu_2]$

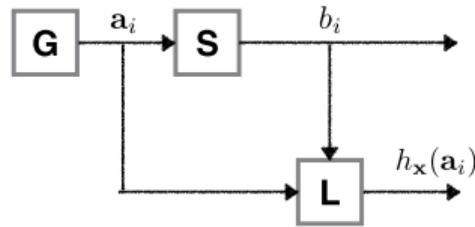


$$h_{\mathbf{x}}(\mathbf{a}) := \begin{bmatrix} \mathbf{X}_2 \end{bmatrix} \sigma \left(\begin{bmatrix} \mathbf{X}_1 \end{bmatrix} \begin{bmatrix} \mathbf{a} \end{bmatrix} + \begin{bmatrix} \mu_1 \end{bmatrix} \right) + \begin{bmatrix} \mu_2 \end{bmatrix}$$

activation \downarrow weight \downarrow input \downarrow bias \downarrow bias \downarrow
 σ $\begin{bmatrix} \mathbf{X}_1 \end{bmatrix}$ $\begin{bmatrix} \mathbf{a} \end{bmatrix}$ $\begin{bmatrix} \mu_1 \end{bmatrix}$ $\begin{bmatrix} \mu_2 \end{bmatrix}$

hidden layer = learned features

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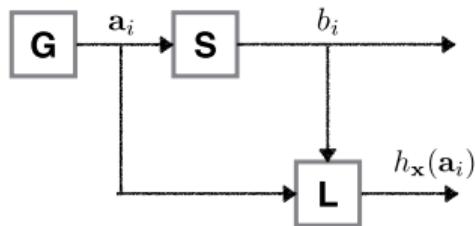
Adversarial Training

Let $h_{\mathbf{x}} : \mathbb{R}^n \rightarrow \mathbb{R}$ be a model with parameters \mathbf{x} and let $\{(\mathbf{a}_i, \mathbf{b}_i)\}_{i=1}^n$, with $\mathbf{a}_i \in \mathbb{R}^p$ and \mathbf{b}_i be the corresponding labels. The adversarial training optimization problem is given by

$$\min_{\mathbf{x}} \left\{ \frac{1}{n} \sum_{i=1}^n f_i(\mathbf{x}) := \frac{1}{n} \sum_{i=1}^n \underbrace{\left[\max_{\delta: \|\delta\| \leq \epsilon} L(h_{\mathbf{x}}(\mathbf{a}_i + \delta), \mathbf{b}_i) \right]}_{=: f_i(\mathbf{x})} \right\}.$$

Note that L is not continuously differentiable due to ReLU, max-pooling, etc.

A deep learning optimization problem in supervised learning



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Example objectives in different tasks

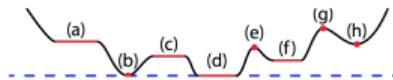
- ▶ $\min_{\mathbf{x}} \left\{ \frac{1}{n} \sum_{i=1}^n \left[\max_{\delta: \|\delta\|_\infty \leq \epsilon} L(h_{\mathbf{x}}(\mathbf{a}_i + \delta), b_i) \right] \right\}$ Adversarial training [44].
- ▶ $\min_{\mathbf{x}} \left\{ \frac{1}{n} \sum_{i=1}^n \left[\max_{\delta: \|\delta\|_2 \leq \epsilon} L(h_{\mathbf{x}+\delta}(\mathbf{a}_i), b_i) \right] \right\}$ ϵ -stability training [10], Sharpness-aware minimization [29].
- ▶ $\min_{\mathbf{x}} \max_{\mathbf{b}^c \in [C]} \frac{1}{n_c} \sum_{i=1}^{n_c} \left[\max_{\delta: \|\delta\| \leq \epsilon} L(h_{\mathbf{x}}(\mathbf{a}_i + \delta), b_i^c) \right]$ Class fairness [67].

Basic questions on solution concepts

- Consider the finite sum setting

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) := \frac{1}{n} \sum_{j=1}^n f_j(\mathbf{x}) \right\}.$$

- Goal:** Find \mathbf{x}^* such that $\nabla f(\mathbf{x}^*) = 0$.

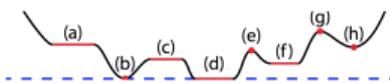


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- Does SGD converge with probability 1? [8, 71, 55, 61]
- Does SGD avoid non-minimum points with probability 1? [51, 31, 61]
- How fast does SGD converge to local minimizers? [31, 32, 61]
- Can SGD converge to global minimizers? [42, 45, 34, 89, 37, 64, 53, 25, 97, 47, 72]

Vanilla (Minibatch) SGD

Input: Stochastic gradient oracle \mathbf{g} , initial point \mathbf{x}^0 , step size α_k

- For $k = 0, 1, \dots$:
obtain the (minibatch) stochastic gradient \mathbf{g}^k
update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k - \gamma_k \mathbf{g}^k$

Perturbed Stochastic Gradient Descent [30]

Input: Stochastic gradient oracle \mathbf{g} , initial point \mathbf{x}^0 , step size α_k

- For $k = 0, 1, \dots$:
sample noise ξ uniformly from unit sphere
update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k - \alpha_k (\mathbf{g}^k + \xi)$

*Stochastic Gradient Langevin Dynamics [80]

Input: Stochastic gradient oracle \mathbf{g} , initial point \mathbf{x}^0 , step size α_k

- For $k = 0, 1, \dots$:
sample noise ξ standard Gaussian
update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k - \alpha_k \mathbf{g}^k + \sqrt{2\alpha_k} \xi$

Solving the outer problem: Gradient computation

Adversarial Training

Let $h_{\mathbf{x}} : \mathbb{R}^p \rightarrow \mathbb{R}$ be a model with parameters \mathbf{x} and let $\{(\mathbf{a}_i, \mathbf{b}_i)\}_{i=1}^n$, with $\mathbf{a}_i \in \mathbb{R}^p$ and \mathbf{b}_i be the corresponding labels. The adversarial training optimization problem is given by

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Note that L is not continuously differentiable due to ReLU, max-pooling, etc.

Question

How can we compute the following stochastic gradient (i.e., $\mathbb{E}_i \nabla_{\mathbf{x}} f_i(\mathbf{x}) = \nabla_{\mathbf{x}} f_i(\mathbf{x})$ for $i \sim \text{Uniform}\{1, \dots, n\}$):

$$\nabla_{\mathbf{x}} f_i(\mathbf{x}) := \nabla_{\mathbf{x}} \left(\max_{\delta: \|\delta\| \leq \epsilon} L(h_{\mathbf{x}}(\mathbf{a}_i + \delta), \mathbf{b}_i) \right)?$$

- **Challenge:** It involves differentiating with respect to a maximization.

Danskin's Theorem (1966): How do we compute the gradient?

Theorem ([21])

Let \mathcal{S} be compact set, $\Phi : \mathbb{R}^p \times \mathcal{S}$ be continuous such that $\Phi(\cdot, \mathbf{y})$ is differentiable for all $\mathbf{y} \in \mathcal{S}$, and $\nabla_{\mathbf{x}}\Phi(\mathbf{x}, \mathbf{y})$ be continuous on $\mathbb{R}^p \times \mathcal{S}$. Define

$$f(\mathbf{x}) := \max_{\mathbf{y} \in \mathcal{S}} \Phi(\mathbf{x}, \mathbf{y}), \quad \mathcal{S}^*(\mathbf{x}) := \arg \max_{\mathbf{y} \in \mathcal{S}} \Phi(\mathbf{x}, \mathbf{y}).$$

Let $\gamma \in \mathbb{R}^p$, and $\|\gamma\|_2 = 1$. The directional derivative $D_\gamma f(\bar{\mathbf{x}})$ of f in the direction γ at $\bar{\mathbf{x}}$ is given by

$$D_\gamma f(\bar{\mathbf{x}}) = \max_{\mathbf{y} \in \mathcal{S}^*(\bar{\mathbf{x}})} \langle \gamma, \nabla_{\mathbf{x}}\Phi(\bar{\mathbf{x}}, \mathbf{y}) \rangle.$$

An immediate consequence

If $\delta^* \in \arg \max_{\delta: \|\delta\| \leq \epsilon} L(h_{\mathbf{x}}(\mathbf{a}_i + \delta), \mathbf{b}_i)$ is unique, then we have

$$\nabla_{\mathbf{x}} f_i(\mathbf{x}) = \nabla_{\mathbf{x}} L(h_{\mathbf{x}}(\mathbf{a}_i + \delta^*), \mathbf{b}_i).$$

Optimized perturbations are typically not unique!

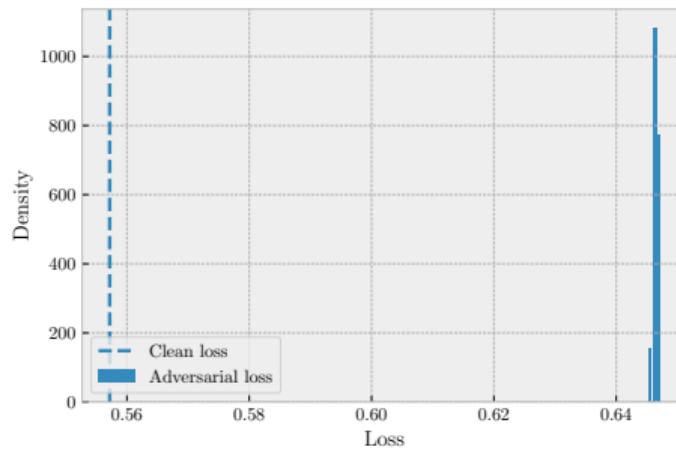
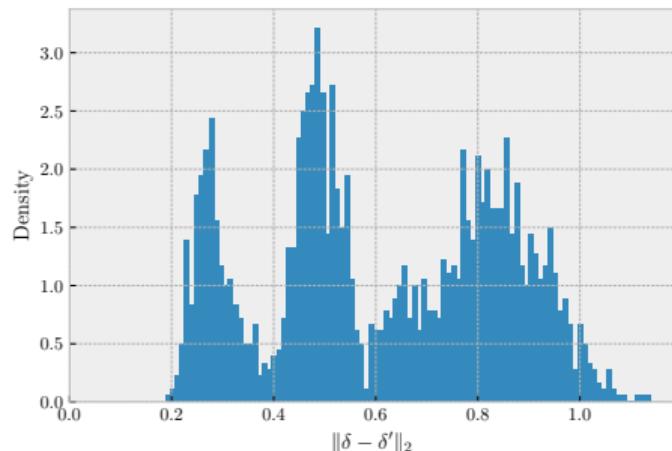


Figure: (left) Pairwise ℓ_2 -distances between “optimized” perturbations with different initializations are bounded away from zero. (right) The losses of multiple perturbations on the same sample concentrate around a value much larger than the clean loss.

Theoretical foundations

$\nabla_{\mathbf{x}} \Phi(\mathbf{x}, \delta^*)$	unique δ^*	non-unique δ^*
$\nabla_{\mathbf{x}} f(\mathbf{x})$		descent direction [58]

Published as a conference paper at ICLR 2018

TOWARDS DEEP LEARNING MODELS RESISTANT TO ADVERSARIAL ATTACKS

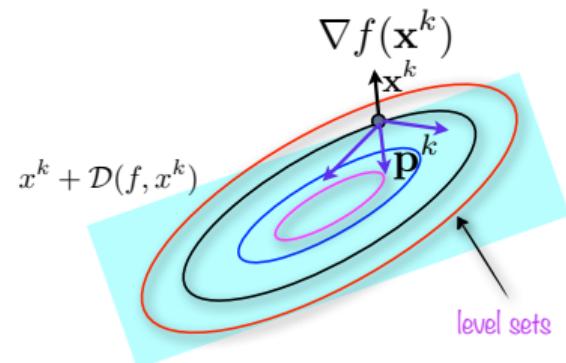
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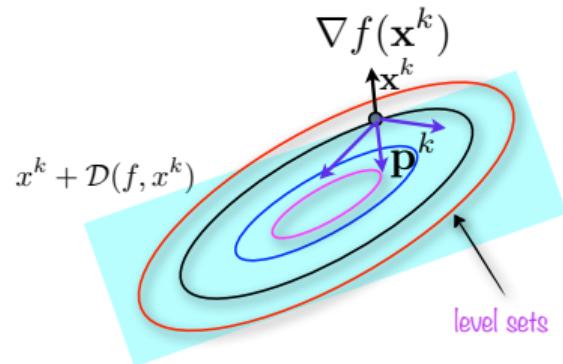
Theoretical foundations ?

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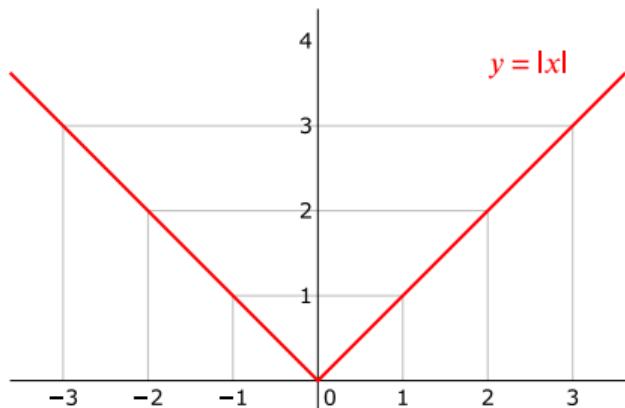
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A counterexample

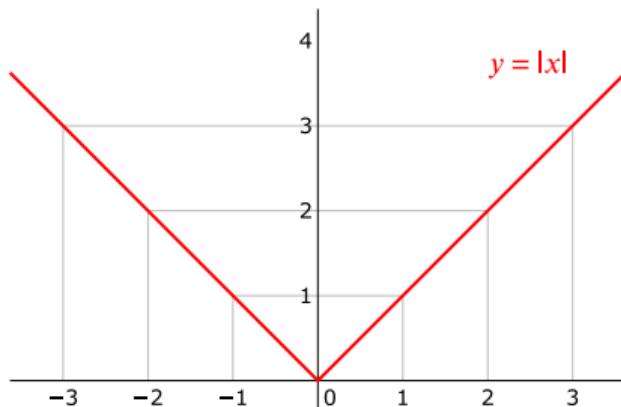
$$f(\mathbf{x}) := \max_{\delta \in [-1, 1]} \mathbf{x}\delta = |\mathbf{x}|.$$



- We have $\mathcal{S} := [-1, 1]$ and $\Phi(\mathbf{x}, \delta) = \mathbf{x}\delta$.
- At $\mathbf{x} = 0$, we have $\mathcal{S}^*(0) = [-1, 1]$.
- We can choose $\delta = 1 \in \mathcal{S}^*(0)$: $\Phi(\mathbf{x}, 1) = \mathbf{x}$.

A counterexample

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- We can choose $\delta = 1 \in \mathcal{S}^*(0)$: $\Phi(\mathbf{x}, 1) = \mathbf{x}$.
 - ▶ $-\nabla_{\mathbf{x}}\Phi(0, 1) = -1 \neq 0$.
 - ▶ Is -1 a descent direction at $\mathbf{x} = 0$?

Our understanding [Latorre, Krawczuk, Dadi, Pethick, Cevher, ICLR (2023)]

- The corollary in [58] is false (it is subtle!).
- We constructed a counter example & proposed an alternative way (DDi) of computing “the gradient”:

unique δ^*	non-unique δ^*
$\nabla_{\mathbf{x}} \Phi(\mathbf{x}, \delta^*)$	$\nabla_{\mathbf{x}} f(\mathbf{x})$ could be ascent direction!

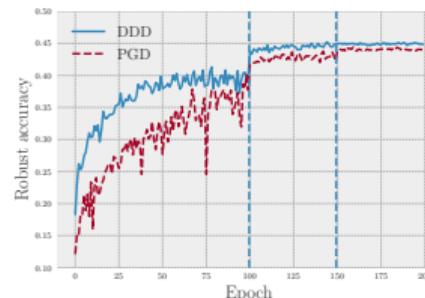
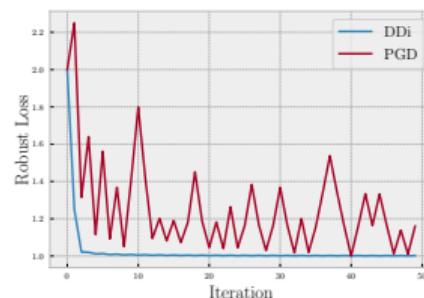
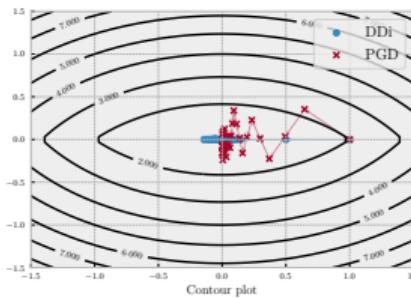


Figure: Left and middle pane: comparison DDi and PGD ([58]) on a synthetic problem. Right pane: DDi vs PGD on CIFAR10.

Comparison with the state-of-the-art

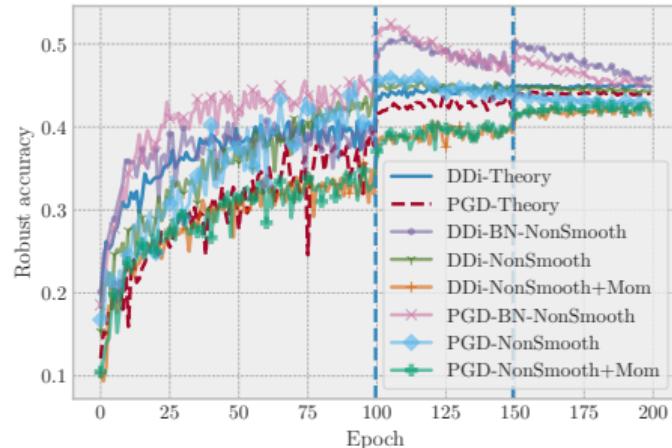
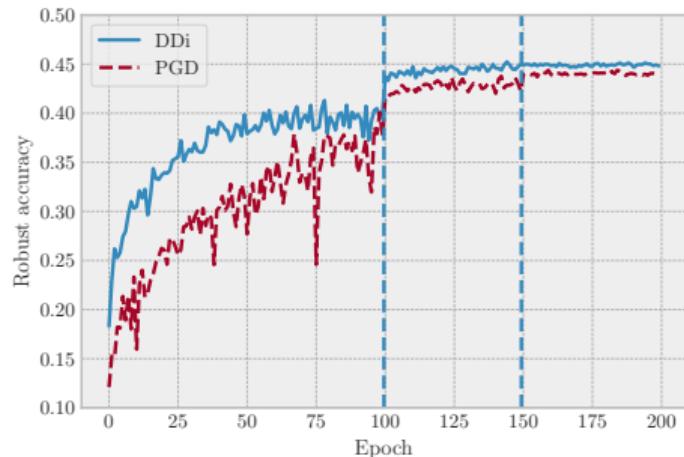


Figure: (left) PGD vs DDi on CIFAR10, in a setting covered by theory. (right) An ablation testing the effect of adding back the elements not covered by theory (BN,ReLU,momentum).

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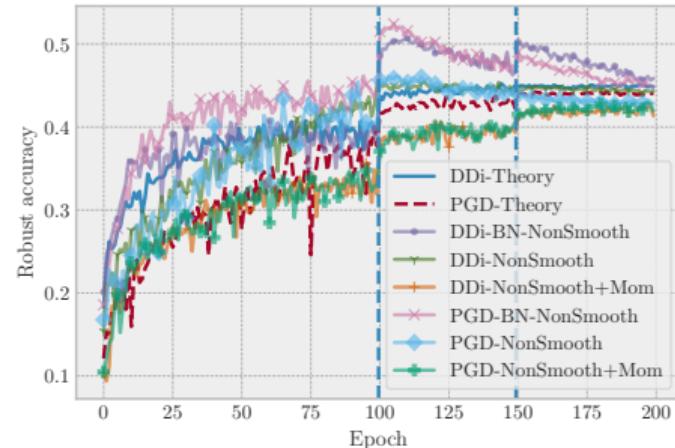
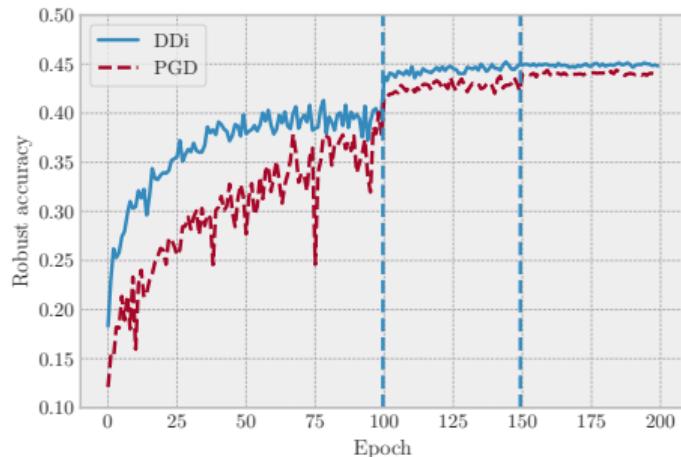
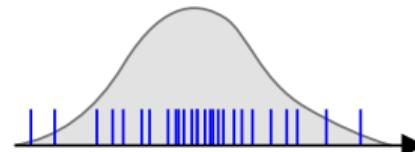


Figure: (left) PGD vs DDi on CIFAR10, in a setting covered by theory. (right) An ablation testing the effect of adding back the elements not covered by theory (BN,ReLU,momentum).

DDi + Graduate Student Descent may improve things (performance or catastrophic overfitting)?

Learning without concentration

- We can minimize $W_1(\hat{\mu}_n, h_{\mathbf{x}} \# p_{\Omega})$ with respect to \mathbf{x} .
- Figure: Empirical distribution (blue), $\hat{\mu}_n = \sum_{i=1}^n \delta_i$



A plug-in empirical estimator

Using the triangle inequality for Wasserstein distances we can upper bound in the follow way,

$$W_1(\mu^\natural, h_{\mathbf{x}} \# p_{\Omega}) \leq W_1(\mu^\natural, \hat{\mu}_n) + W_1(\hat{\mu}_n, h_{\mathbf{x}} \# p_{\Omega}), \quad (1)$$

where $\hat{\mu}_n$ is the empirical estimator of μ^\natural obtained from n independent samples from μ^\natural .

Theorem (Slow convergence of empirical measures in 1-Wasserstein [79, 26])

Let μ^\natural be a measure defined on \mathbb{R}^p and let $\hat{\mu}_n$ be its empirical measure. Then the $\hat{\mu}_n$ converges, in the worst case, at the following rate,

$$W_1(\mu^\natural, \hat{\mu}_n) \gtrsim n^{-1/p}. \quad (2)$$

Remarks:

- Using an empirical estimator in high-dimensions is terrible in the worst case.
- However, it does not directly say that $W_1(\mu^\natural, h_{\mathbf{x}} \# p_{\Omega})$ will be large.
- So we can still proceed and hope our parameterization interpolates harmlessly.

Duality of 1-Wasserstein

- How do we get a sub-gradient of $W_1(\hat{\mu}_n, h_{\mathbf{x}} \# \rho_\Omega)$ with respect to \mathbf{x} ?

Theorem (Kantorovich-Rubinstein duality)

$$W_1(\mu, \nu) = \sup_{\mathbf{d}} \{ \langle \mathbf{d}, \mu \rangle - \langle \mathbf{d}, \nu \rangle : \mathbf{d} \text{ is 1-Lipschitz} \} \quad (3)$$

Remark: \mathbf{d} is the “dual” variable. In the literature, it is commonly referred to as the “discriminator.”

Inner product is an expectation

$$\langle \mathbf{d}, \mu \rangle = \int \mathbf{d} d\mu = \int \mathbf{d}(\mathbf{a}) d\mu(\mathbf{a}) = E_{\mathbf{a} \sim \mu} [\mathbf{d}(\mathbf{a})]. \quad (4)$$

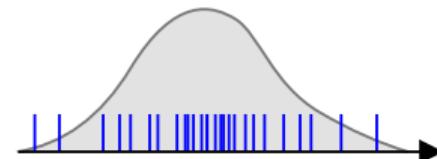
Kantorovich-Rubinstein duality applied to our objective

$$W_1(\hat{\mu}_n, h_{\mathbf{x}} \# \omega) = \sup \left\{ E_{\mathbf{a} \sim \hat{\mu}_n} [\mathbf{d}(\mathbf{a})] - E_{\mathbf{a} \sim h_{\mathbf{x}} \# \omega} [\mathbf{d}(\mathbf{a})] : \mathbf{d} \text{ is 1-Lipschitz} \right\} \quad (5)$$

Another minimax example: Generative adversarial networks (GANs)

- Ingredients:

- ▶ fixed *noise* distribution p_{Ω} (e.g., normal)
- ▶ target distribution $\hat{\mu}_n$ (natural images)
- ▶ \mathcal{X} parameter class inducing a class of functions (generators)
- ▶ \mathcal{Y} parameter class inducing a class of functions (dual variables)



Wasserstein GANs formulation [3]

Define a parameterized function $d_y(a)$, where $y \in \mathcal{Y}$ such that $d_y(a)$ is 1-Lipschitz. In this case, the Wasserstein GAN training problem is given by

$$\min_{x \in \mathcal{X}} \left(\max_{y \in \mathcal{Y}} E_{a \sim \hat{\mu}_n} [d_y(a)] - E_{\omega \sim p_{\Omega}} [d_y(h_x(\omega))] \right). \quad (6)$$

This problem is already captured by the template $\min_{x \in \mathcal{X}} \max_{y \in \mathcal{Y}} \Phi(x, y)$. Note that the original problem is a direct non-smooth minimization problem and the Rubinstein-Kantarovic duality results in the minimax template.

Remarks:

- Cannot solve in a manner similar to adversarial training a la Danksin. Need a direct approach.
- Scalability, mode collapse, catastrophic forgetting. Heuristics galore!
- Enforce Lipschitz constraint weight clipping, gradient penalty, spectral normalization [3, 36, 62].

Abstract minmax formulation

Minimax formulation

$$\min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \Phi(\mathbf{x}, \mathbf{y}), \quad (7)$$

where

- ▶ Φ is differentiable and nonconvex in \mathbf{x} and nonconcave in \mathbf{y} ,
- ▶ The domain is unconstrained, specifically $\mathcal{X} = \mathbb{R}^m$ and $\mathcal{Y} = \mathbb{R}^n$.

○ Key questions:

1. Where do the algorithms converge?
2. When do the algorithm converge?

Solving the minimax problem: Solution concepts

- Consider the unconstrained setting:

$$\Phi^* = \min_{\mathbf{x}} \max_{\mathbf{y}} \Phi(\mathbf{x}, \mathbf{y})$$

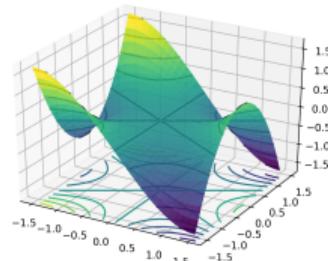


Figure: The monkey saddle
 $\Phi(x, y) = x^3 - 3xy^2$.

- Goal: Find an LNE point $(\mathbf{x}^*, \mathbf{y}^*)$.

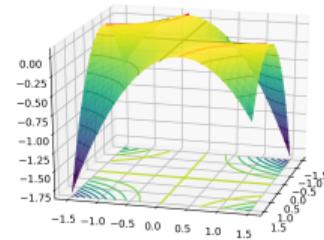


Figure: The weird saddle
 $\Phi(x, y) = -x^2y^2 + xy$.

Definition (Local Nash Equilibrium)

A pure strategy $(\mathbf{x}^*, \mathbf{y}^*)$ is called a local Nash equilibrium if

$$\Phi(\mathbf{x}^*, \mathbf{y}) \leq \Phi(\mathbf{x}^*, \mathbf{y}^*) \leq \Phi(\mathbf{x}, \mathbf{y}^*) \quad (\text{LNE})$$

for all \mathbf{x} and \mathbf{y} within some neighborhood of \mathbf{x}^* and \mathbf{y}^* , i.e., $\|\mathbf{x} - \mathbf{x}^*\| \leq \varepsilon$ and $\|\mathbf{y} - \mathbf{y}^*\| \leq \varepsilon$ for some $\varepsilon > 0$.

Necessary conditions

Through a Taylor expansion around \mathbf{x}^* and \mathbf{y}^* one can show that a LNE implies

$$\nabla_{\mathbf{x}}\Phi(\mathbf{x}, \mathbf{y}), -\nabla_{\mathbf{y}}\Phi(\mathbf{x}, \mathbf{y}) = 0;$$

$$\nabla_{\mathbf{xx}}\Phi(\mathbf{x}, \mathbf{y}), -\nabla_{\mathbf{yy}}\Phi(\mathbf{x}, \mathbf{y}) \succeq 0.$$

Abstract minmax formulation

Minimax formulation

$$\min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \Phi(\mathbf{x}, \mathbf{y}), \quad (8)$$

where

- ▶ Φ is differentiable and nonconvex in \mathbf{x} and nonconcave in \mathbf{y} ,
- ▶ The domain is unconstrained, specifically $\mathcal{X} = \mathbb{R}^m$ and $\mathcal{Y} = \mathbb{R}^n$.

○ Key questions:

1. Where do the algorithms converge?
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A buffet of negative results [22]

"Even when the objective is a Lipschitz and smooth differentiable function, deciding whether a min-max point exists, in fact even deciding whether an approximate min-max point exists, is NP-hard. More importantly, an approximate local min-max point of large enough approximation is guaranteed to exist, but finding one such point is PPAD-complete. The same is true of computing an approximate fixed point of the (Projected) Gradient Descent/Ascent update dynamics."

Basic algorithms for minimax

- Given $\min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \Phi(\mathbf{x}, \mathbf{y})$, define $V(\mathbf{z}) = [\nabla_{\mathbf{x}} \Phi(\mathbf{x}, \mathbf{y}), -\nabla_{\mathbf{y}} \Phi(\mathbf{x}, \mathbf{y})]$ with $\mathbf{z} = [\mathbf{x}, \mathbf{y}]$.

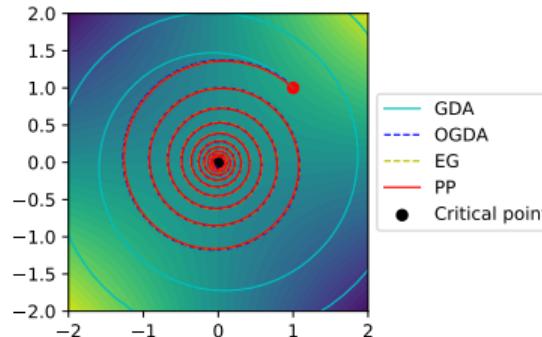


Figure: Trajectory of different algorithms for a simple bilinear game $\min_x \max_y xy$.

- (In)Famous algorithms
 - Gradient Descent Ascent (GDA)
 - Proximal point method (PPM)
 - Extra-gradient (EG)
 - Optimistic GDA (OGDA)
 - Reflected-Forward-Backward-Splitting (RFBS)
- EG and OGDA are approximations of the PPM
 - [69, 35] ► $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha V(\mathbf{z}^k)$.
 - [48] ► $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha V(\mathbf{z}^{k+1})$.
 - [94, 59] ► $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha V(\mathbf{z}^k - \alpha V(\mathbf{z}^{k-1}))$.
 - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha [2V(\mathbf{z}^k) - V(\mathbf{z}^{k-1})]$.
 - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha V(2\mathbf{z}^k - \mathbf{z}^{k-1})$.

Where do the algorithms converge?

- Recall: Given $\min_{\mathbf{x} \in \mathcal{X}} \max_{\mathbf{y} \in \mathcal{Y}} \Phi(\mathbf{x}, \mathbf{y})$, define $V(\mathbf{z}) = [\nabla_{\mathbf{x}} \Phi(\mathbf{x}, \mathbf{y}), -\nabla_{\mathbf{y}} \Phi(\mathbf{x}, \mathbf{y})]$ with $\mathbf{z} = [\mathbf{x}, \mathbf{y}]$.
- Given $V(\mathbf{z})$, define stochastic estimates of $V(\mathbf{z}, \zeta) = V(\mathbf{z}) + U(\mathbf{z}, \zeta)$, where
 - ▶ $U(\mathbf{z}, \zeta)$ is a bias term,
 - ▶ We often have unbiasedness: $EU(\mathbf{z}, \zeta) = 0$,
 - ▶ The bias term can have bounded moments,
 - ▶ We often have bounded variance: $P(\|U(\mathbf{z}, \zeta)\| \geq t) \leq 2 \exp -\frac{t^2}{2\sigma^2}$ for $\sigma > 0$.
- An abstract template for generalized Robbins-Monro schemes, dubbed as \mathcal{A} :

$$\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha_k V(\mathbf{z}^k, \zeta^k).$$

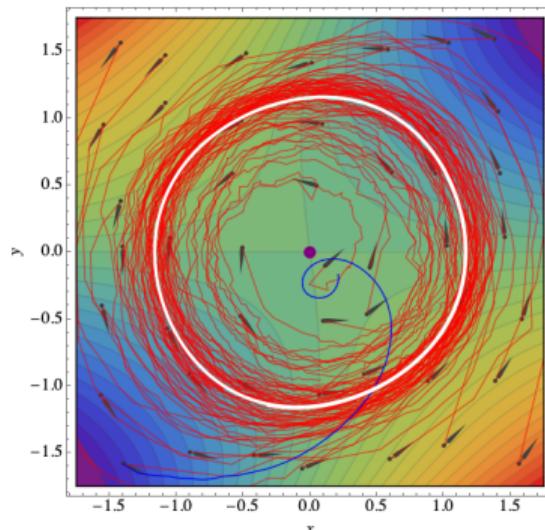
The dessert section in the buffet of negative results: [41]

1. Bounded trajectories of \mathcal{A} always converge to an internally chain-transitive (ICT) set.
2. Trajectories of \mathcal{A} may converge with arbitrarily high probability to spurious attractors that contain no critical point of Φ .

Minimax is more difficult than just optimization [41]

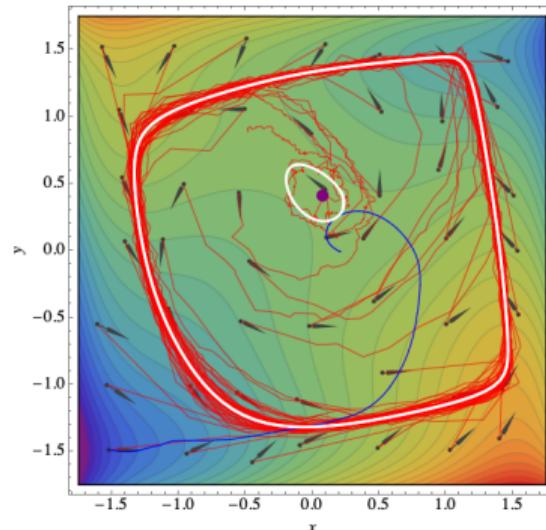
- Internally chain-transitive (ICT) sets characterize the convergence of dynamical systems [9].
 - ▶ For optimization, {attracting ICT} \equiv {solutions}
 - ▶ For minimax, {attracting ICT} \equiv {solutions} \cup {spurious sets}
- “Almost” bilinear \neq bilinear:

$$\Phi(x, y) = xy + \epsilon\phi(x), \phi(x) = \frac{1}{2}x^2 - \frac{1}{4}x^4$$



- The “forsaken” solutions:

$$\Phi(y, x) = y(x-0.5) + \phi(y) - \phi(x), \phi(u) = \frac{1}{4}u^2 - \frac{1}{2}u^4 + \frac{1}{6}u^6$$

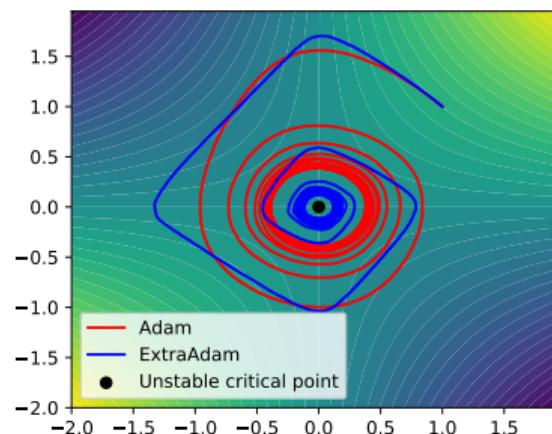


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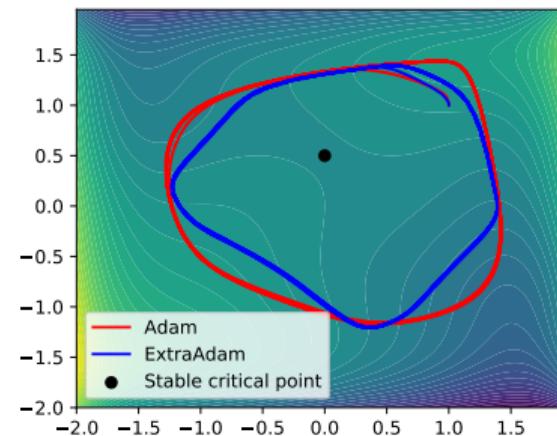
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When do the algorithms converge?

Assumption (weak Minty variational inequality)

For some $\rho \in \mathbb{R}$, weak MVI implies

$$\langle V(\mathbf{z}), \mathbf{z} - \mathbf{z}^* \rangle \geq \rho \|V(\mathbf{z})\|^2, \quad \text{for all } \mathbf{z} \in \mathbb{R}^n. \quad (9)$$

- A variant EG+ converges when $\rho > -\frac{1}{8L}$
 - ▶ Diakonikolas, Daskalakis, Jordan, AISTATS 2021.
- It still cannot handle the examples of [41].

- Complete picture under weak MVI (ICLR'22 and '23)
 - ▶ Pethick, Lalafat, Patrinos, Fercoq, and Cevher.
 - ▶ constrained and regularized settings with $\rho > -\frac{1}{2L}$
 - ▶ matching lower bounds
 - ▶ stochastic variants handling the examples of [41]
 - ▶ adaptive variants handling the examples of [41]

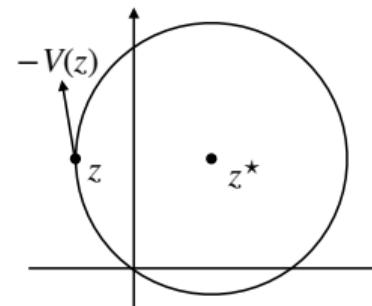
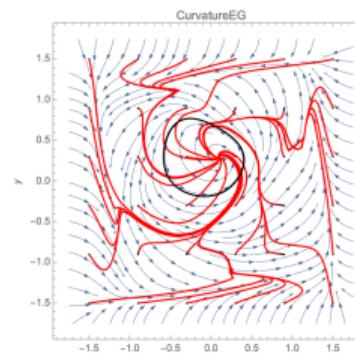


Figure: The operator $V(z)$ is allowed to point away from the solution by some amount when ρ is negative.



GANs with SEG+ [68]

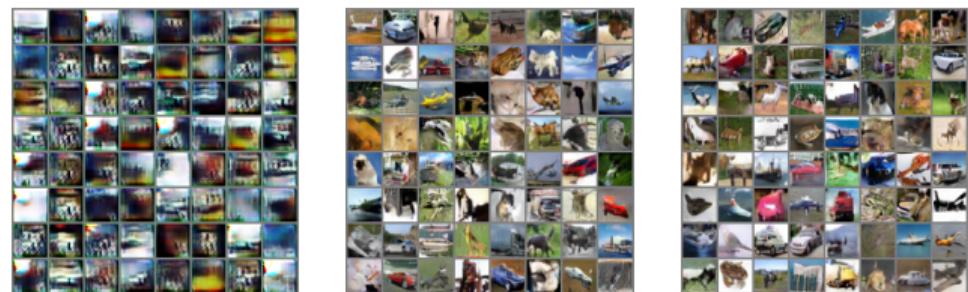
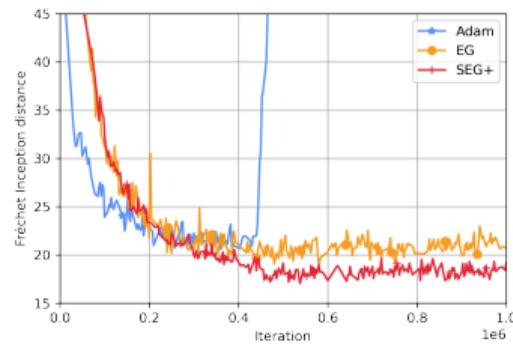


Figure: A performance comparison of GAN training by Adam, EG with stochastic gradients, and SEG+.

Robustness of the worst-performing class [67]

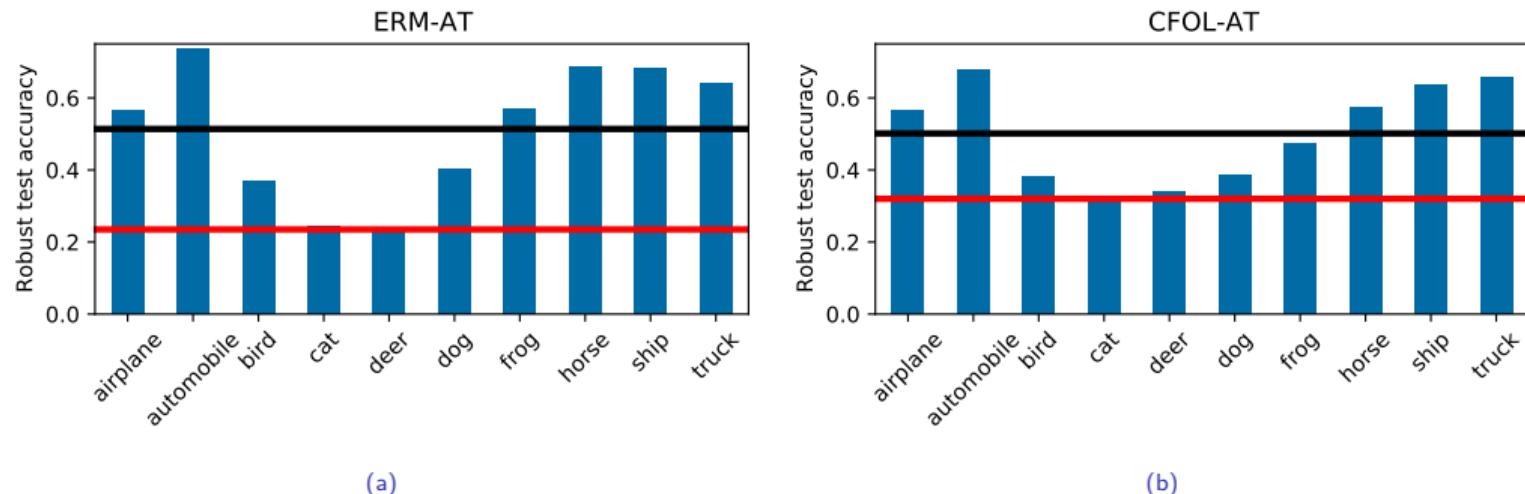


Figure: Robust test accuracy of (a) Empirical Risk Minimization and (b) the class focused online learning.

Code: <https://github.com/LIONS-EPFL/class-focused-online-learning-code>

Out of the frying pan into the fire



Original Formulation of Adversarial Training (I)

$$\min_{\mathbf{x}} \mathbb{E} \left[\max_{\delta: \|\delta\| \leq \epsilon} L(\mathbf{x}, \mathbf{a} + \delta, \mathbf{b}) \right]$$

Original Formulation of Adversarial Training (I)

$$\min_{\mathbf{x}} \mathbb{E} \left[\max_{\delta: \|\delta\| \leq \epsilon} L(\mathbf{x}, \mathbf{a} + \delta, \mathbf{b}) \right]$$

which loss L ?

Original Formulation of Adversarial Training (II)

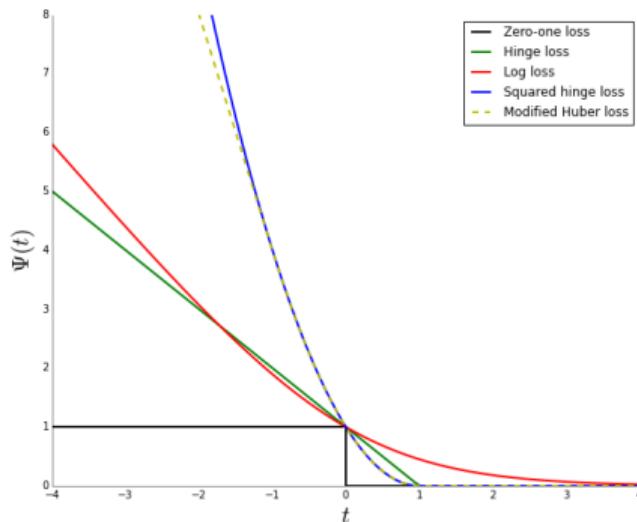
$$\min_{\mathbf{x}} \mathbb{E} \left[\max_{\delta: \|\delta\| \leq \epsilon} L_{01}(\mathbf{x}, \mathbf{a} + \delta, \mathbf{b}) \right]$$

Original Formulation of Adversarial Training (II)

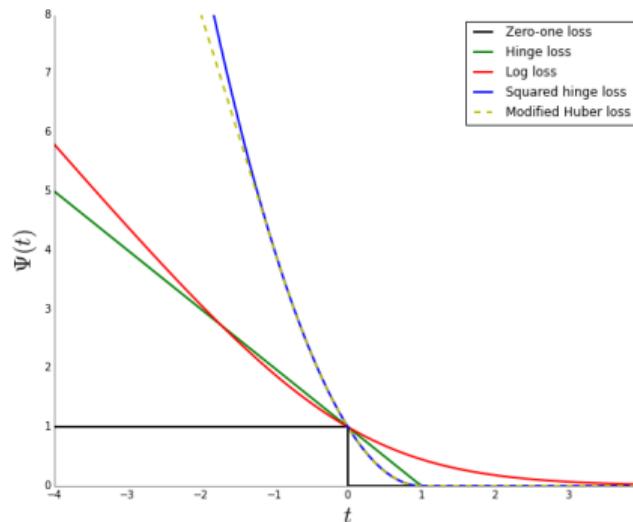
$$\min_{\mathbf{x}} \mathbb{E} \left[\max_{\delta: \|\delta\| \leq \epsilon} L_{01}(\mathbf{x}, \mathbf{a} + \boldsymbol{\delta}, \mathbf{b}) \right]$$

$$\min_{\mathbf{x}} \mathbb{E} \left[\max_{\delta: \|\delta\| \leq \epsilon} L_{CE}(\mathbf{x}, \mathbf{a} + \boldsymbol{\delta}, \mathbf{b}) \right]$$

Surrogate-based optimization for Risk Minimization



Surrogate-based optimization for Risk Minimization

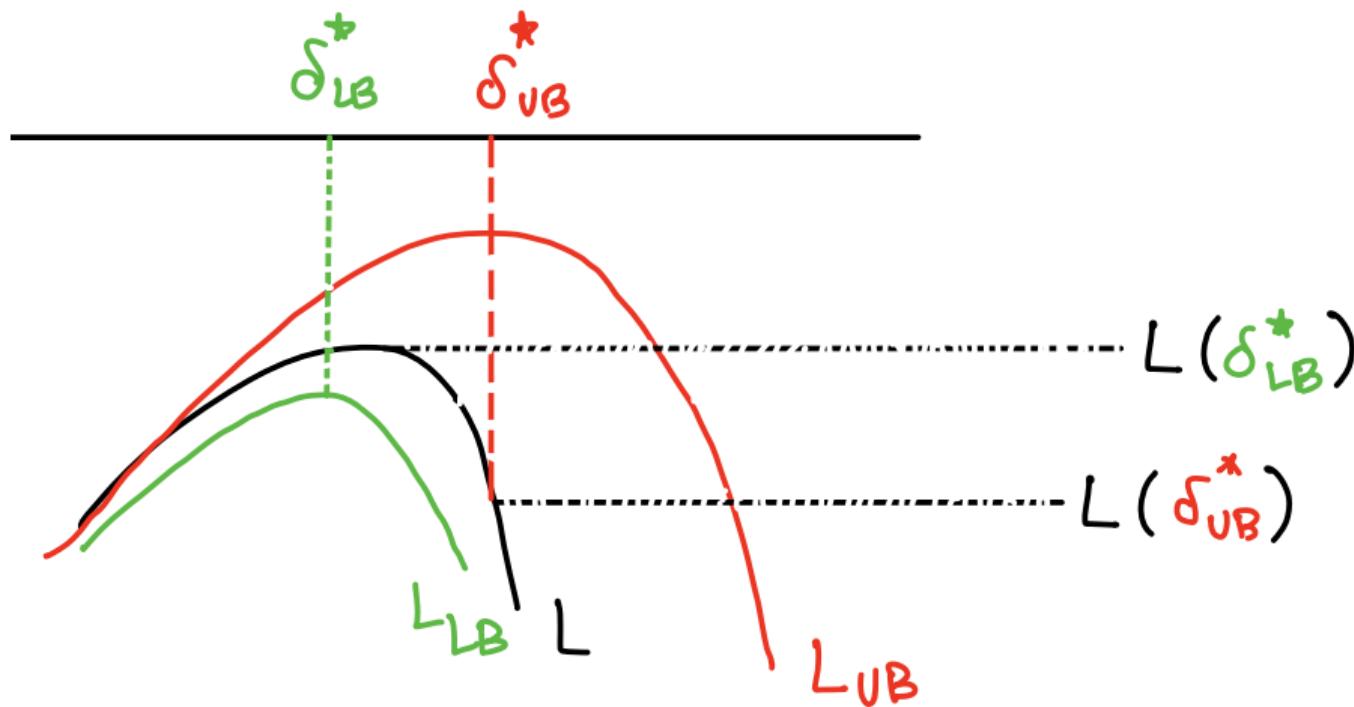


$$\mathbb{E} [L_{01}(\mathbf{x}^*, \mathbf{a}, \mathbf{b})] \leq \min_{\mathbf{x}} \mathbb{E} [L_{CE}(\mathbf{x}, \mathbf{a}, \mathbf{b})]$$

Adversary maximizes an upper bound (I)

$$L_{01}(\mathbf{x}, \mathbf{a} + \boldsymbol{\delta}^*, \mathbf{b}) \leq \max_{\boldsymbol{\delta}: \|\boldsymbol{\delta}\| \leq \epsilon} L_{CE}(\mathbf{x}, \mathbf{a} + \boldsymbol{\delta}, \mathbf{b})$$

Adversary maximizes an upper bound (II)



Why maximizing Cross-Entropy leads to weak adversaries

Suppose $\mathbf{b}_1 = 1$, $c = 4$:

$$h_{\mathbf{x}}(\mathbf{a} + \boldsymbol{\delta}_A) = (0.26, 0.24, 0.25, 0.25)$$

$$h_{\mathbf{x}}(\mathbf{a} + \boldsymbol{\delta}_B) = (0.49, 0.51, 0, 0)$$

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$$h_{\mathbf{x}}(\mathbf{a} + \boldsymbol{\delta}_B) = (0.49, 0.51, 0, 0)$$

$$L_{\text{CE}}(\mathbf{x}, \mathbf{a} + \boldsymbol{\delta}_A, \mathbf{b}) = 1.38$$

$$L_{\text{CE}}(\mathbf{x}, \mathbf{a} + \boldsymbol{\delta}_B, \mathbf{b}) = 1.18$$

Adversary's problem can be “solved” without using surrogates

Theorem (Reformulation of the Adversary's problem)

$$\boldsymbol{\delta}^* \in \arg \max_{\boldsymbol{\delta}: \|\boldsymbol{\delta}\| \leq \epsilon} \max_{j \neq b} h_{\mathbf{x}}(\mathbf{a} + \boldsymbol{\delta})_j - h_{\mathbf{x}}(\mathbf{a} + \boldsymbol{\delta})_b \Rightarrow$$

$$\boldsymbol{\delta}^* \in \arg \max_{\boldsymbol{\delta}: \|\boldsymbol{\delta}\| \leq \epsilon} L_{01}(\mathbf{x}, \mathbf{a} + \boldsymbol{\delta}, \mathbf{b})$$

$$\min_{\mathbf{x} \in \mathbf{X}} \frac{1}{n} \sum_{i=1}^n L_{\text{CE}}(\mathbf{x}, \mathbf{a}_i + \boldsymbol{\delta}_{i,j^\star}^\star, \mathbf{b}_i)$$

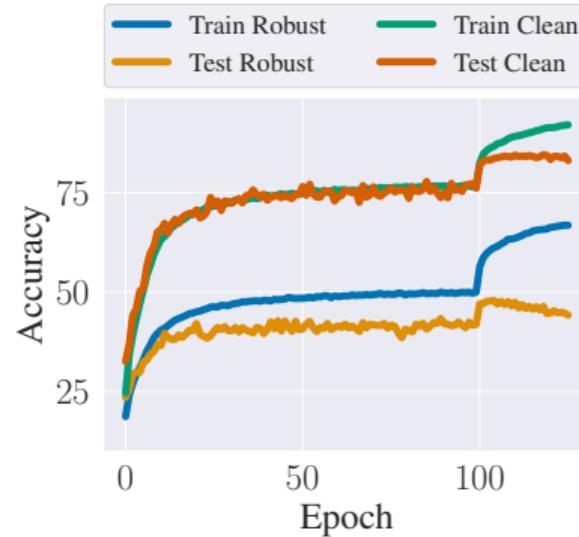
such that $\boldsymbol{\delta}_{i,j}^\star \in \arg \max_{\boldsymbol{\delta}: \|\boldsymbol{\delta}\| \leq \epsilon} h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\delta})_j - h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\delta})_{\mathbf{b}_i}$

$j^\star \in \arg \max_{j \in [K] - \{\mathbf{b}_i\}} h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\delta}_{i,j^\star})_j - h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\delta}_{i,j^\star})_{\mathbf{b}_i}$

¹<https://infoscience.epfl.ch/record/302995> or <https://tinyurl.com/33yup77v>

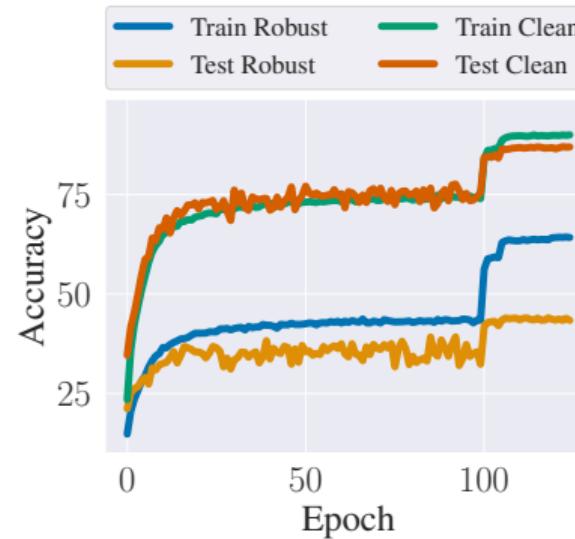
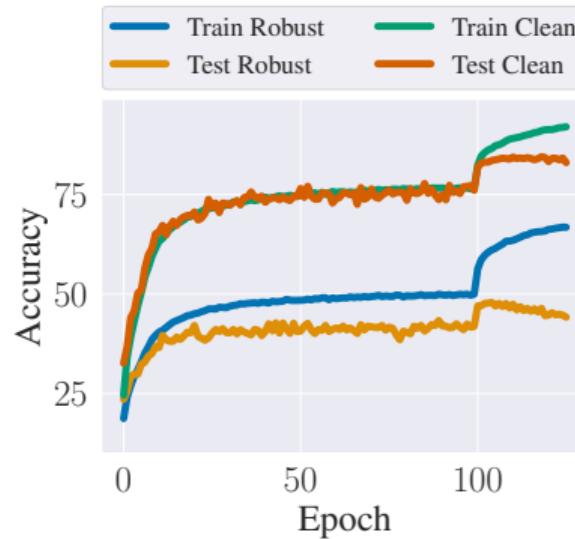
Practical Consequences of the Bilevel Formulation (I)

Figure: Learning curves of PGD¹⁰-AT (Left) and BETA¹⁰-AT



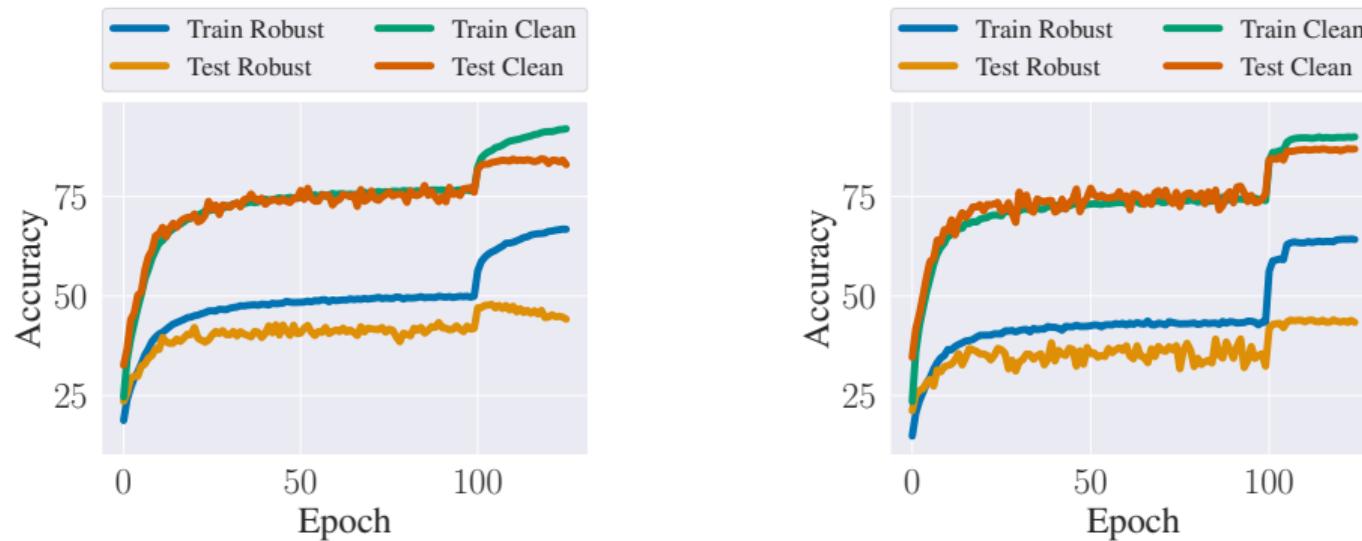
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Practical Consequences of the Bilevel Formulation (I)

Figure: Learning curves of PGD¹⁰-AT (Left) and BETA¹⁰-AT (Right). Robust accuracy estimated with PGD²⁰



No Robust Overfitting occurs!

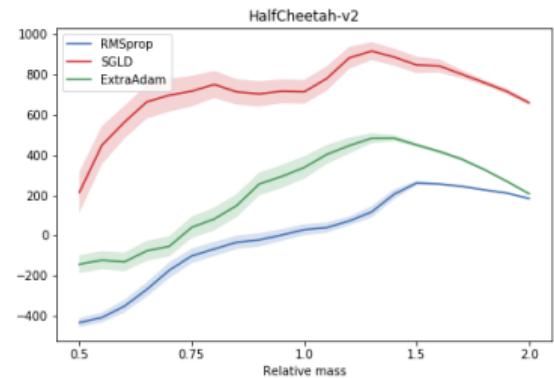
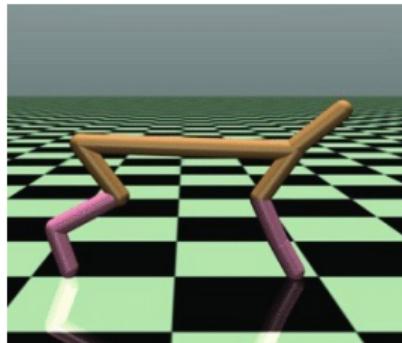
Practical Consequences of the Bilevel Formulation (I)

Training algorithm	Test accuracy					
	Clean		BETA ¹⁰		APGD	
	Best	Last	Best	Last	Best	Last
FGSM	81.96	75.43	40.30	0.04	41.56	0.00
PGD ¹⁰	83.71	83.21	43.64	40.21	44.36	42.62
TRADES ¹⁰	81.64	81.42	44.31	40.97	43.34	41.33
MART ¹⁰	78.80	77.20	44.81	41.22	45.00	42.90
BETA-AT ⁵	87.02	86.67	42.62	42.61	41.44	41.02
BETA-AT ¹⁰	85.37	85.30	44.54	44.36	44.32	44.12
BETA-AT ²⁰	82.11	81.72	46.91	45.90	45.27	45.25

Figure: Adversarial performance on CIFAR-10.

Take home messages

- Even the simplified view of robust & adversarial ML is challenging
- min-max-type has spurious attractors with no equivalent concept in min-type
- Not all step-size schedules are considered in our work: Possible to “converge” under some settings
- Other successful attempts¹ consider “mixed Nash” concepts²



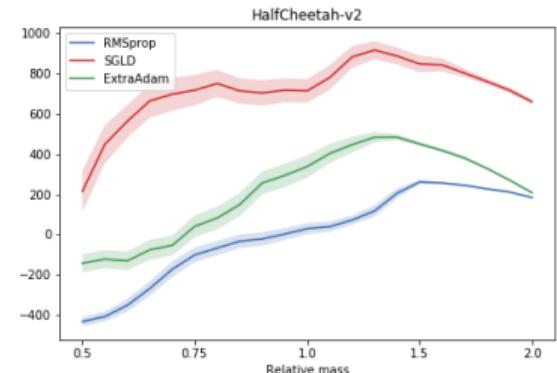
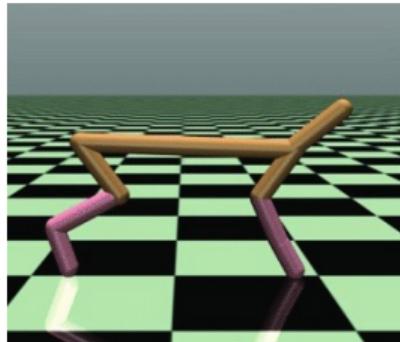
- Existing theory and methods for adversarial training is wrong!

¹Y-P. Hsieh, C. Liu, and V. Cevher, “Finding mixed Nash equilibria of generative adversarial networks,” International Conference on Machine Learning, 2019.

²K. Parameswaran, Y-T. Huang, Y-P. Hsieh, P. Rolland, C. Shi, V. Cevher, “Robust Reinforcement Learning via Adversarial Training with Langevin Dynamics,” NeurIPS, 2020.

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- Existing theory and methods for adversarial training is wrong! ... SAM too...

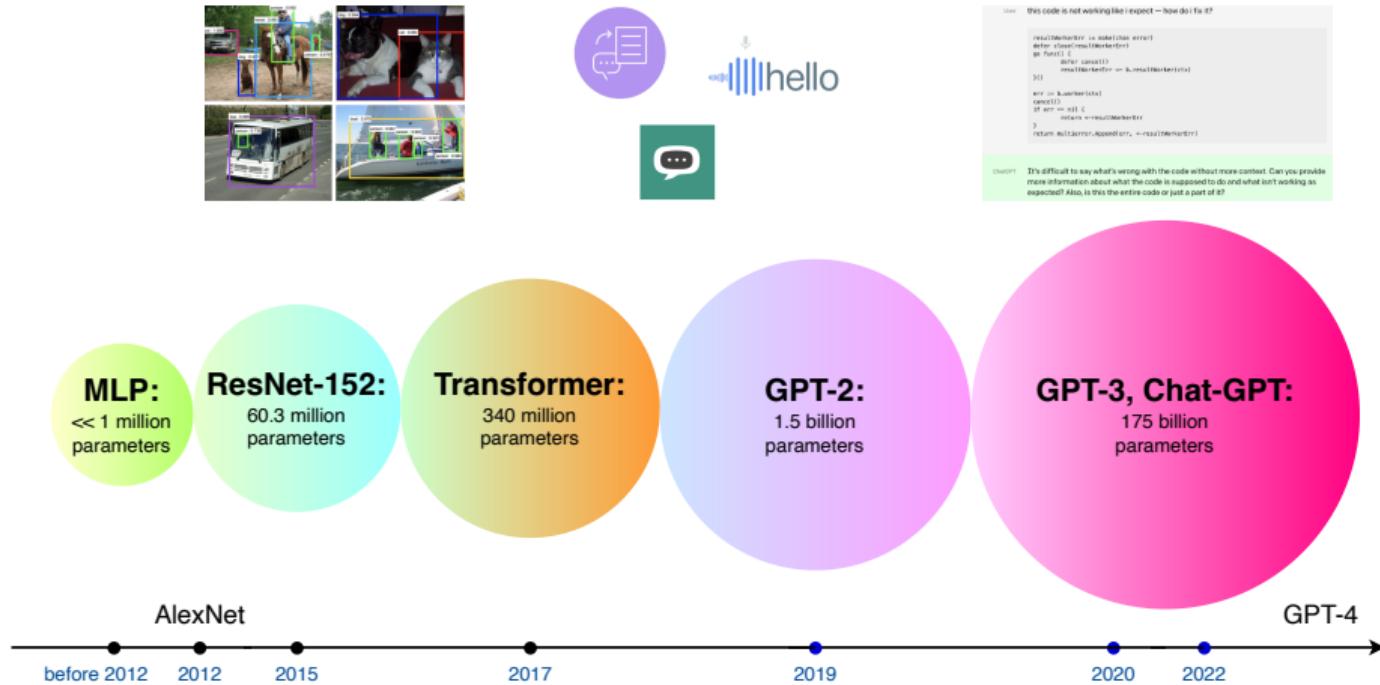
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Break



Over-parameterization: more parameters than training data



Over-parameterization: more parameters than training data

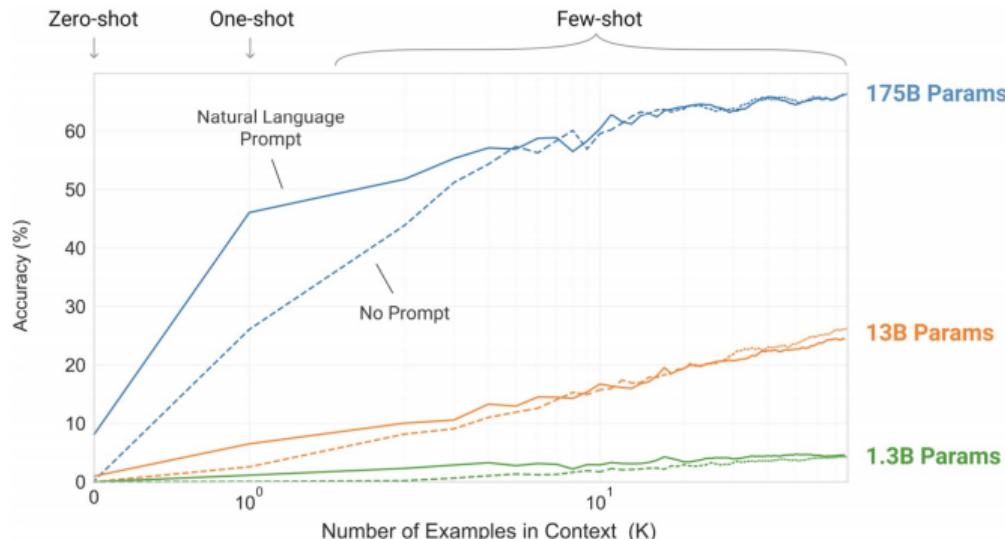


Figure: Larger models make increasingly efficient use of in-context information: source from [Open AI](#).

Recall DNNs: the good in **fitting** ...

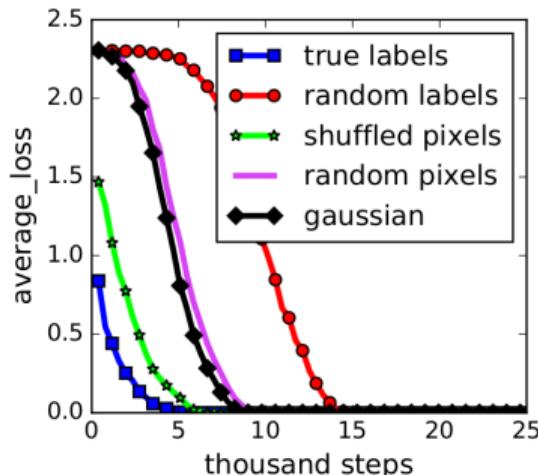
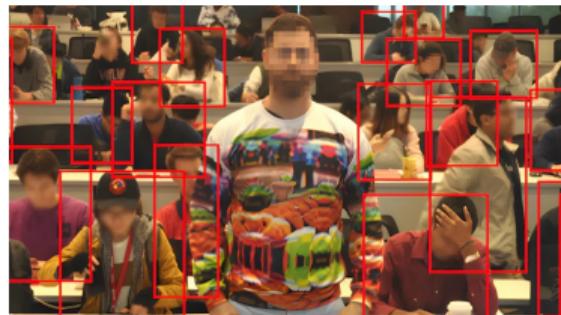


Figure: DNN Training curves on CIFAR10, from [90]

- A gap between theory and practice:
 - ▶ DNNs can fit random labels
 - ▶ SGD: zero training error and low test error

Recall DNNs: the bad in **robustness**...



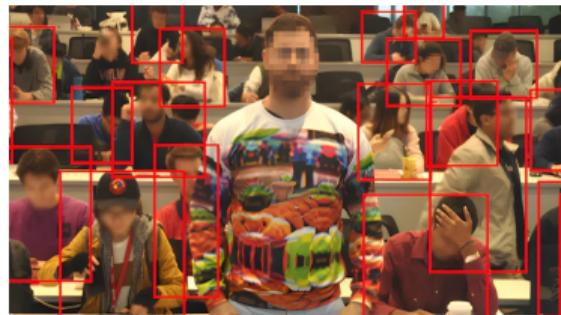
(a) Invisibility [83]



(b) Stop sign classified as 45 mph sign [28]



Recall DNNs: the bad in **robustness**...



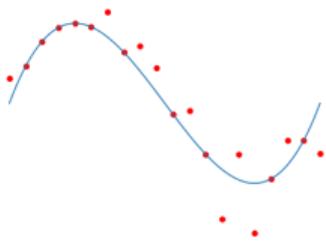
(a) Invisibility [83]



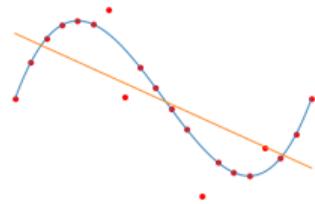
(b) Stop sign classified as 45 mph sign [28]

the ugly in over-parameterization?

A toy example: curve fitting

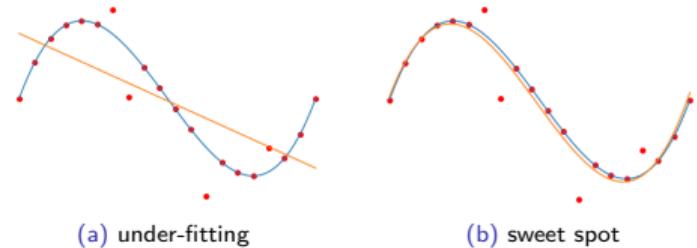


A toy example: curve fitting

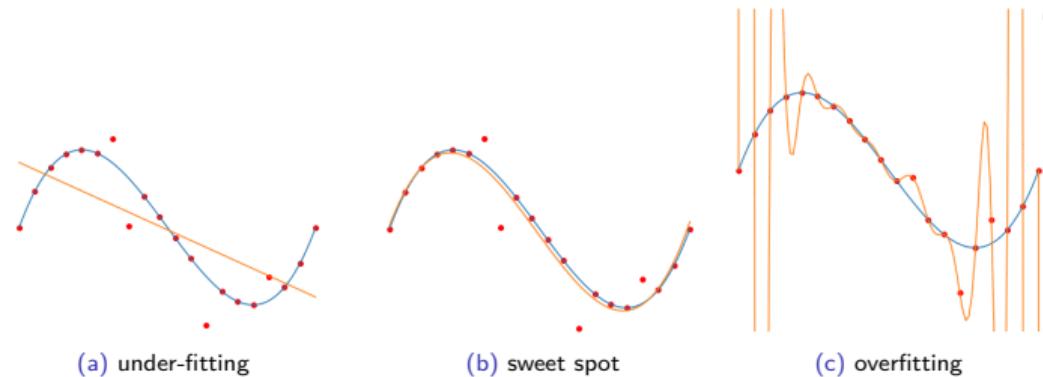


(a) under-fitting

A toy example: curve fitting



A toy example: curve fitting



(a) under-fitting

(b) sweet spot

(c) overfitting

A toy example: curve fitting

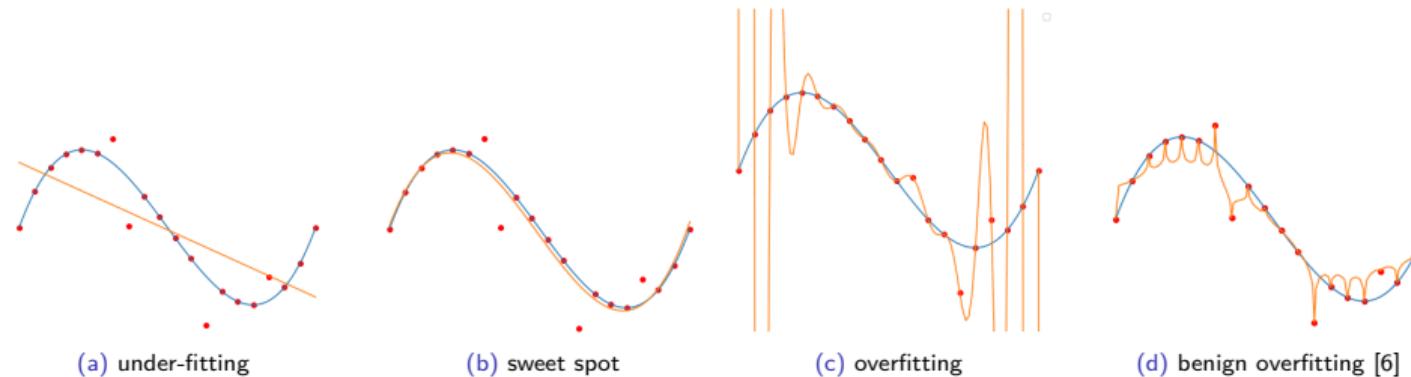


Figure: Test performance on curve fitting: source from [Open AI](#).

Recall: the formulation of FCNN

$$h^{(0)}(\mathbf{a}) = \mathbf{a},$$

$$h^{(l)}(\mathbf{a}) = \sigma \left(\begin{array}{c} \text{activation} \\ \downarrow \\ \mathbf{X}_l \end{array} \right) \left[\begin{array}{c} \text{weight} \\ \downarrow \\ h^{(l-1)}(\mathbf{a}) \end{array} \right], \quad (L\text{-Layer NN})$$

$$h_{\mathbf{x}}(\mathbf{a}) = h^{(L)}(\mathbf{a}) = \frac{1}{\alpha} \sigma \left(\mathbf{X}_L h^{(L-1)}(\mathbf{a}) \right), \quad \mathbf{x} := [\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_L].$$

- Elements of NN architectures we will discuss in the sequel:

- Parameters: $\mathbf{X}_1 \in \mathbb{R}^{m \times p}$, $\mathbf{X}_L \in \mathbb{R}^{1 \times m}$, $\mathbf{X}_l \in \mathbb{R}^{m \times m}$ for $l = 2, 3, \dots, L-1$ (weights).
- Initialization: $\mathbf{X}_1 \sim \mathcal{N}(0, \beta_1^2)$, $\mathbf{X}_L \sim \mathcal{N}(0, \beta_L^2)$, $\mathbf{X}_l \sim \mathcal{N}(0, \beta^2)$ for $l = 2, 3, \dots, L-1$ (weights).
- Activation function ReLU: $\sigma(\cdot) = \max(\cdot, 0) : \mathbb{R} \rightarrow \mathbb{R}$.
- Without loss of generality, we will avoid the bias variables in the sequel.

Initialization in deep ReLU NNs

- Initialization: $\mathbf{X}_1 \sim \mathcal{N}(0, \beta_1^2)$, $\mathbf{X}_L \sim \mathcal{N}(0, \beta_L^2)$, $\mathbf{X}_l \sim \mathcal{N}(0, \beta_l^2)$ for $l = 2, 3, \dots, L-1$ (weights).

Table: Some commonly used initializations in neural networks.

Initialization name	β_1^2	β^2	β_L^2	α
LeCun [50]	$\frac{1}{p}$	$\frac{1}{m}$	$\frac{1}{m}$	1
He [38]	$\frac{2}{p}$	$\frac{2}{m}$	$\frac{2}{m}$	1
NTK [2]	$\frac{2}{m}$	$\frac{2}{m}$	1	1
Xavier [33]	$\frac{2}{m+p}$	$\frac{1}{m}$	$\frac{2}{m+1}$	1
Mean-field [60]	1	1	1	m
E et al. [27]	1	1	β_c^2	1

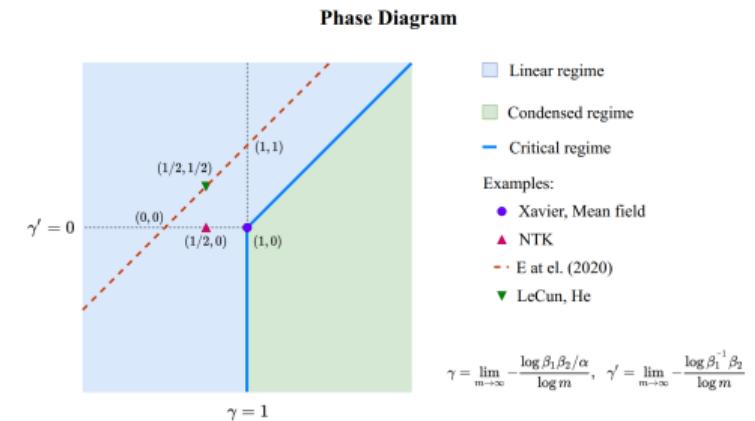


Figure: Phase diagram of two-layer ReLU NNs at infinite-width limit in [56].

Lazy training

Definition (Lazy-training (Linear) regime [56])

Define an L -layer fully-connected ReLU NN via (L -Layer NN). After training time t , as $m \rightarrow \infty$, if the following condition holds

$$\sup_{t \in [0, +\infty)} \frac{\|\mathbf{X}_l(t) - \mathbf{X}_l(0)\|_2}{\|\mathbf{X}_l(0)\|_2} \rightarrow 0, \quad \forall l \in [L].$$

then the NN training dynamics falls into the lazy-training regime.

- Remarks:**
- In this regime, training h and h_0 is equivalent if taking Taylor expansion.
 - Which conditions allow for lazy training to occur ?

Lazy training: a consequence of overparametrization or scaling?

Theorem (Lazy training for two-layer ReLU networks [18], modified version)

Two layer networks $h(\mathbf{a}, \{\mathbf{x}, \mathbf{v}\}) : \mathbf{a} \mapsto \alpha(m) \sum_{j=1}^m v_j \text{ReLU}(\mathbf{x}_j^\top \mathbf{a})$ with Gaussian initialization $v_i, \mathbf{x}_i \sim \mathcal{N}(0, \beta^2)$ will fall within the lazy regime as long as

$$\lim_{m \rightarrow \infty} m\beta = \infty.$$

- Remarks:
- The loss changes a lot but the neural network output changes little.
 - Other conditions for deep neural networks can be found here [18, 7].

Lazy training regime: visualization

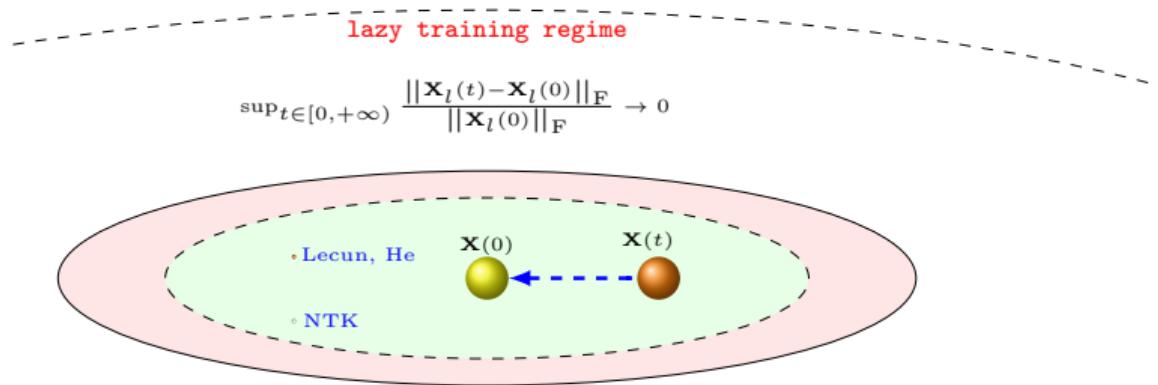
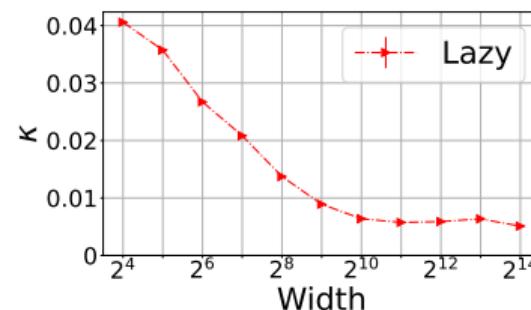
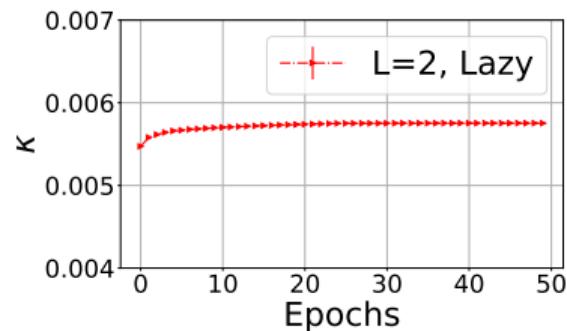


Figure: Training dynamics of two-layer ReLU NNs under different initializations [46, 19, 57].

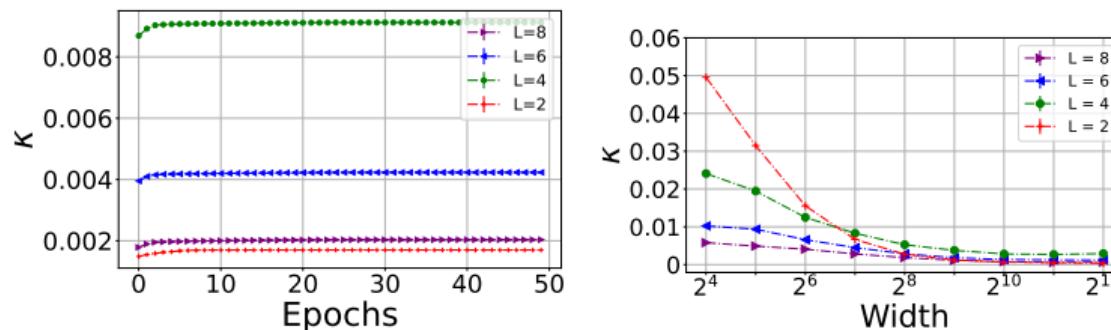
Lazy training regime: experiments

$$\text{lazy training ratio } \kappa := \frac{\sum_{l=1}^L \|\mathbf{X}_l(t) - \mathbf{X}_l(0)\|_F}{\sum_{l=1}^L \|\mathbf{X}_l(0)\|_F}$$



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Non-lazy training regime: visualization

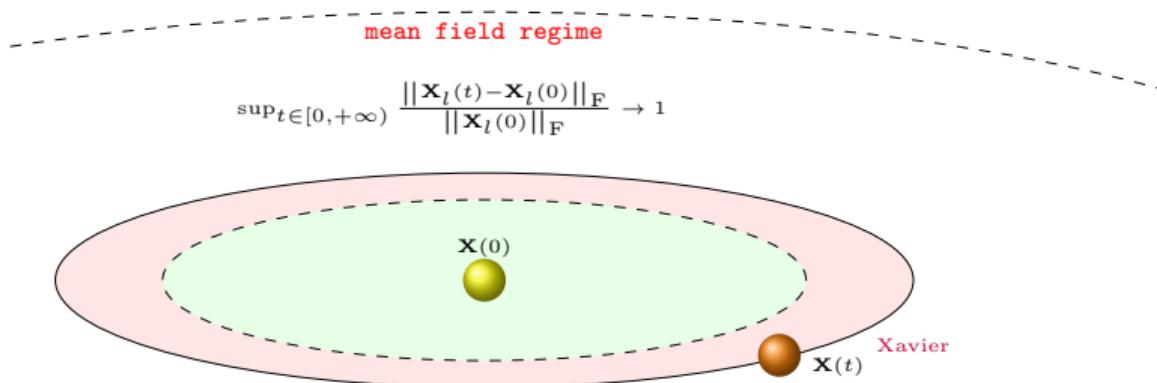


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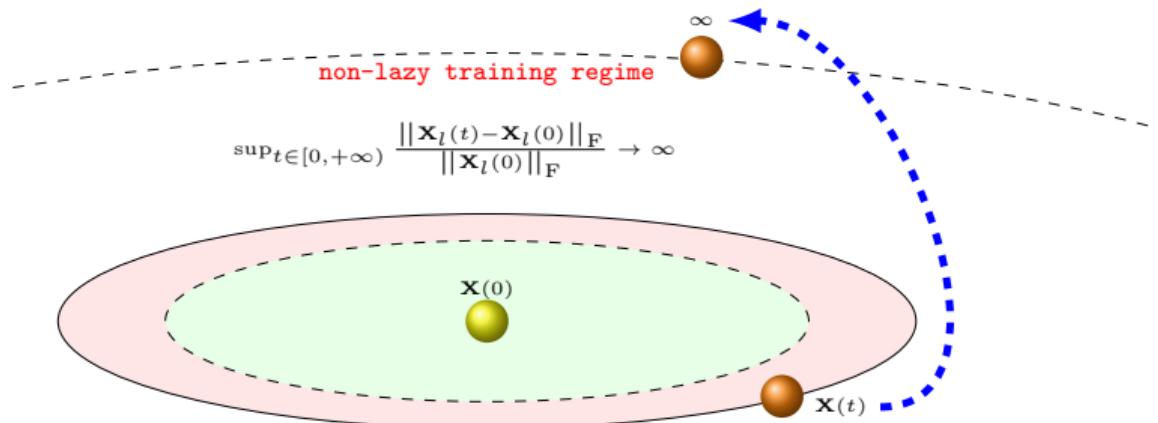


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Neural Tangent Kernel [46]

- Define feature mapping $\mathbf{a} \mapsto \frac{\partial h}{\partial \mathbf{x}}(\mathbf{a}, \mathbf{x}_0)$, the (empirical) neural tangent kernel is defined as

$$\Theta(\mathbf{a}_i, \mathbf{a}_j) := \langle \nabla_{\mathbf{x}} h(\mathbf{a}_i, \mathbf{x}), \nabla_{\mathbf{x}} h(\mathbf{a}_j, \mathbf{x}) \rangle, \forall i, j \in [n].$$

Training dynamics

Under NTK initialization and large enough width, we have

$$\lim_{\text{width} \rightarrow \infty} \Theta_{\mathbf{x}(0)}(\mathbf{a}_i, \mathbf{a}_j) = \mathbb{E}_{\mathbf{x}}[\Theta_{\mathbf{x}(0)}(\mathbf{a}_i, \mathbf{a}_j)] =: K_{\infty}.$$

Under the squared loss, the dynamics of $h(\mathbf{a}, \mathbf{x})$ is equivalent to **kernel regression**

$$\dot{h}(\mathbf{a}, \mathbf{x}(t)) = \nabla_{\mathbf{x}} h(\mathbf{a}, \mathbf{x}) \dot{\mathbf{x}}(t) = K_{\infty}(\mathbf{a}, \mathbf{a}_i)(h(\mathbf{a}, \mathbf{x}(t)) - b).$$

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Remarks:

- NTK stays unchanged during training

- General loss functions: equivalence between infinite NNs and kernel methods [17]
 - e.g., NN trained by soft margin loss vs. SVM trained by subgradient descent

Convolutional neural tangent kernel

- Convolutional neural networks (CNNs) [4]
 - ▶ without global average pooling (GAP)
 - ▶ with GAP, without training the first/last year

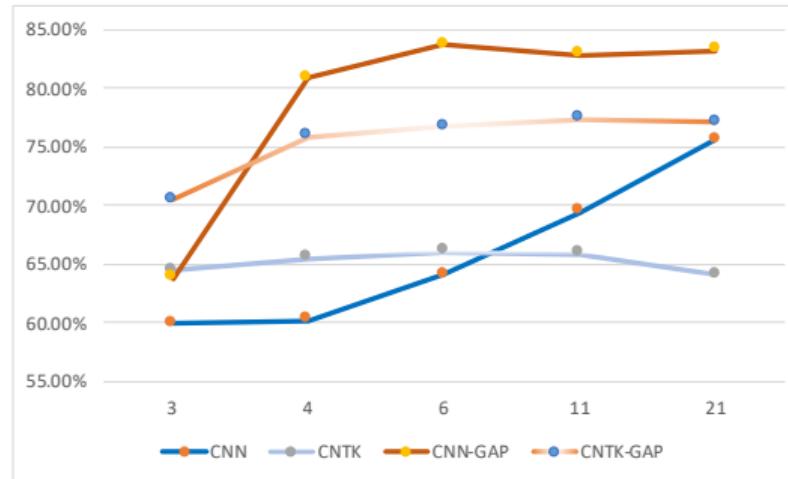


Figure: Classification accuracies of CNNs and CNTK on the CIFAR-10 dataset [4].

- Remarks:**
- This performance is below the accuracy of finite width networks ($> 98\%$).
 - NTK for general architectures, e.g., RNNs [1], GNNs [24, 49], PNNs [82]

Optimization and generalization by NTK

Theorem (optimization and generalization [2, 13])

For a DNN with a large enough width trained by (S)GD, under proper data assumption and step-size η ,

- ▶ global convergence

$$L(\mathbf{x}(t)) \leq [1 - \eta \lambda_{\min}(K_\infty)]^t L(\mathbf{x}(0)), \quad \text{whp.}$$

where $\lambda_{\min}(K_\infty)$ is the minimum eigenvalue of K_∞ .

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Remarks: ◦ The objective is “almost convex”.

◦ The minimum eigenvalue of NTK plays an important role!

How much overparametrization of fully-connected NNs is enough?

Reference	Number of parameters	Depth L	Result
[53]	$\tilde{\Omega}(\text{poly}(n))$	1	(S)GD global convergence
[2, 96]	$\tilde{\Omega}(\text{poly}(n, L))$	Any L	(S)GD global convergence
[23]	$\tilde{\Omega}(n^8 2^{O(L)})$	Any L	(S)GD global convergence
[97]	$\tilde{\Omega}(n^8 L^{12})$	Any L	(S)GD global convergence
[47]	$\tilde{\Omega}(n)$ (Training last layer)	Any L	(S)GD global convergence
[11]	$\tilde{\Omega}(n)$ (Training all layers)	Any L	(S)GD global convergence

Table: Summary of results on overparametrization. Minimum number of parameters required as a function of data size n and depth L . [11]: smooth activation function; Lipschitz concentrated data; a loose pyramidal topology.

Remarks:

- Practical datasets are structured: the width need no be large for a good approximation [63]

Function space: from kernel methods to neural networks

- Feature mapping $\mathbf{a} \mapsto \frac{\partial h}{\partial \mathbf{x}}(\mathbf{a}, \mathbf{x}_0)$: captures the first-order approximation of NN's training.

Kernel Methods

reproducing kernel Hilbert space (RKHS)

Neural Networks

Neural tangent kernel (NTK)

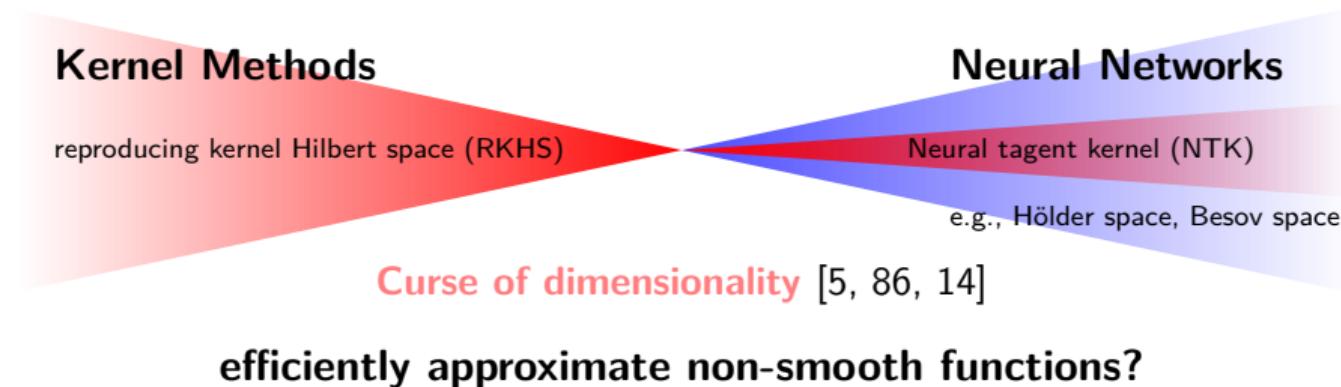
e.g., Hölder space, Besov space

Curse of dimensionality [5, 86, 14]

efficiently approximate non-smooth functions?

Function space: from kernel methods to neural networks

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What can linearized neural networks actually say about CV tasks?

What can we benefit from NTK for computer vision?

- efficient algorithm
 - ▶ fine-tuning: gradient as features [63, 87]
 - ▶ efficient training in low-dimensional spaces [52], neural networks pruning [54]
 - ▶ robustness: generate adversarial examples [75], black-box generalization attack [88]
 - ▶ small-scale dataset [66], dataset distillation [65]
 - ▶ image denoising [73]
 - ▶ neural architecture search in a "train-free" fashion [92, 16]

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Over-parameterization helps or hurts robustness?

Helps! [12]



Hurts! [81, 43]

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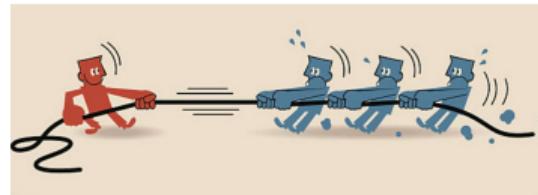


Hurts! [81, 43]

- ▶ initialization (e.g., lazy training, non-lazy training)
- ▶ architecture (e.g., width, depth)

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Definition (perturbation stability [93])

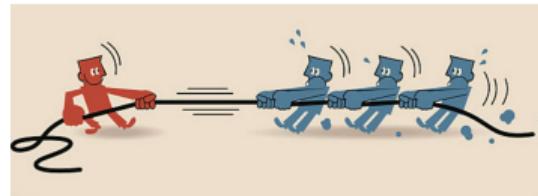
The perturbation stability of a ReLU DNN $h_{\mathbf{x}}(\mathbf{a})$ is:

$$\mathcal{P}(h, \epsilon) = \mathbb{E}_{\mathbf{a}, \hat{\mathbf{a}}, \mathbf{x}} \left\| \nabla_{\mathbf{a}} h_{\mathbf{x}}(\mathbf{a})^\top (\mathbf{a} - \hat{\mathbf{a}}) \right\|_2, \quad \forall \mathbf{a} \sim \mathcal{D}_A, \quad \hat{\mathbf{a}} \sim \text{Unif}(\mathbb{B}(\epsilon, \mathbf{a})).$$

where ϵ is the perturbation radius.

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Definition (perturbation stability: lazy training regime)

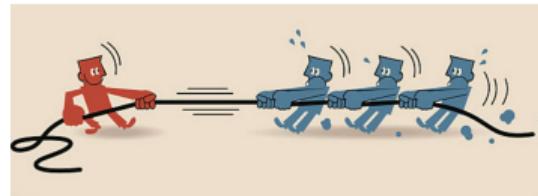
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Main results (Lazy-training regime)

Theorem: perturbation stability $\lesssim \text{Func}(\mathbf{m}, \mathbf{L}, \beta)$

Assumption	Initialization	Our bound for $\mathcal{P}(f, \epsilon)/\epsilon$	Trend of width \mathbf{m} [1]	Trend of depth \mathbf{L} [1]
$\ \mathbf{x}\ _2 = 1$	Lecun initialization	$\left(\sqrt{\frac{\mathbf{L}^3 \mathbf{m}}{p}} e^{-\mathbf{m}/\mathbf{L}^3} + \sqrt{\frac{1}{p}} \right) \left(\frac{\sqrt{2}}{2} \right) \mathbf{L}^{-2}$	$\nearrow \searrow$	\searrow
	He initialization	$\sqrt{\frac{\mathbf{L}^3 \mathbf{m}}{d}} e^{-\mathbf{m}/\mathbf{L}^3} + \sqrt{\frac{1}{d}}$	$\nearrow \searrow$	\nearrow
	NTK initialization	$\sqrt{\frac{\mathbf{L}^3 \mathbf{m}}{p}} e^{-\mathbf{m}/\mathbf{L}^3} + 1$	$\nearrow \searrow$	\nearrow

[1] The larger perturbation stability means worse average robustness.

- Takeaway messages: **the good (width), the bad (depth), the ugly (initialization)**

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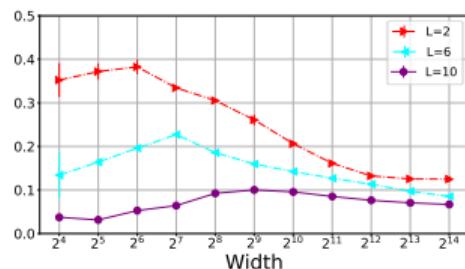
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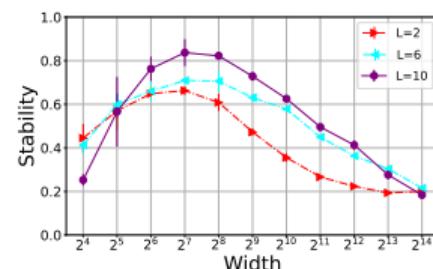
- Takeaway messages: **the good (width), the bad (depth), the ugly (initialization)**
 - ▶ width **helps** robustness in the over-parameterized regime
 - ▶ depth **helps** robustness in Lecun initialization but **hurts** robustness in He/NTK initialization

Experiments: lazy training experiment for FCNN

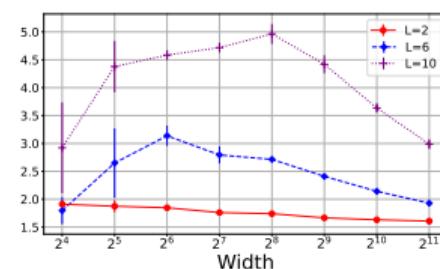
Metrics	Ours (NTK initialization)	[81]	[43]
$\mathcal{P}(f, \epsilon) / \epsilon$	$\sqrt{\frac{L^3 m}{p}} e^{-m/L^3} + 1$	$L^2 m^{1/3} \sqrt{\log m} + \sqrt{m L}$	$2^{\frac{3L-5}{2}} \sqrt{L}$



(a) LeCun initialization

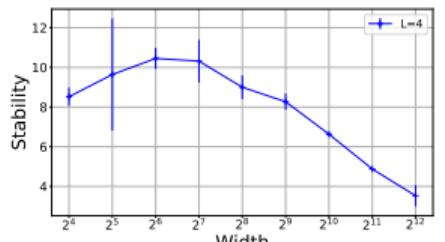


(b) He initialization

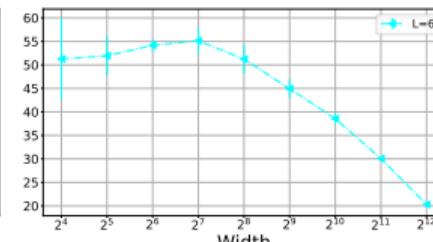


(c) NTK initialization

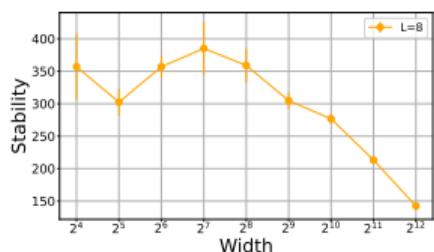
Experiments: lazy training experiment for CNN



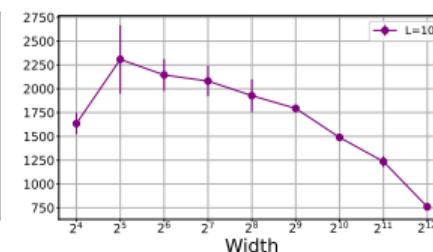
(a) $L = 4$



(b) $L = 6$



(c) $L = 8$



(d) $L = 10$

Figure: Relationship between the *perturbation stability* and width of CNN under He initialization for different depths of $L = 4, 6, 8$ and 10 . More experimental results on ResNet can be found in [93].

Main results (Non-lazy training regime)

A sufficient condition for DNNs

For large enough m and $m \gg p$, w.h.p, DNNs fall into **non-lazy training regime** if $\alpha \gg (m^{3/2} \sum_{i=1}^L \beta_i)^L$.

Remarks: $\circ L = 2, \alpha = 1, \beta_1 = \beta_2 = \beta \sim \frac{1}{m^c}$ with $c > 1.5$

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Theorem (non-lazy training regime for two-layer NNs)

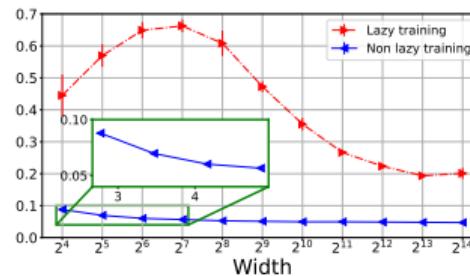
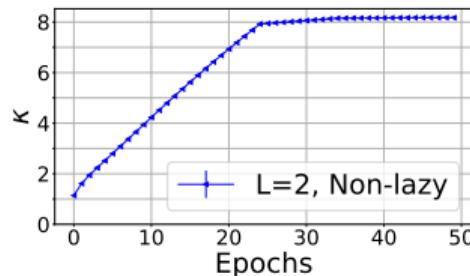
Under this setting with $m \gg n^2$ and standard assumptions, then

$$\text{perturbation stability} \leq \widetilde{\mathcal{O}}\left(\frac{n}{m^{c+1.5}}\right), \text{ whp.}$$

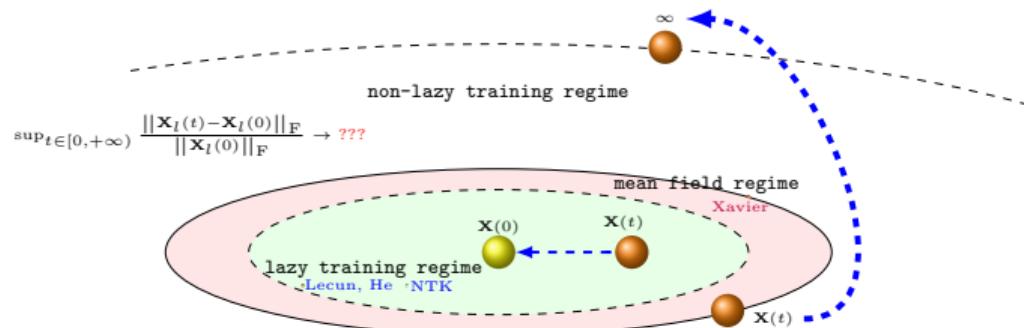
Remarks: \circ Width **helps** robustness in the over-parameterized regime in both lazy/non-lazy training regime

Experiment: Non-lazy training regime

$$\text{lazy training ratio } \kappa := \frac{\sum_{l=1}^L \| \mathbf{X}_l(t) - \mathbf{X}_l(0) \|_F}{\sum_{l=1}^L \| \mathbf{X}_l(0) \|_F}$$



	good	bad	ugly
neural networks	performance	analysis	over-parameterization
generalization	benign overfitting	catastrophic overfitting	model complexity
robustness	width	depth	initialization



Break



Neural Architecture Search (NAS) [95]

- ▶ An architecture has a significant impact on the performance and the inductive bias of the model [39, 77, 78, 20].

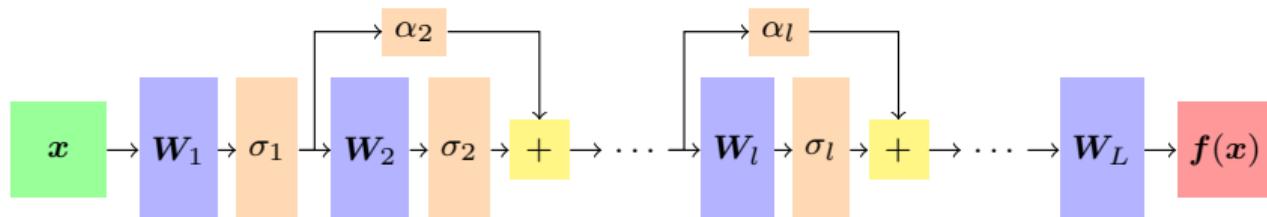
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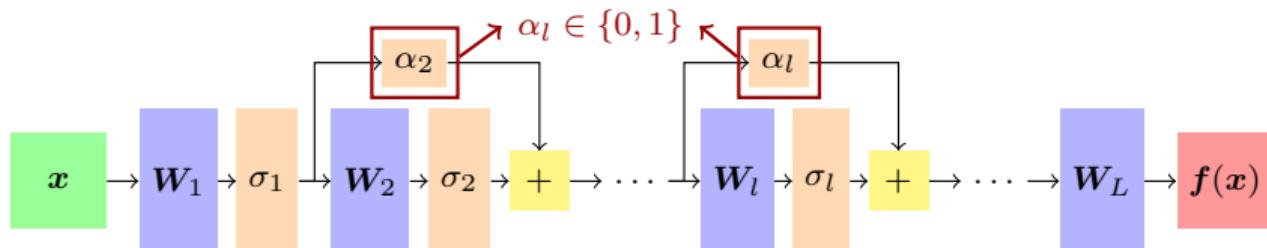
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- ▶ Manually designed architectures require domain expertise and might not be optimal.
- ▶ Instead, we can define a search procedure to select the architecture.

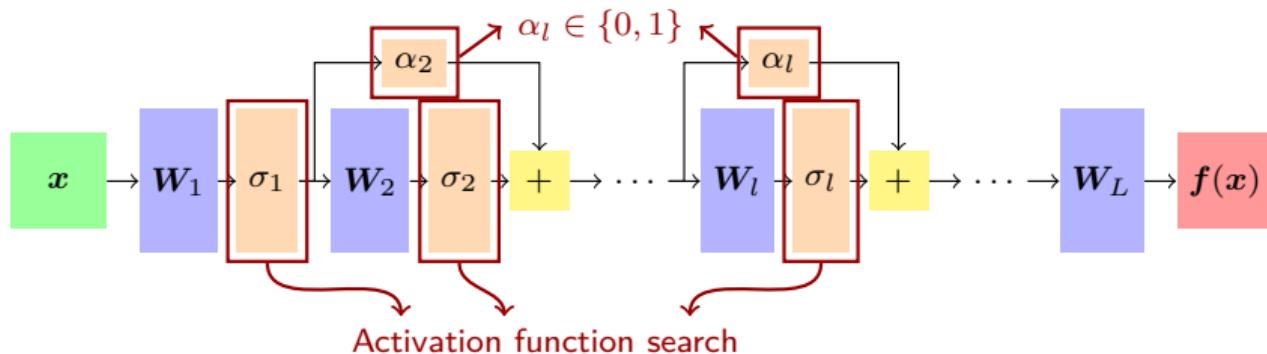
Towards a principled Neural Architecture Search (NAS) [92]



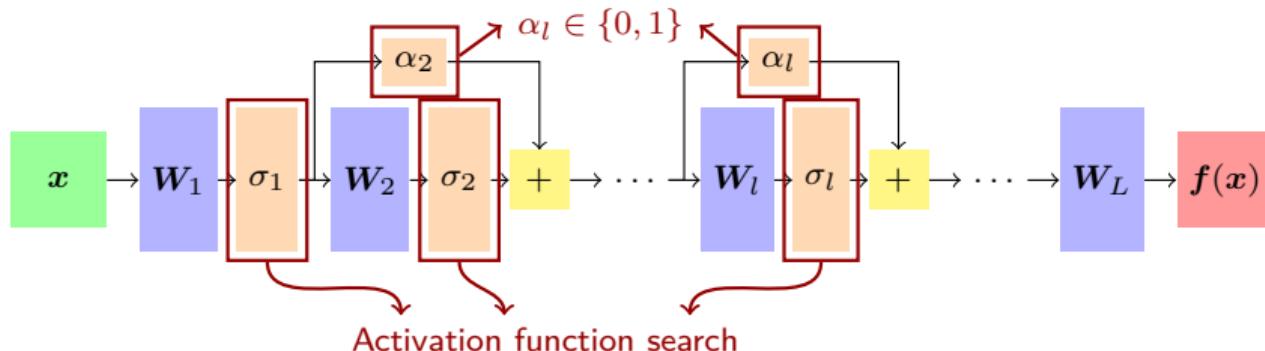
Towards a principled Neural Architecture Search (NAS) [92]



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- Generalization error (of the unified architecture) with respect to the minimum eigenvalue λ_{\min} of NTK:

$$\text{generalization error} \lesssim \mathcal{O}\left(\frac{1}{\sqrt{\lambda_{\min}}}\right), w.h.p.$$

Towards a principled Neural Architecture Search (NAS) [92]

- Beyond the depth L , the minimum eigenvalue is also affected by the constants $\beta_1, \beta_2, \beta_3$ that are only determined by the activation function. Specifically, $f_{\text{lower}}(\beta_3) \leq \lambda_{\min} \leq f_{\text{upper}}(\beta_1, \beta_2)$.

σ	Trend of lower bound	ReLU	LeakyReLU	Sigmoid	Tanh	Swish
$\beta_3(\sigma)$	\nearrow	1	> 1	$\leq 1/16$	≤ 1	$1/2$

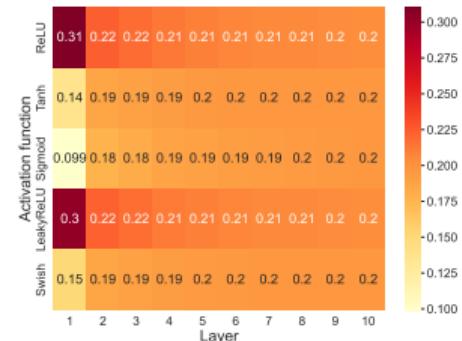


Figure: Probability of selecting activation per layer numerically.

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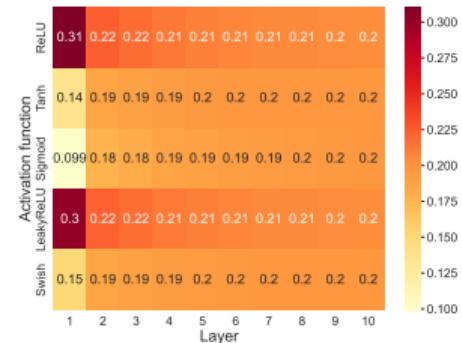


Figure: Probability of selecting activation per layer numerically.

Overall insights:

- The depth L and the skip connections via α_l affect significantly the bounds.
- The first activation function σ_1 is more important than the rest activation functions.

Train-free Neural Architecture Search (NAS) [92]

Algorithm 1 Eigen-NAS Algorithm

Require: Search space \mathcal{S} , training data $\mathcal{D}_{tr} = \{(x_i, y_i)_{i=1}^{N_t}\}$, validation data $\mathcal{D}_{val} = \{(x_j, y_j)_{j=1}^{N_v}\}$.

Initialize `max_iteration` = M
Initialize candidate set $\mathcal{C} = []$
for `search_iteration` in $1, 2, \dots, \text{max_iteration}$ **do**
 Randomly sample architecture s from search space \mathcal{S} .
 Compute *Eigen* := minimum eigenvalue of NTK.
 $\mathcal{C}.\text{append}(s, \text{Eigen})$
 update \mathcal{C} to kept top-K best architectures
end for
 $s^* = \text{best}_s(\mathcal{C}, \mathcal{D}_{tr}, \mathcal{D}_{val})$ # Choose the best architecture based on validation error after training 20 epochs.
Output s^*

Extrapolation

Let us assume training data $\{(x_i, y_i)\}_{i=1}^{|\mathcal{X}|}$ and any direction $v \in \mathbb{R}^d$ that satisfies $\|v\|_2 = \max\{\|x_i\|^2\}$. Let $x = (t + h)v$ with $t > 1$ and $h > 0$ be the extrapolation data points.

Theorem (N -layer MLP [84])

*The output $f(x)$, when f is a trained N -layer ReLU-NN, follows a **linear** function with respect to h .*

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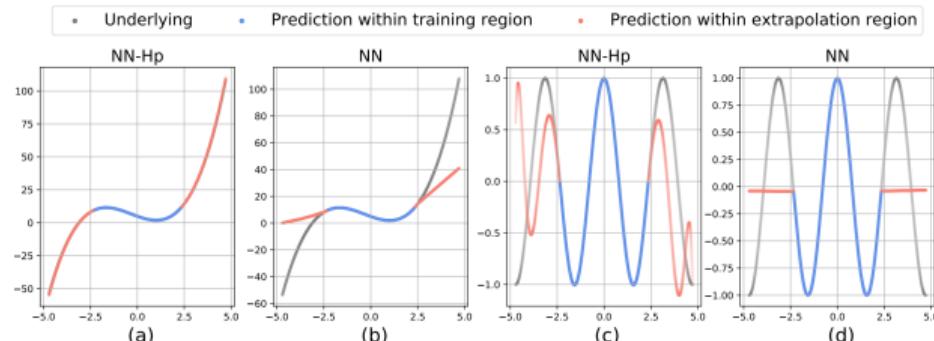


Figure: (a) and (b): fitting $f_\rho(x) = x^3 + x^2 - 10x + 5$. (c) and (d): fitting $f_\rho(x) = \cos(2x)$.

Extrapolation – experimental validation

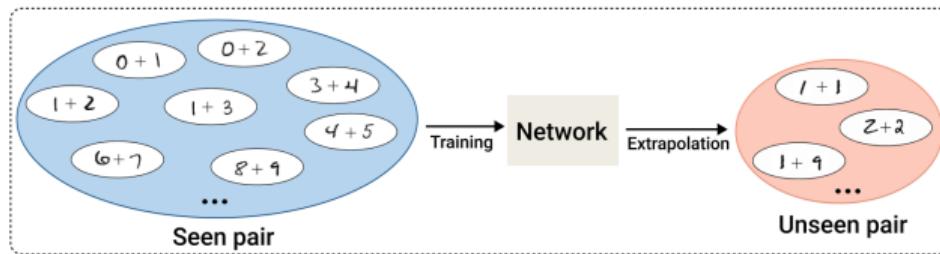


Table: Experimental evaluation of visual addition.

Method	Accuracy (Rounding)
NN (Dense)	0.436 ± 0.065
PNN (Dense)	0.554 ± 0.011
NN (Conv)	0.617 ± 0.103
PNN (Conv)	0.825 ± 0.109

Visualizing the components of adversarial perturbations [75]



$$+ 4/255 \cdot \text{sign}($$



$$) =$$

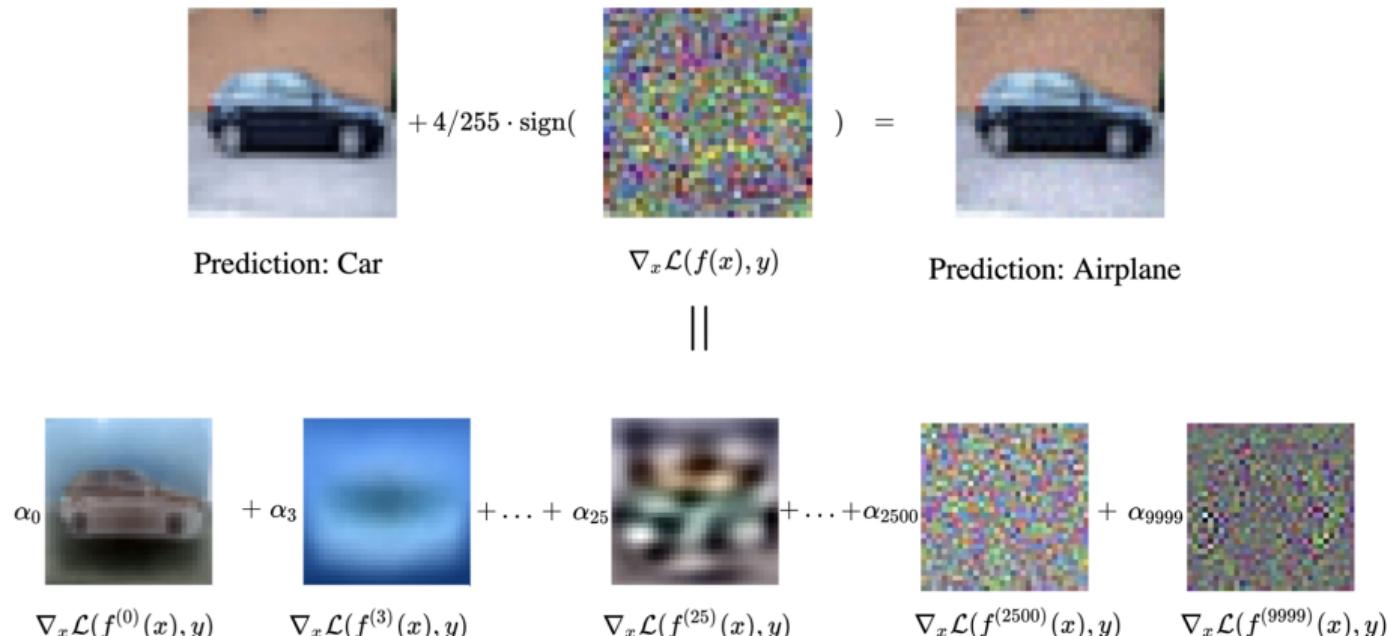


Prediction: Car

$$\nabla_x \mathcal{L}(f(x), y)$$

Prediction: Airplane

Visualizing the components of adversarial perturbations [75]



Visualizing the features [75]

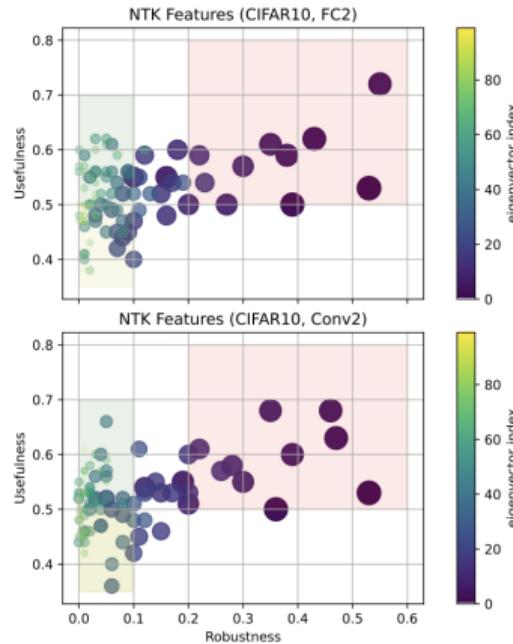
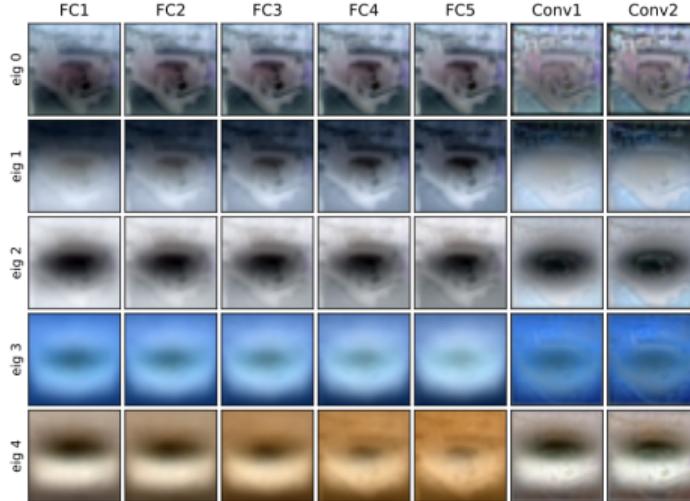
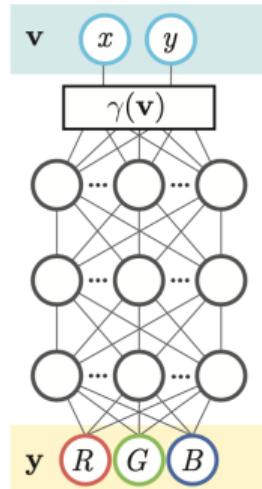


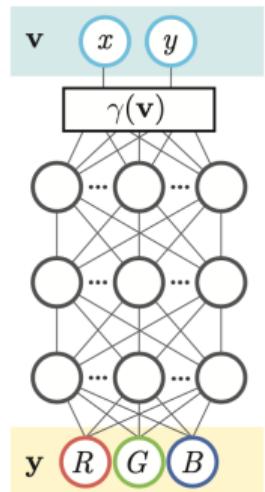
Figure: (Left) Top 5 features for 7 different kernel architectures for a car image. (Right) Features according to their robustness (x-axis) and usefulness (y-axis).

The role of positional encodings in implicit representations [74]

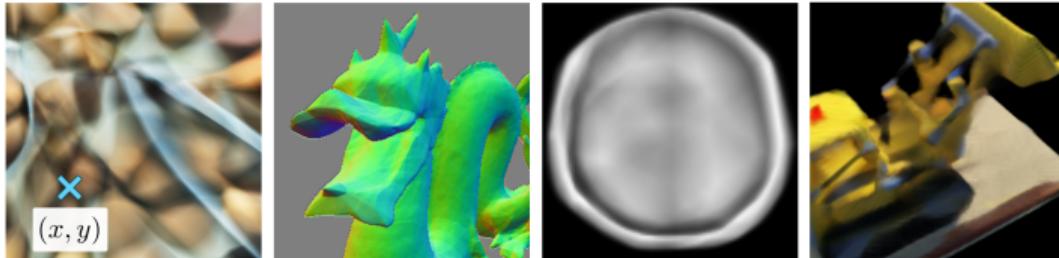


(a) Coordinate-based MLP

The role of positional encodings in implicit representations [74]

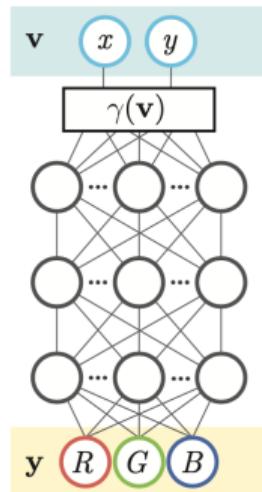


No Fourier features
 $\gamma(\mathbf{v}) = \mathbf{v}$



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The role of positional encodings in implicit representations [74]



(a) Coordinate-based MLP

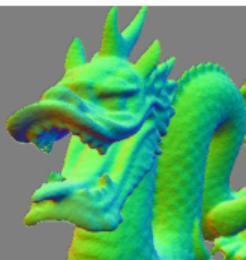
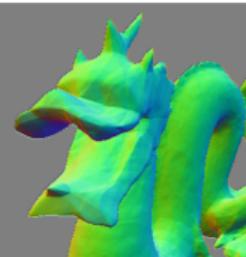
No Fourier features
 $\gamma(\mathbf{v}) \equiv \mathbf{v}$



(b) Image regression

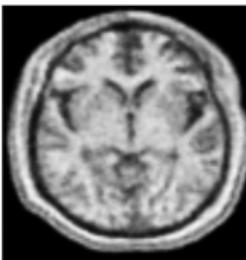
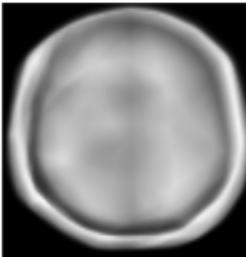
$$(x, y) \rightarrow \text{RGB}$$

With Fourier features
 $\gamma(\mathbf{v}) \equiv \text{FF}(\mathbf{v})$



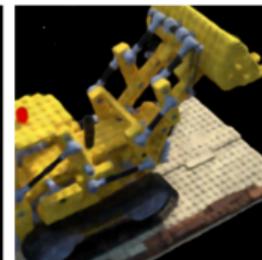
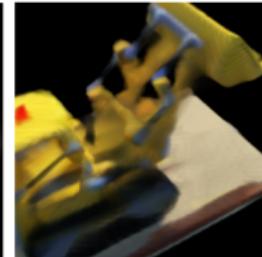
(c) 3D shape regression

$$(x, y, z) \rightarrow \text{occupancy}$$



(d) MRI reconstruction

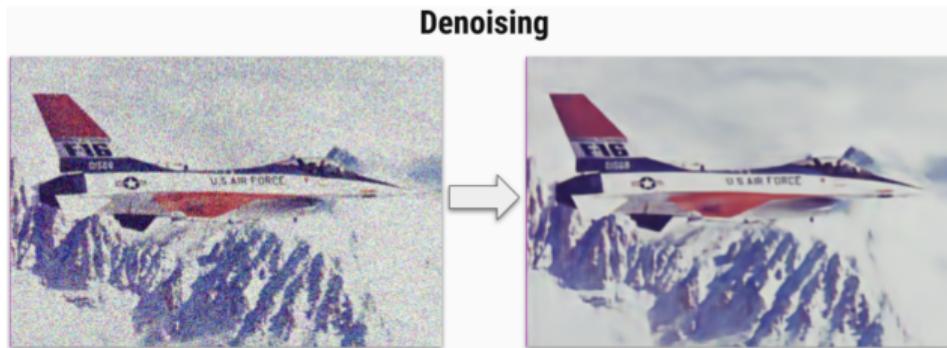
$$(x, y, z) \rightarrow \text{density}$$



(e) Inverse rendering

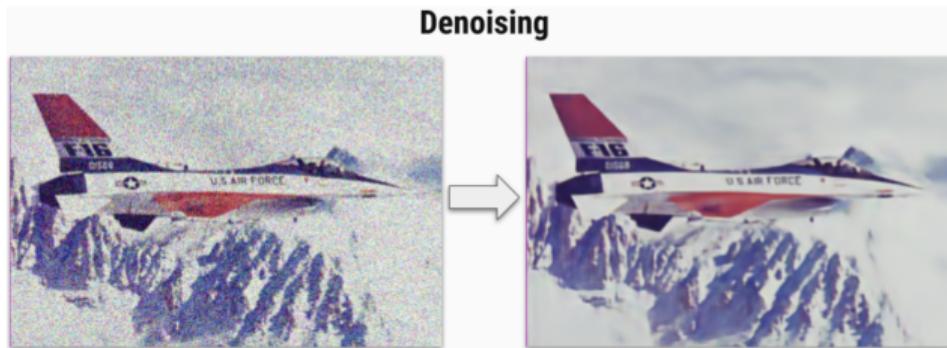
$$(x, y, z) \rightarrow \text{RGB}, \text{density}$$

Denoising with Deep Image Prior (DIP) [76]



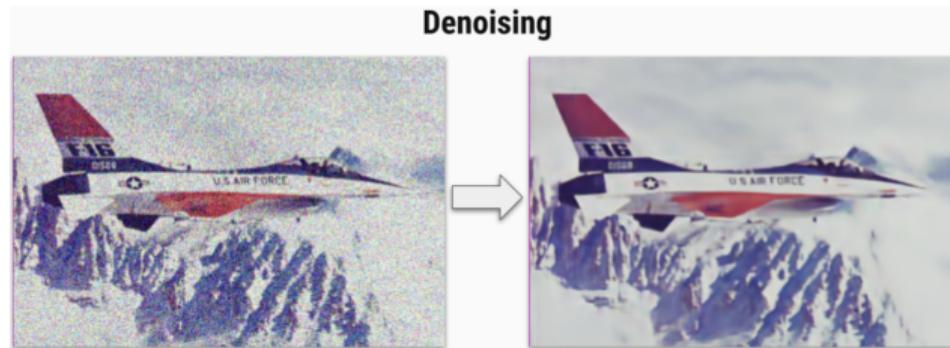
- ▶ Inverse problems have immense applications in imaging tasks.
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Denoising with Deep Image Prior (DIP) [76]



- ▶ Inverse problems have immense applications in imaging tasks.
- ▶ Deep Image Prior (DIP) does not require training with massive data. The noisy (input) image is sufficient.
- ▶ *How* does DIP work?
- ▶ *Why* does DIP work?

The Neural Tangent Link Between DIP and Non-Local Filters [73]

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- ▶ Compute the NTK Gram matrix instead of learning. Use directly that version for denoising.
- ▶ Use insights from the derivation to explain why the optimizer is crucial and why DIP works primarily with Adam and not SGD.

Beyond linear layers

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- ▶ Analysis of contemporary components, e.g. layer normalization, remains elusive.
- ▶ The assumptions on the components are often restrictive and do not reflect their utilization in actual applications.

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- ▶ Simplifying assumptions in the transformer block, e.g., width of the layers.
- ▶ Little insight into what is special about transformers when compared to other architectures.

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- ▶ The theoretical analysis on the non-lazy regime seems to be much more diverse, which creates a requirement for a more thorough taxonomy.

Practical considerations

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- ▶ How can the theoretical insights extend beyond classification to problems relevant to vision? For instance, (conditional) generation, dense reconstruction or tracking?
- ▶ Can tight generalization bounds be used for guiding practical implementations [91]?
- ▶ How can we relax the existing theoretical tools to reflect practical implementations (e.g., having a finite width)?

Thanks for your attention!

Q & A

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