Challenges in Robust Machine Learning

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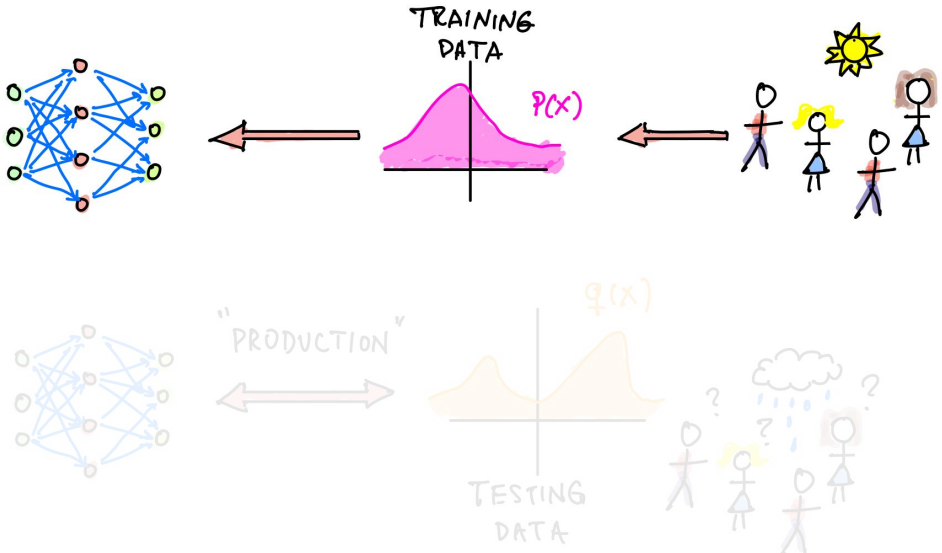
Why do we need robustness?



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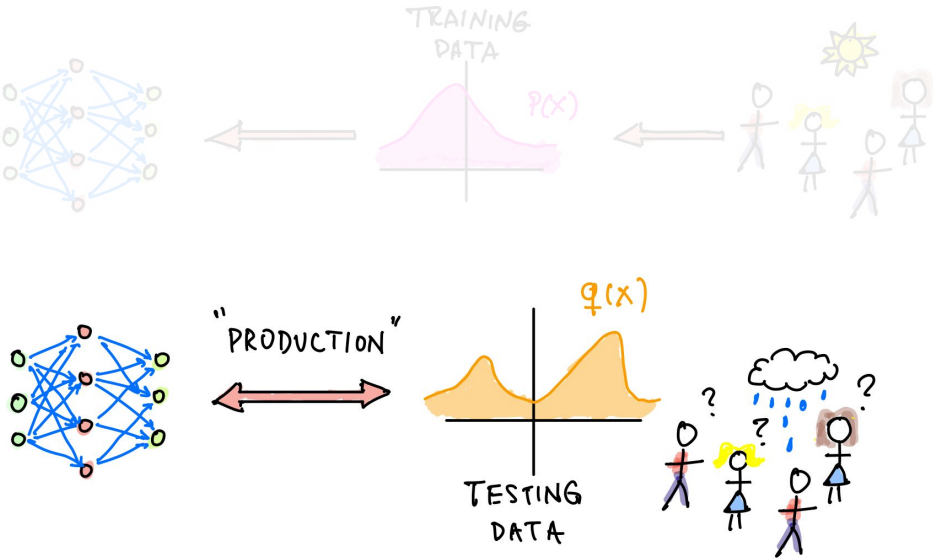

Robustness meets the adversaries

Kids

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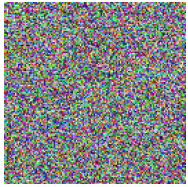

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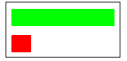

NFL

+0.01x

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Robustness meets the adversaries

Kids

Yuan et al. (2019)

+0.01x

=

safe
+18

safe
+18

NFL

Saadatpanah, Shafahi and Goldstein. (ICML 2020)

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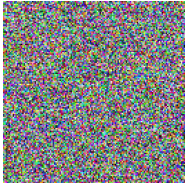

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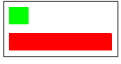

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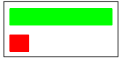

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Today: “Basic” robust machine learning

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

- 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

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

Warm up: Flexibility of the template

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

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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

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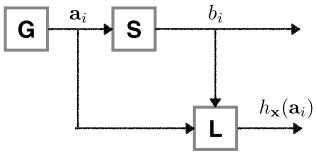
A deep learning optimization problem in supervised learning



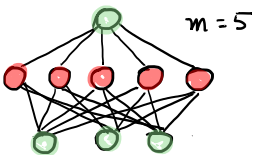
Definition (Optimization formulation)

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

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

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

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

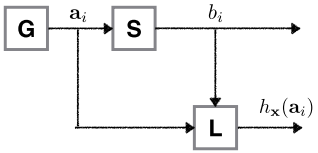


$$h_{\mathbf{x}}(\mathbf{a}) := \begin{bmatrix} \mathbf{X}_2 \end{bmatrix} \sigma \left(\begin{bmatrix} \mathbf{X}_1 \end{bmatrix} \begin{bmatrix} \mathbf{a} \end{bmatrix} + \begin{bmatrix} \mu_1 \end{bmatrix} \right) + \begin{bmatrix} \mu_2 \end{bmatrix}$$

activation (over σ); weight (over $\mathbf{X}_1$); input (over $\mathbf{a}$); bias (over μ_1); bias (over μ_2)

hidden layer = learned features

A deep learning optimization problem in supervised learning



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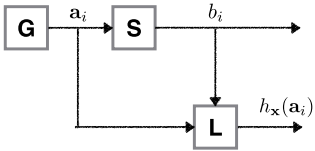
Adversarial Training

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

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

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

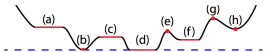
- $\min_{\mathbf{x}} \left\{ \frac{1}{n}\sum_{i=1}^{n} \left[\max_{\boldsymbol{\delta}:\|\boldsymbol{\delta}\|_\infty \le \epsilon} L\left(h_{\mathbf{x}}\left(\mathbf{a}_i+\boldsymbol{\delta}\right), \mathbf{b}_i\right) \right] \right\}$ — Adversarial training [11].
- $\min_{\mathbf{x}} \left\{ \frac{1}{n}\sum_{i=1}^{n} \left[\max_{\boldsymbol{\delta}:\|\boldsymbol{\delta}\|_2 \le \epsilon} L(h_{\mathbf{x}+\boldsymbol{\delta}}\left(\mathbf{a}_i\right), \mathbf{b}_i) \right] \right\}$ — ϵ-stability training [3], Sharpness-aware minimization [7].
- $\min_{\mathbf{x}} \max_{\mathbf{b}^c\in[C]} \frac{1}{n_c}\sum_{i=1}^{n_c} \left[\max_{\boldsymbol{\delta}:\|\boldsymbol{\delta}\| \le \epsilon} L\left(h_{\mathbf{x}}\left(\mathbf{a}_i+\boldsymbol{\delta}\right), \mathbf{b}_i^c\right) \right]$ — Class fairness [16].

Basic questions on solution concepts

- Consider the finite sum setting

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

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



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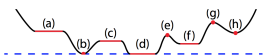

Vanilla (Minibatch) SGD
Input: Stochastic gradient oracle $\mathbf{g}$, initial point x^0, step size α_k
1. For $k = 0, 1, \ldots$: obtain the (minibatch) stochastic gradient $\mathbf{g}^k$ update $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k - \gamma_k \mathbf{g}^k$

Solving the outer problem: Gradient computation

Adversarial Training

Let $h_{\mathbf{x}} : \mathbb{R}^p \to \mathbb{R}$ be a model with parameters $\mathbf{x}$ and let $\{(\boldsymbol{a}_i, \mathbf{b}_i)\}_{i=1}^n$, with $\boldsymbol{a}_i \in \mathbb{R}^p$ 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 $i \sim \text{Uniform}\{1, \ldots, n\}$):

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

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

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

Theorem ([5])

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

$$f(\mathbf{x}) \coloneqq \max_{\mathbf{y} \in \mathcal{S}} \Phi(\mathbf{x}, \mathbf{y}), \qquad \mathcal{S}^\star(\mathbf{x}) \coloneqq \arg\max_{\mathbf{y} \in \mathcal{S}} \Phi(\mathbf{x}, \mathbf{y}).$$

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

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

An immediate consequence

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

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

Optimized perturbations are typically not unique!

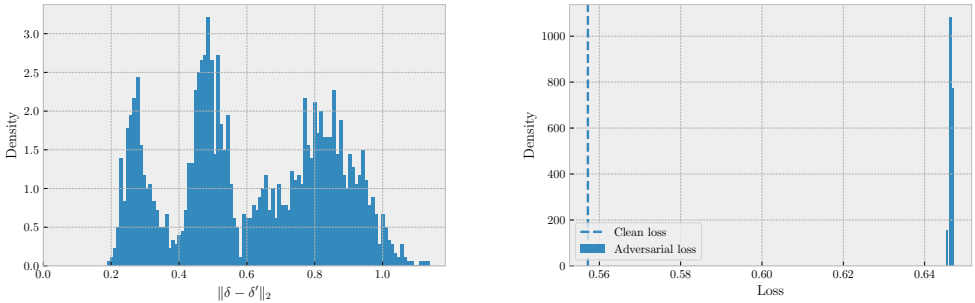

Figure: (*left*) Pairwise ℓ_2-distances between "optimized" perturbations with different initializations are bounded away from zero. (*right*) The losses of multiple perturbations on the same sample concentrate around a value much larger than the clean loss.

Theoretical foundations

	unique $\delta^\star$	non-unique $\delta^\star$
$\nabla_{\mathbf{x}}\Phi(\mathbf{x},\delta^\star)$	$\nabla_{\mathbf{x}} f(\mathbf{x})$	descent direction [13]

Published as a conference paper at ICLR 2018

TOWARDS DEEP LEARNING MODELS RESISTANT TO ADVERSARIAL ATTACKS

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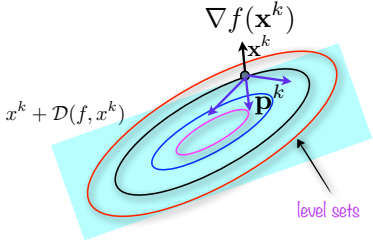

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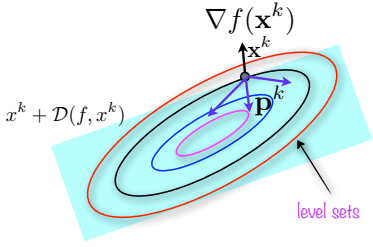
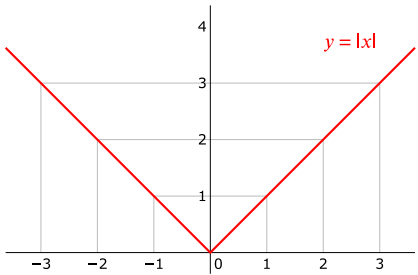


A counterexample

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



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

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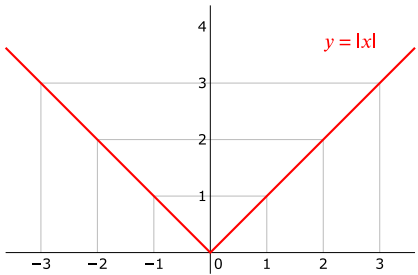

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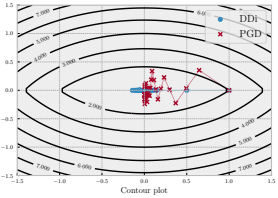
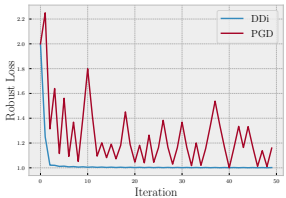
- At $\mathbf{x} = 0$, we have $\mathcal{S}^\star(0) = [-1, 1]$.
- We can choose $\delta = 1 \in \mathcal{S}^\star(0)$: $\Phi(\mathbf{x}, 1) = \mathbf{x}$.
  - $-\nabla_{\mathbf{x}} \Phi(0, 1) = -1 \neq 0$.
  - Is -1 a descent direction at $\mathbf{x} = 0$?

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

- The corollary in [13] is false (it is subtle!).
- We constructed a counter example & proposed an alternative way (DDi) of computing "the gradient":

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





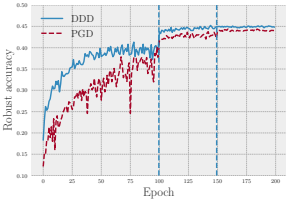


Figure: Left and middle pane: comparison DDi and PGD ([13]) on a synthetic problem. Right pane: DDi vs PGD on CIFAR10.

Comparison with the state-of-the-art

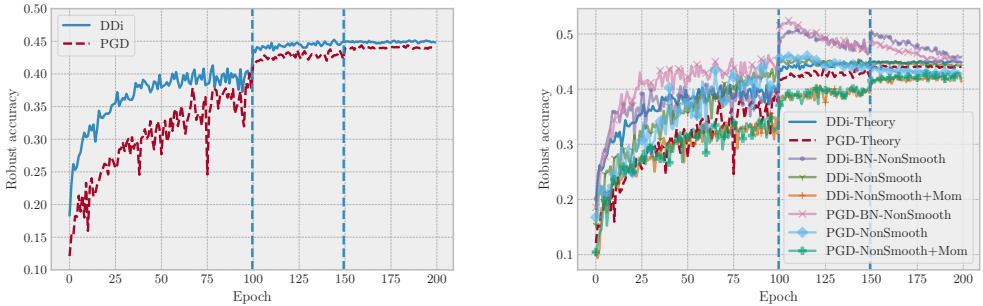
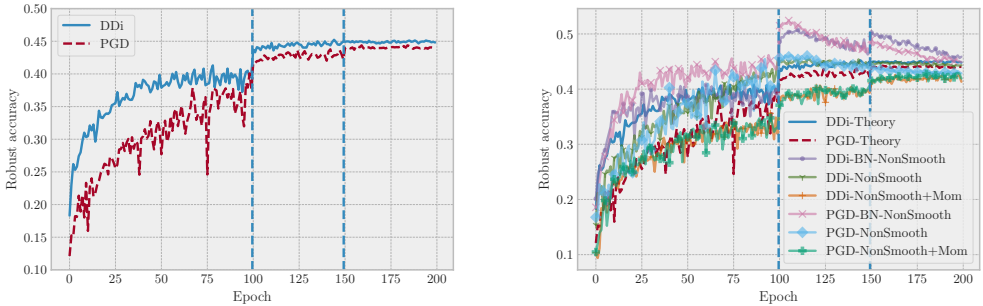


Figure: (left) PGD vs DDi on CIFAR10, in a setting covered by theory. (right) An ablation testing the effect of adding back the elements not covered by theory (BN,ReLU,momentum).

Comparison with the state-of-the-art



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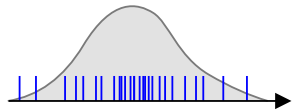
DDi + Graduate Student Descent may improve things (performance or catastrophic overfitting)?

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 [1]

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

$$\min_{\mathbf{x}\in\mathcal{X}} \left(\max_{\mathbf{y}\in\mathcal{Y}} \boldsymbol{E}_{\mathbf{a}\sim\hat{\mu}_n} \left[\mathsf{d}_{\mathbf{y}}(\mathbf{a})\right] - \boldsymbol{E}_{\boldsymbol{\omega}\sim\mathsf{p}_\Omega} \left[\mathsf{d}_{\mathbf{y}}(h_{\mathbf{x}}(\boldsymbol{\omega}))\right] \right). \tag{1}$$

This problem is already captured by the template $\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x}, \mathbf{y})$. 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 Danskin. Need a direct approach.
- Scalability, mode collapse, catastrophic forgetting. Heuristics galore!
- Enforce Lipschitz constraint weight clipping, gradient penalty, spectral normalization [1, 9, 15].

Abstract minmax formulation

Minimax formulation

$$\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y}), \tag{2}$$

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:

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

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

Definition (Local Nash Equilibrium)

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

$$\Phi\left(\mathbf{x}^\star, \mathbf{y}\right) \leq \Phi\left(\mathbf{x}^\star, \mathbf{y}^\star\right) \leq \Phi\left(\mathbf{x}, \mathbf{y}^\star\right) \qquad \text{(LNE)}$$

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

Abstract minmax formulation

Minimax formulation

$$\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} \Phi(\mathbf{x},\mathbf{y}), \tag{3}$$

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?

A buffet of negative results [6]

"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 $\mathbf{z} = [\mathbf{x},\mathbf{y}]$.

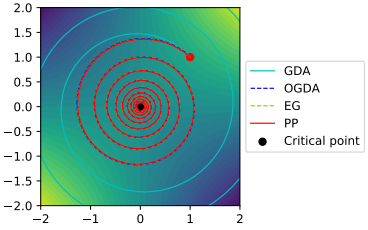


Figure: Trajectory of different algorithms for a simple bilinear game $\min_x \max_y xy$.

- (In)Famous algorithms
  - Gradient Descent Ascent (GDA)
  - Proximal point method (PPM) [18, 8]
  - Extra-gradient (EG) [12]
  - Optimistic GDA (OGDA) [19, 14]
  - Reflected-Forward-Backward-Splitting (RFBS) [4]
- EG and OGDA are approximations of the PPM
  - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha V(\mathbf{z}^k)$.
  - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha V(\mathbf{z}^{k+1})$.
  - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha V(\mathbf{z}^k - \alpha V(\mathbf{z}^k))$.
  - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha[2V(\mathbf{z}^k) - V(\mathbf{z}^{k-1})]$.
  - $\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha V(2\mathbf{z}^k - \mathbf{z}^{k-1})$.

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: $\boldsymbol{E}U(\mathbf{z},\zeta) = 0$,
  - 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: [10]

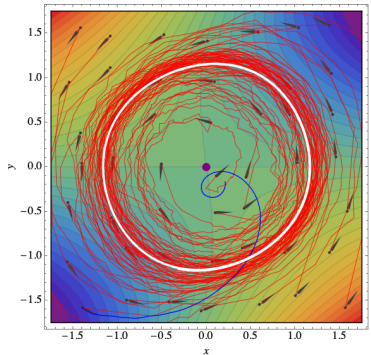
1. Bounded trajectories of $\mathcal{A}$ always converge to an internally chain-transitive (ICT) set.
2. Trajectories of $\mathcal{A}$ may converge with arbitrarily high probability to spurious attractors that contain no critical point of Φ.

Minimax is more difficult than just optimization [10]

- Internally chain-transitive (ICT) sets characterize the convergence of dynamical systems [2].
  - For optimization, {attracting ICT} $\equiv$ {solutions}
  - For minimax, {attracting ICT} $\equiv$ {solutions} $\cup$ {spurious sets}

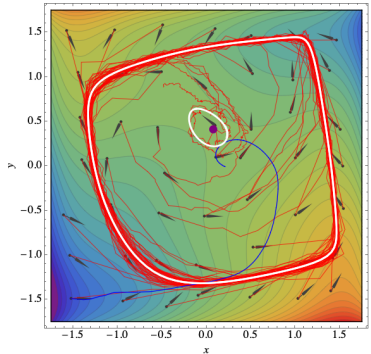
- "Almost" bilinear $\neq$ bilinear:

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



- 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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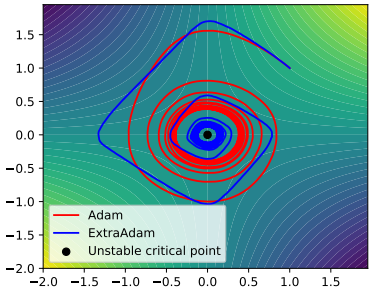

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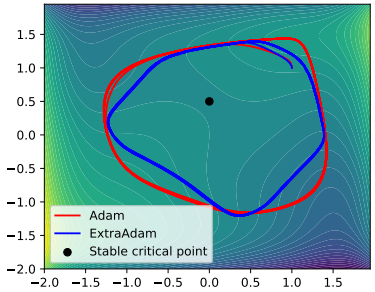


When do the algorithms converge?

Assumption (weak Minty variational inequality)

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

$$\langle V(\mathbf{z}), \mathbf{z} - \mathbf{z}^\star \rangle \geqslant \rho \|V(\mathbf{z})\|^2, \quad \textit{for all } \mathbf{z} \in \mathbb{R}^n. \qquad (4)$$

- A variant EG+ converges when $\rho > -\frac{1}{8L}$
  - Diakonikolas, Daskalakis, Jordan, AISTATS 2021.
- It still cannot handle the examples of [10].

- 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 [10]
  - adaptive variants handling the examples of [10]

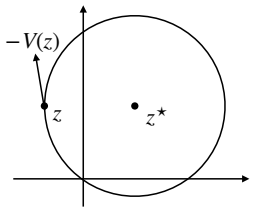
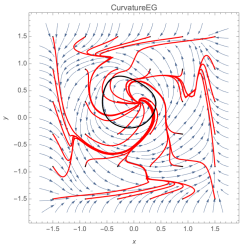
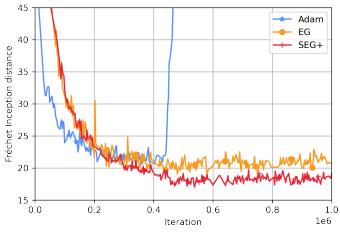
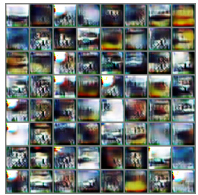


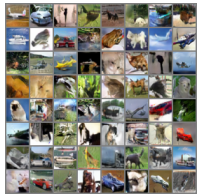
Figure: The operator $V(z)$ is allowed to point away from the solution by some amount when ρ is negative.



GANs with SEG+ [17]







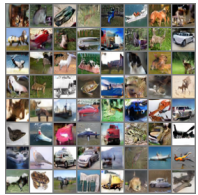


Figure: A performance comparison of GAN training by Adam, EG with stochastic gradients, and SEG+.

Robustness of the worst-performing class [16]

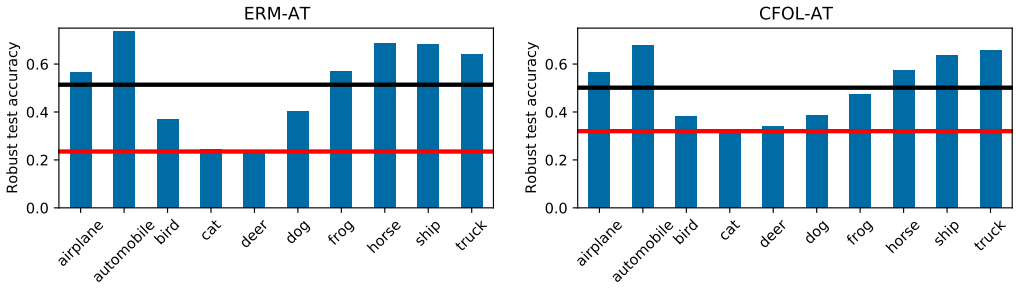


Figure: Robust test accuracy of (a) Empirical Risk Minimization and (b) the class focused online learning.

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)

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

Original Formulation of Adversarial Training (I)

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

which loss L?

Original Formulation of Adversarial Training (II)

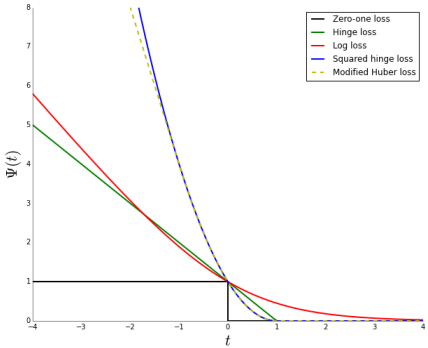
$$\min_{\mathbf{x}} \mathbb{E}\left[\max_{\boldsymbol{\delta}:\|\boldsymbol{\delta}\|\leq\epsilon} L_{01}(\mathbf{x}, \mathbf{a}+\boldsymbol{\delta}, \mathbf{b})\right]$$

Original Formulation of Adversarial Training (II)

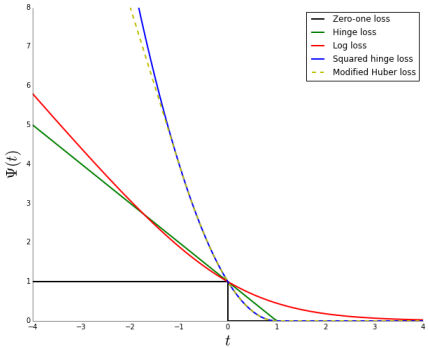
$$\min_{\mathbf{x}} \mathbb{E}\left[\max_{\boldsymbol{\delta}:\|\boldsymbol{\delta}\|\leq\epsilon} L_{01}(\mathbf{x}, \mathbf{a}+\boldsymbol{\delta}, \mathbf{b})\right]$$

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

Surrogate-based optimization for Risk Minimization



Surrogate-based optimization for Risk Minimization

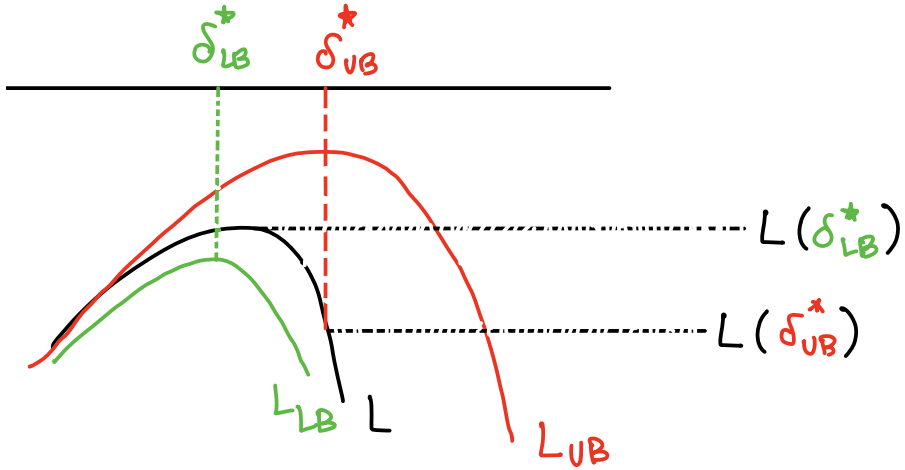


$$\mathbb{E}\left[L_{01}(\mathbf{x}^\star, \mathbf{a}, \mathbf{b})\right] \leq \min_{\mathbf{x}} \mathbb{E}\left[L_{\mathsf{CE}}(\mathbf{x}, \mathbf{a}, \mathbf{b})\right]$$

Adversary maximizes an upper bound (I)

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

Adversary maximizes an upper bound (II)



Why maximizing cross-entropy leads to weak adversaries

x

δ_A

$+$ $=$

$(.49, .51, \quad 0, \quad 0)$

$\mathcal{L}_{\mathrm{CE}}(\theta, x + \delta_A, \text{🐶}) = 1.18$

δ_B

$+$ $=$

$(.26, .24, \quad .25, \quad .25)$

$\mathcal{L}_{\mathrm{CE}}(\theta, x + \delta_B, \text{🐶}) = 1.38$

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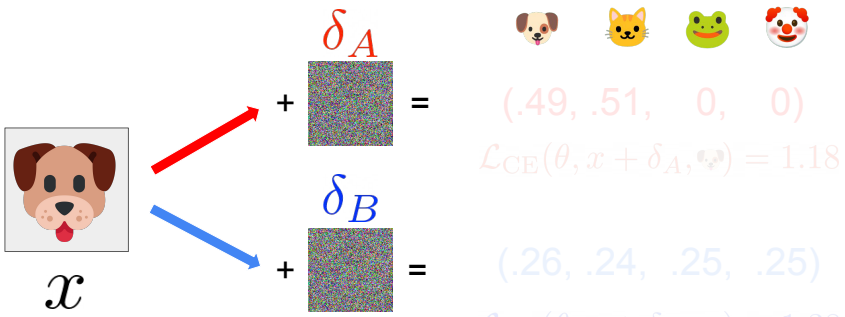

Why maximizing cross-entropy leads to weak adversaries

x

$+ \; \delta_A =$

$+ \; \delta_B =$

🐶 🐱 🐸 🤡

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Adversary's problem can be "solved" without using surrogates

Theorem (Reformulation of the Adversary's problem)

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

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

Bilevel Optimization [Robey,* Latorre,* Pappas, Hassani, Cevher(2023)][1]

- Best targeted attack (BETA) optimization formulation:

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

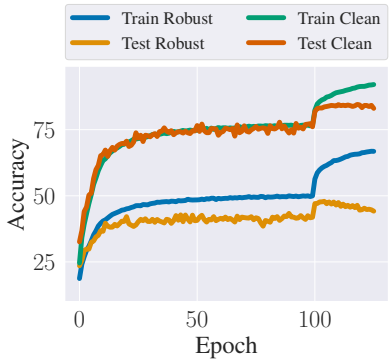
$$\text{such that } \boldsymbol{\delta}^{\star}_{i,j} \in \underset{\boldsymbol{\delta}:\, \|\boldsymbol{\delta}\|\leq\epsilon}{\arg\max}\, h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\delta})_j - h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\delta})_{\mathbf{b}_i}$$

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

[1] https://infoscience.epfl.ch/record/302995 or https://tinyurl.com/33yup77v

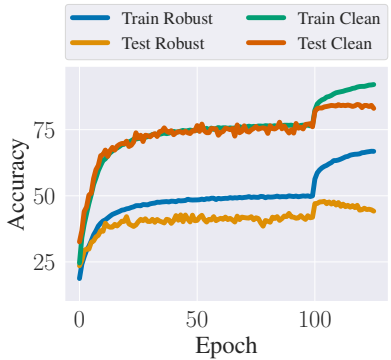
Practical Consequences of the Bilevel Formulation (I)

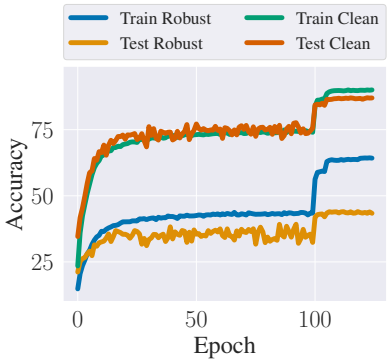
Figure: Learning curves of PGD^{10}-AT (Left) and BETA^{10}-AT



Practical Consequences of the Bilevel Formulation (I)

Figure: Learning curves of PGD^{10}-AT (Left) and BETA^{10}-AT (Right). Robust accuracy estimated with PGD^{20}





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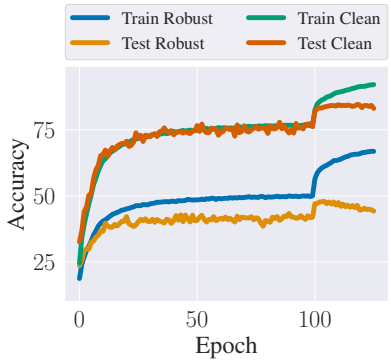
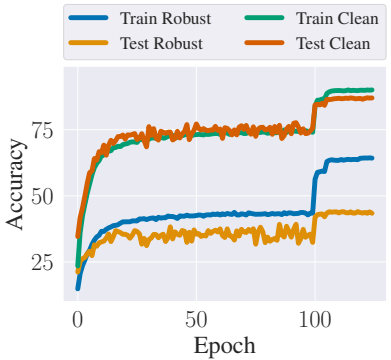




No Robust Overfitting occurs!

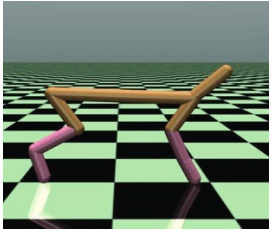
Practical Consequences of the Bilevel Formulation (I)

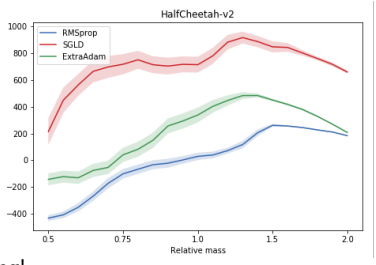
Training algorithm	Test accuracy					
	Clean		BETA^{10}		APGD	
	Best	Last	Best	Last	Best	Last
FGSM	81.96	75.43	40.30	0.04	41.56	0.00
PGD^{10}	83.71	83.21	43.64	40.21	44.36	42.62
TRADES^{10}	81.64	81.42	44.31	40.97	43.34	41.33
MART^{10}	78.80	77.20	44.81	41.22	45.00	42.90
BETA-AT^{5}	87.02	86.67	42.62	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 attempts[1] consider "mixed Nash" concepts[2]





- Existing theory and methods for adversarial training is wrong!

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

[2] K. 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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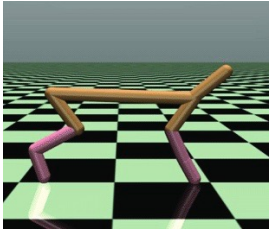
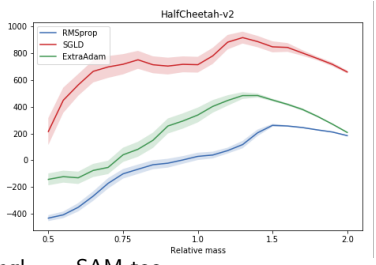
- $\min$-$\max$-type has spurious attractors with no equivalent concept in $\min$-type
- Not all step-size schedules are considered in our work: Possible to "converge" under some settings
- Other successful attempts[1] consider "mixed Nash" concepts[2]





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

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