Adversarial training should be cast as a non-zero sum game

Volkan Cevher

volkan.cevher@epfl.ch

Applied Algorithms for Machine Learning

Laboratory for Information and Inference Systems (LIONS)
École Polytechnique Fédérale de Lausanne (EPFL)
Switzerland

Paris, France

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- Many talented collaborators
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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

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

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

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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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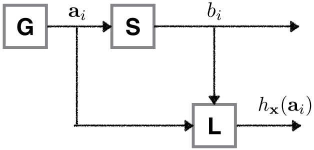
A deep learning optimization problem in supervised learning



Definition (Optimization formulation)

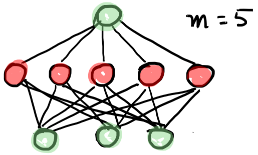
The "deep-learning" problem with a neural network $h_{\mathbf{x}}(\mathbf{a})$ is given by

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

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

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

$$h_{\mathbf{x}}(\mathbf{a}) := \begin{bmatrix} \mathbf{X}_2 \end{bmatrix} \underbrace{\overset{\text{activation}}{\sigma}\left(\begin{bmatrix} \overset{\text{weight}}{\mathbf{X}_1} \end{bmatrix} \overset{\text{input}}{\begin{bmatrix} \mathbf{a} \end{bmatrix}} + \overset{\text{bias}}{\begin{bmatrix} \mu_1 \end{bmatrix}} \right) + \overset{\text{bias}}{\begin{bmatrix} \mu_2 \end{bmatrix}}}_{\text{hidden layer} \,=\, \text{learned features}}$$



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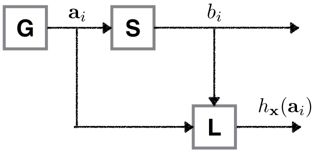

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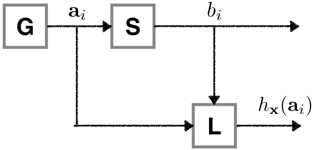
Adversarial Training

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

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

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

Example objectives in different tasks

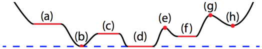
- $\min_{\mathbf{x}} \left\{ \frac{1}{n}\sum_{i=1}^{n} \left[\max_{\boldsymbol{\delta}:\|\boldsymbol{\delta}\|_\infty\le\epsilon} L\left(h_{\mathbf{x}}\left(\mathbf{a}_i+\boldsymbol{\delta}\right),\mathbf{b}_i\right)\right]\right\}$ Adversarial training [14].
- $\min_{\mathbf{x}} \left\{ \frac{1}{n}\sum_{i=1}^{n} \left[\max_{\boldsymbol{\delta}:\|\boldsymbol{\delta}\|_2\le\epsilon} L(h_{\mathbf{x}+\boldsymbol{\delta}}\left(\mathbf{a}_i\right),\mathbf{b}_i)\right]\right\}$ ϵ-stability training [5], Sharpness-aware minimization [9].
- $\min_{\mathbf{x}} \max_{\mathbf{b}^c\in[C]} \frac{1}{n_c}\sum_{i=1}^{n_c}\left[\max_{\boldsymbol{\delta}:\|\boldsymbol{\delta}\|\le\epsilon} L\left(h_{\mathbf{x}}\left(\mathbf{a}_i+\boldsymbol{\delta}\right),\mathbf{b}_i^c\right)\right]$ Class fairness [20].

Basic questions on solution concepts

- Consider the finite sum setting

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

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



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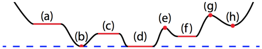

Vanilla (Minibatch) SGD

Input: Stochastic gradient oracle $\mathbf{g}$, initial point $\boldsymbol{x}^0$, 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

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

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

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 $i \sim \text{Uniform}\{1, \ldots, n\}$):

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

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

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

Theorem ([7])

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

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

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

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

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

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Observation: ○ Solving the inner problem can be expensive!

A cheap alternative: Fast gradient sign method (FGSM) [10]

Projected gradient descent (PGD) attack: A misnomer

Let $\boldsymbol{\delta}^{(0)} = \mathbf{0}$, the PGD update rule is given by:

$$\begin{aligned}
\hat{\boldsymbol{\delta}}^{(t)} &= \boldsymbol{\delta}^{(t-1)} + \alpha \cdot \mathsf{sign}\left(\nabla_{\boldsymbol{\delta}} L\left(h_{\mathbf{x}}\left(\mathbf{a} + \boldsymbol{\delta}^{(t-1)}\right), b\right)\right) && \text{[Gradient step]} \\
\boldsymbol{\delta}^{(t)} &= \max\left\{\min\left\{\hat{\boldsymbol{\delta}}^{(t)}, \epsilon\right\}, -\epsilon\right\}, && \text{[Projection step]}
\end{aligned}$$

where α is the step-size and the procedure is ran for T steps. If $T = 1$ and $\alpha = \epsilon$ we recover the FGSM:

$$\boldsymbol{\delta}_{\mathsf{FGSM}} = \epsilon \cdot \mathsf{sign}\left(\nabla_{\boldsymbol{\delta}} L\left(h_{\mathbf{x}}(\mathbf{a}), b\right)\right).$$

Problems:

- In Adversarial Training: $\times T$ overhead in training time.
- If $T = 1$, we can observe **Catastrophic Overfitting (CO)**.

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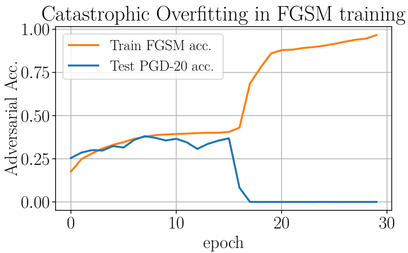
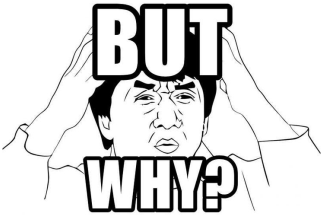
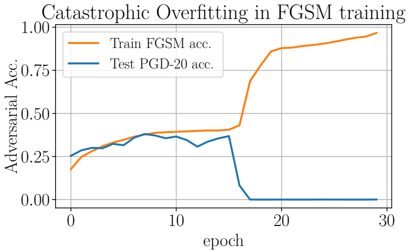
Example:

- PreActResNet18 on CIFAR10 at $\epsilon = 8/255$.
- 100% robust to FGSM attacks.
- 0% robust to PGD-20 attacks.



More on CO





Linearizations may not be accurate

The single step solution $\boldsymbol{\delta}_{\text{FGSM}}$ only makes sense if our loss is locally linear, i.e.:

$$L\left(h_{\mathbf{x}^k}(\mathbf{a}+\boldsymbol{\delta}), b\right) \approx L\left(h_{\mathbf{x}^k}(\mathbf{a}), b\right) + \boldsymbol{\delta}^\top \nabla_{\mathbf{a}} L\left(h_{\mathbf{x}^k}(\mathbf{a}), b\right) \,, \quad \forall \boldsymbol{\delta} : ||\boldsymbol{\delta}||_\infty \leq \epsilon \,. \quad \text{[1st order Taylor expansion]}$$

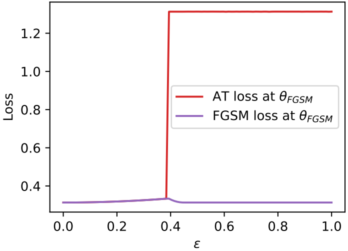
Observation: This property is lost during AT with FGSM and CO appears [2].

A phase transition in adversarial training

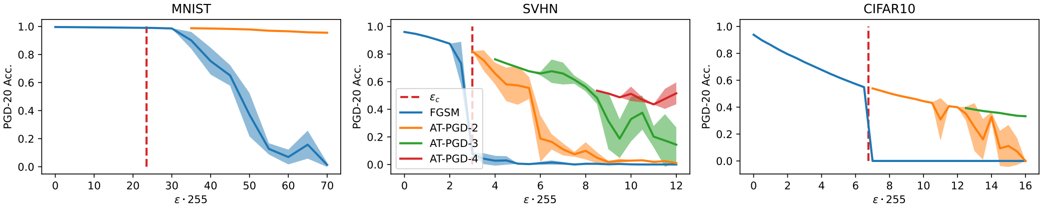
- There is a qualitative increase in difficulty in computation

A toy model for CO (Levi, Abad Rocamora and Cevher, 2024)

Let $\mathrm{a}_2 = \pi/2 = -\mathrm{a}_1$ with labels $b_1 = -1$ and $b_2 = 1$. Let the classifier $h_{\mathrm{x}}(\mathrm{a}) = \sin(\mathrm{x} \cdot \mathrm{a})$ with a single trainable parameter x. CO happens in FGSM AT for $\epsilon > \epsilon_c = \pi/8$.

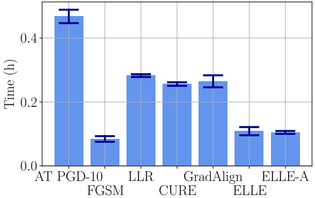


- We provide ϵ_c estimates for the MNIST, SVHN and CIFAR10 datasets.



The ELLE way [Abad Rocamora, Liu, Chrysos, Olmos and Cevher, ICLR 2024]

- If it does not succeed by itself, enforce it...



(a) Training time comparison

ϵ	8		16	
Method	AutoAttack	Clean	AutoAttack	Clean
LLR	42.18 ± (0.20)	75.02 ± (0.09)	16.92 ± (0.20)	42.81 ± (9.62)
CURE	43.60 ± (0.17)	77.74 ± (0.11)	18.25 ± (0.45)	52.49 ± (0.04)
GradAlign	**44.66** ± (0.21)	**80.50** ± (0.07)	17.46 ± (1.71)	44.35 ± (15.32)
ELLE	42.78 ± (0.95)	80.13 ± (0.32)	**18.28** ± (0.17)	**59.73** ± (0.16)
ELLE-A	44.32 ± (0.04)	79.81 ± (0.10)	18.03 ± (0.15)	59.21 ± (1.23)
AT PGD-10	46.95 ± (0.11)	79.11 ± (0.08)	24.77 ± (0.26)	59.64 ± (0.46)

(b) PreActResNet18 in CIFAR10

Algorithmic approaches:

- Local linearization (LLR) [22]
- Curvature regularization (CURE) [19]
- Gradient alignment (GradAlign) [2]
- Efficient local linearity regularization (ELLE) [1]

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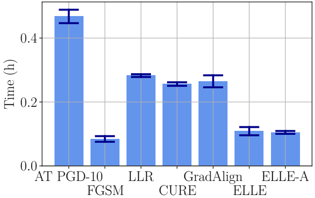

(c) Training time comparison

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- Gradient alignment (GradAlign) [2]
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Question:

- Does the ultimate robustness lie in increasing the inner iterations T (e.g., PGD-10)?

Optimized perturbations are typically not unique!

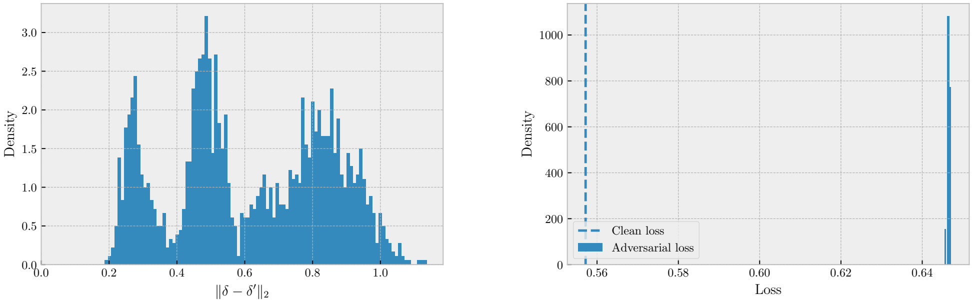
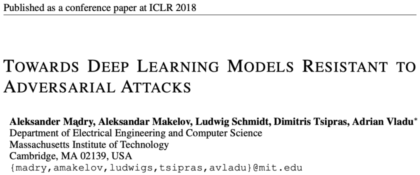


Figure: (*left*) Pairwise ℓ_2-distances between "optimized" perturbations with different initializations are bounded away from zero. (*right*) The losses of multiple perturbations on the same sample concentrate around a value much larger than the clean loss.

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 [16]



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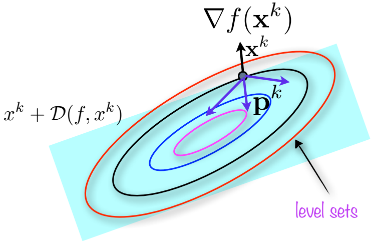
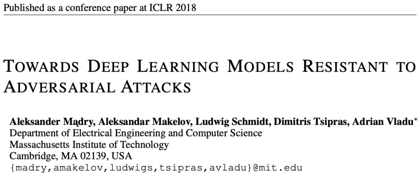
Towards Deep Learning Models Resistant to Adversarial Attacks

Aleksander Mądry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, Adrian Vladu[*]
Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology
Cambridge, MA 02139, USA
`{madry,amakelov,ludwigs,tsipras,avladu}@mit.edu`



Theoretical foundations ?

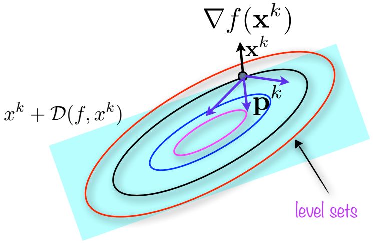
	unique $\delta^\star$	non-unique $\delta^\star$
$\nabla_{\mathbf{x}}\Phi(\mathbf{x},\delta^\star)$	$\nabla_{\mathbf{x}} f(\mathbf{x})$	descent direction [16]



Published as a conference paper at ICLR 2018

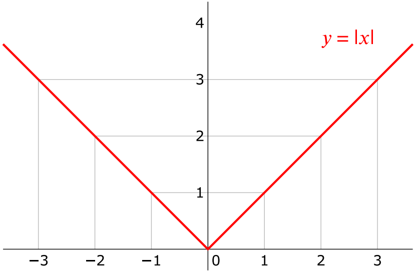
TOWARDS DEEP LEARNING MODELS RESISTANT TO ADVERSARIAL ATTACKS

Aleksander Mądry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, Adrian Vladu*
Department of Electrical Engineering and Computer Science
Massachusetts Institute of Technology
Cambridge, MA 02139, USA
{madry,amakelov,ludwigs,tsipras,avladu}@mit.edu



A counterexample

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



- ◦ We have $\mathcal{S} := [-1, 1]$ 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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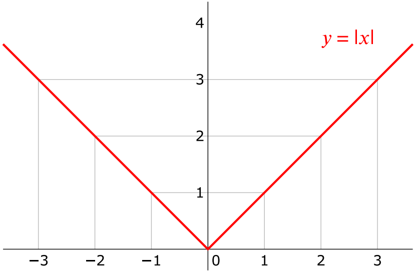

- ○ We have $\mathcal{S} := [-1, 1]$ and $\Phi(\mathbf{x}, \boldsymbol{\delta}) = \mathbf{x}\boldsymbol{\delta}$.
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- ○ We can choose $\delta = 1 \in \mathcal{S}^\star(0)$: $\Phi(\mathbf{x}, 1) = \mathbf{x}$.
  - ▶ $-\nabla_{\mathbf{x}}\Phi(0, 1) = -1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

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

- The corollary in [16] 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!

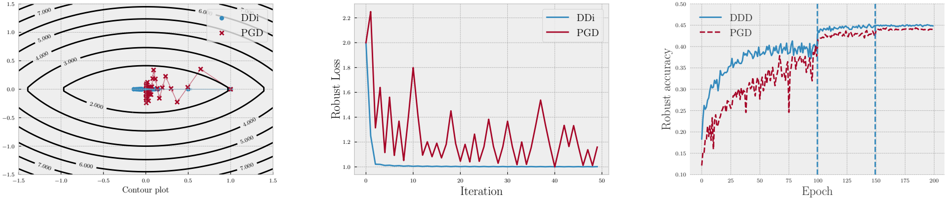

Figure: Left and middle pane: comparison DDi and PGD ([16]) on a synthetic problem. Right pane: DDi vs PGD on CIFAR10.

Comparison with the state-of-the-art

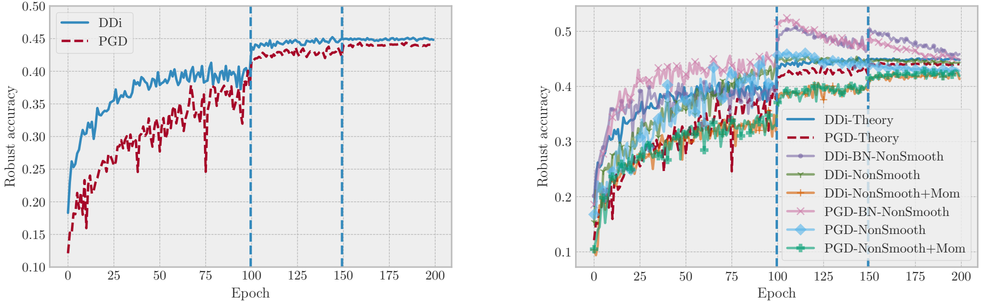

Figure: (left) PGD vs DDi on CIFAR10, in a setting covered by theory. (right) An ablation testing the effect of adding back the elements not covered by theory (BN,ReLU,momentum).

Comparison with the state-of-the-art

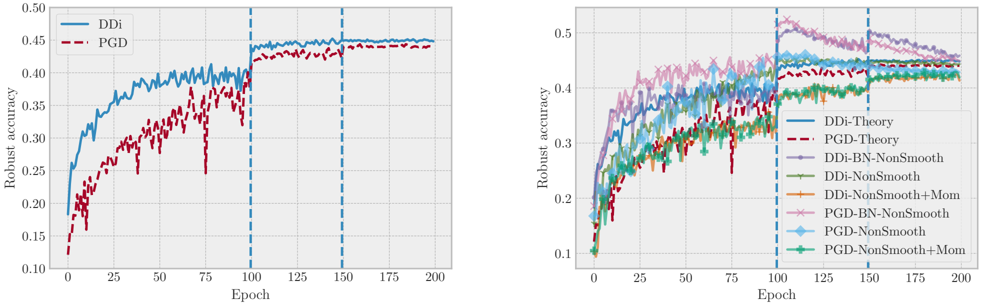

Figure: (left) PGD vs DDi on CIFAR10, in a setting covered by theory. (right) An ablation testing the effect of adding back the elements not covered by theory (BN,ReLU,momentum).

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

Out of the frying pan into the fire

Original Formulation of Adversarial Training (I)

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

Original Formulation of Adversarial Training (I)

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

which loss L?

Original Formulation of Adversarial Training (II)

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

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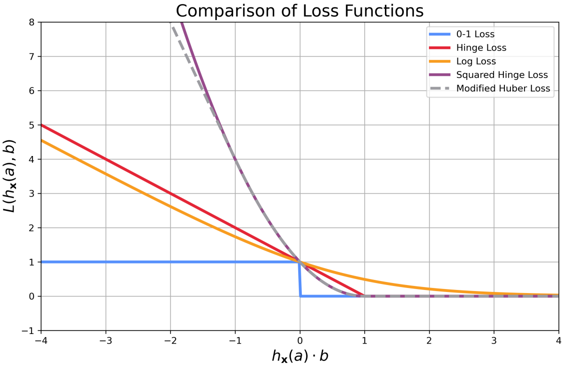
$$\min_{\mathbf{x}} \mathbb{E}\left[\max_{\boldsymbol{\delta}:\|\boldsymbol{\delta}\|\leq\epsilon} L_{01}(h_{\mathbf{x}}(\mathbf{a}+\boldsymbol{\delta}), b)\right]$$

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

Surrogate-based optimization for Risk Minimization



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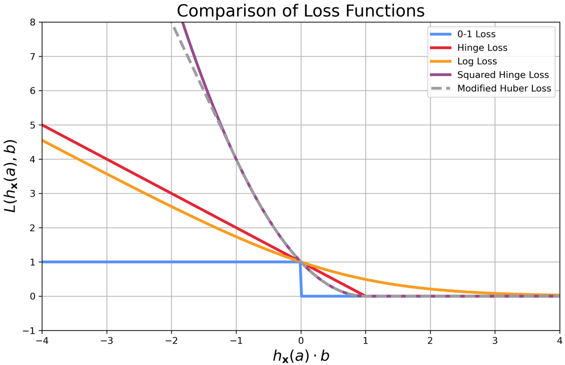
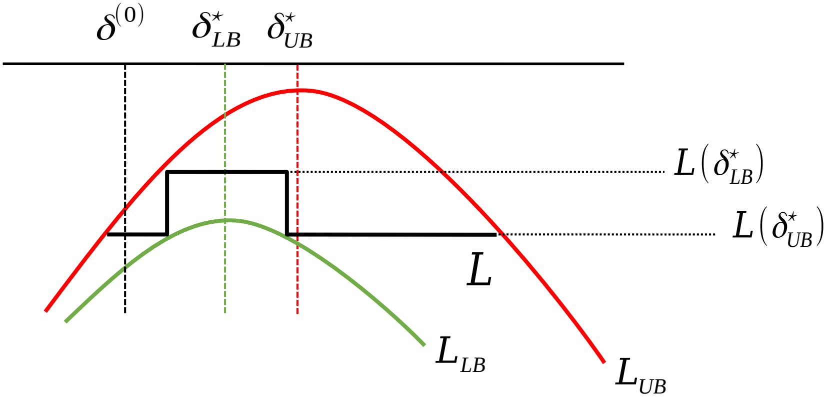


$$\mathbb{E}\left[L_{01}(h_{\mathbf{x}^\star}(\mathbf{a}+\boldsymbol{\delta}), b)\right] \leq \min_{\mathbf{x}} \mathbb{E}\left[L_{\mathsf{CE}}(h_{\mathbf{x}}(\mathbf{a}+\boldsymbol{\delta}), b)\right]$$

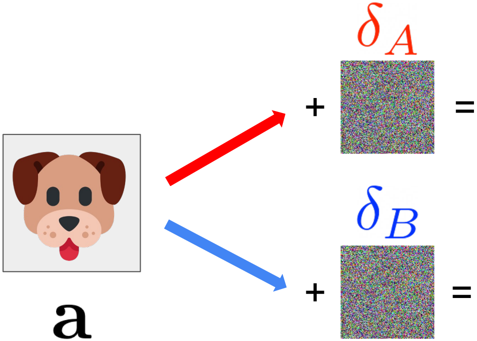
Adversary maximizes an upper bound (I)

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

Adversary maximizes an upper bound (II)



Why maximizing cross-entropy leads to weak adversaries



🐶 🐱 🐸 🤡

(.49, .51, 0, 0)

$L_{\mathrm{CE}}(h_{\mathbf{x}}(\mathbf{a}+\delta_A),$ 🐶 $) = 1.18$

(.26, .24, .25, .25)

$L_{\mathrm{CE}}(h_{\mathbf{x}}(\mathbf{a}+\delta_B),$ 🐶 $) = 1.38$

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:

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

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

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

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

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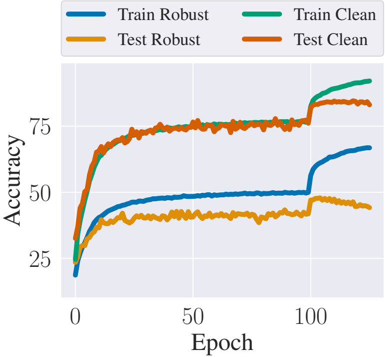
$$j^\star \in \underset{j\in[K]-\{\mathbf{b}_i\}}{\arg\max}\, h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\delta}_{i,j^\star})_j - h_{\mathbf{x}}(\mathbf{a}_i + \boldsymbol{\delta}_{i,j^\star})_{\mathbf{b}_i}$$

Best paper award at ICML AdvML 2023

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

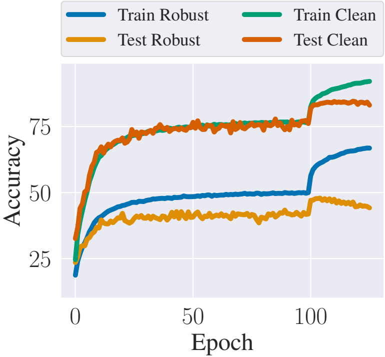
Practical Consequences of the Bilevel Formulation (I)

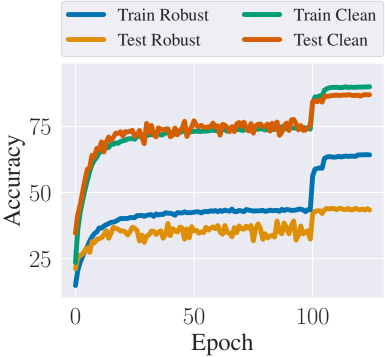
Figure: Learning curves of PGD^{10}-AT (Left) and BETA^{10}-AT



Practical Consequences of the Bilevel Formulation (I)

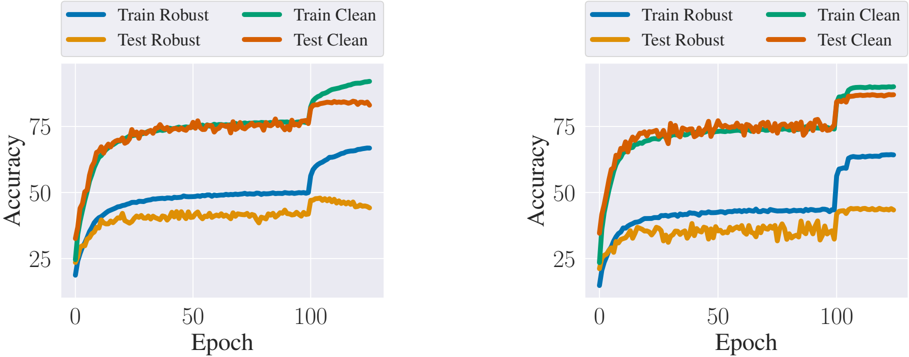
Figure: Learning curves of PGD^{10}-AT (Left) and BETA^{10}-AT (Right). Robust accuracy estimated with PGD^{20}





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}



No Robust Overfitting occurs!

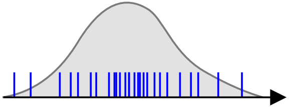
Practical Consequences of the Bilevel Formulation

Table: Adversarial performance on CIFAR-10.

Training algorithm	Test accuracy											
	Clean		FGSM		PGD^{10}		PGD^{40}		BETA^{10}		APGD	
	Best	Last	Best	Last	Best	Last	Best	Last	Best	Last	Best	Last
FGSM	81.96	75.43	**94.26**	**94.22**	42.64	1.49	42.66	1.62	40.30	0.04	41.56	0.00
PGD^{10}	83.71	83.21	51.98	47.39	46.74	39.90	45.91	39.45	43.64	40.21	44.36	42.62
TRADES^{10}	81.64	81.42	52.40	51.31	47.85	42.31	47.76	42.92	44.31	40.97	43.34	41.33
MART^{10}	78.80	77.20	53.84	53.73	49.08	41.12	48.41	41.55	44.81	41.22	45.00	42.90
BETA-AT^{5}	**87.02**	**86.67**	51.22	51.10	44.02	43.22	43.94	42.56	42.62	42.61	41.44	41.02
BETA-AT^{10}	85.37	85.30	51.42	51.11	45.67	45.39	45.22	45.00	44.54	44.36	44.32	44.12
BETA-AT^{20}	82.11	81.72	54.01	53.99	**49.96**	**48.67**	**49.20**	**48.70**	**46.91**	**45.90**	**45.27**	**45.25**

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

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

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 [3, 12, 18].

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 $\mathbf{y}$,
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○ Key questions:

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A buffet of negative results [8]

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

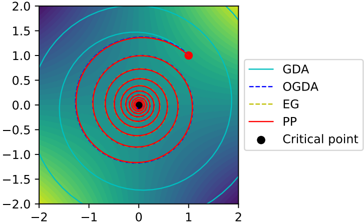


Figure: Trajectory of different algorithms for a simple bilinear game $\min_x \max_y xy$.

- (In)Famous algorithms
  - Gradient Descent Ascent (GDA)
  - Proximal point method (PPM) [23, 11]
  - Extra-gradient (EG) [15]
  - Optimistic GDA (OGDA) [24, 17]
  - Reflected-Forward-Backward-Splitting (RFBS) [6]

- 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: [13]

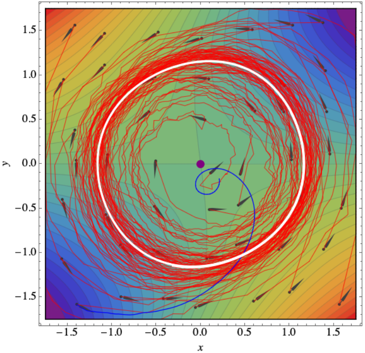
1. Bounded trajectories of $\mathcal{A}$ always converge to an internally chain-transitive (ICT) set.
2. Trajectories of $\mathcal{A}$ may converge with arbitrarily high probability to spurious attractors that contain no critical point of Φ.

Minimax is more difficult than just optimization [13]

- Internally chain-transitive (ICT) sets characterize the convergence of dynamical systems [4].
  - For optimization, {attracting ICT} $\equiv$ {solutions}
  - For minimax, {attracting ICT} $\equiv$ {solutions} $\cup$ {spurious sets}

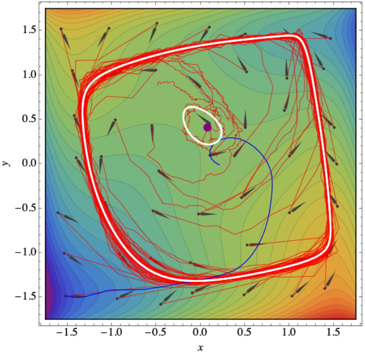
- "Almost" bilinear $\neq$ bilinear:

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



- 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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○ "Almost" bilinear ≠ bilinear:

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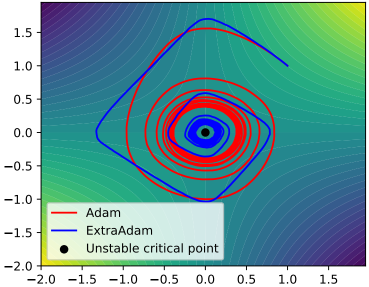

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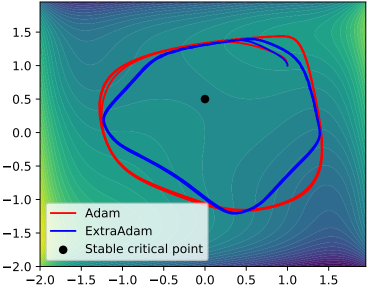


When do the algorithms converge?

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 [13].

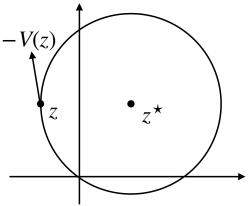
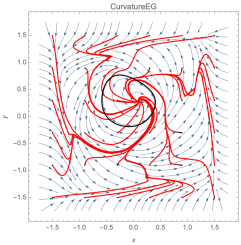


Figure: The operator $V(z)$ is allowed to point away from the solution by some amount when ρ is negative.

- 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 [13]
  - adaptive variants handling the examples of [13]



GANs with SEG+ [21]

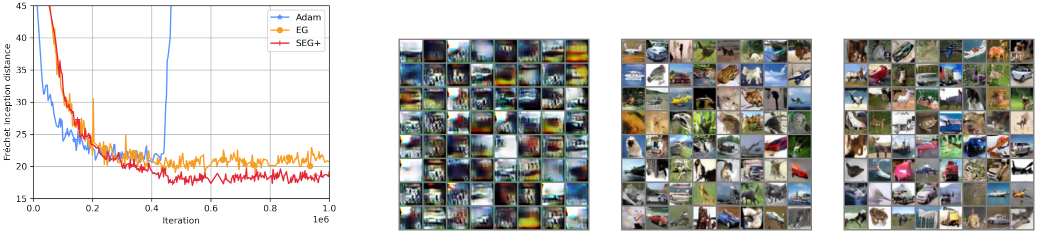
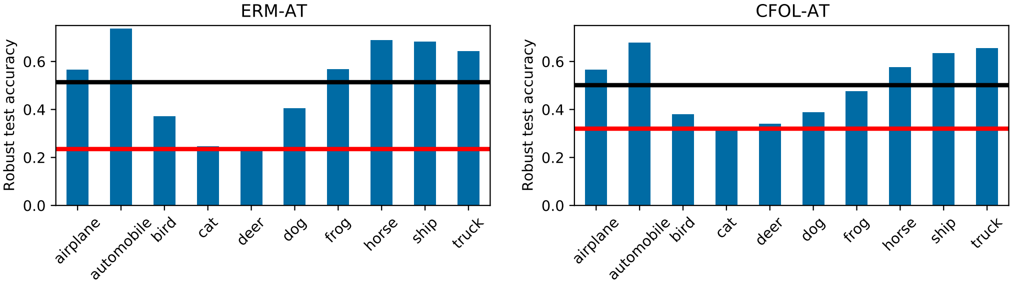


Figure: A performance comparison of GAN training by Adam, EG with stochastic gradients, and SEG+.

Robustness of the worst-performing class [20]



(a)

(b)

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`

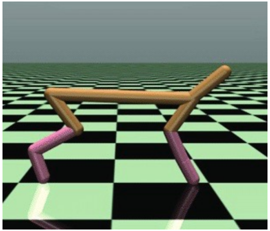
Take home messages

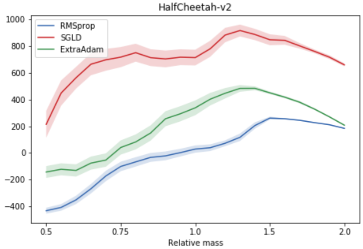
- Even the simplified view of robust & adversarial ML is challenging

- $\min$-$\max$-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! **... SAM too...**[3]

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