Distribution-Dissimilarities in Machine Learning

Carl-Johann SIMON-GABRIEL

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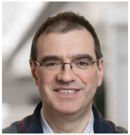
Organizers and Collaborators: Thanks!


Yann Ollivier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Outline

1. Introduction: classifier-based distribution-dissimilarities

2. Maximum Mean Discrepancies (MMD)

3. Adversarial Vulnerability of Neural Networks

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2. Maximum Mean Discrepancies (MMD)

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GANs and distribution-dissimilarities

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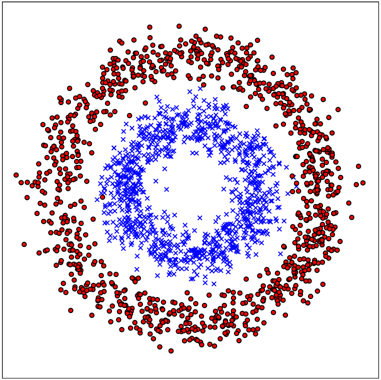

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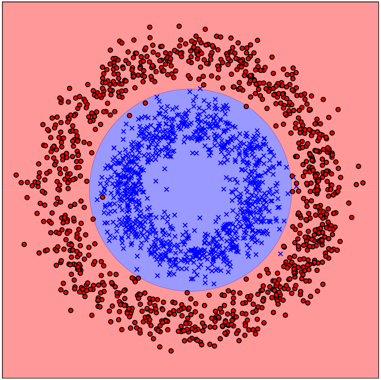

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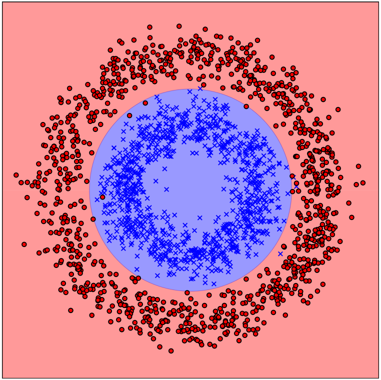

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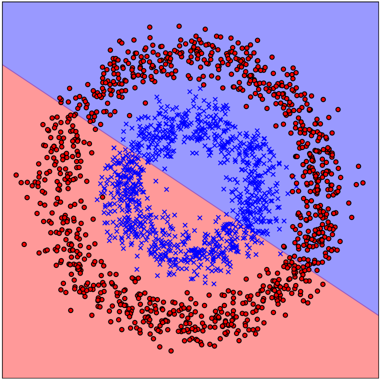

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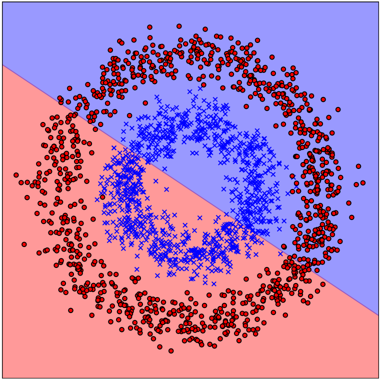

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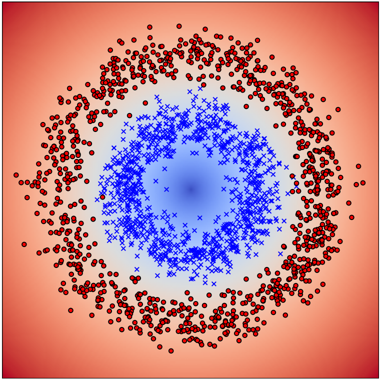

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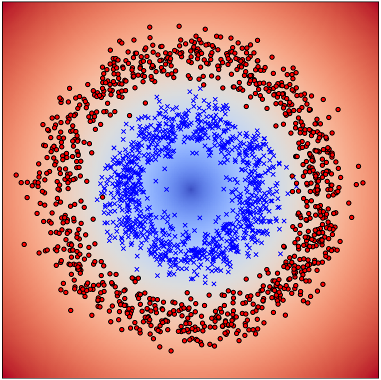

$$D(P, Q) = \sup_{\varphi \in \mathcal{F}} \mathbb{E}_{X,Y} \, \mathcal{R}(\varphi(X), Y)$$

Classifier-based distribution-dissimilarities: Examples

- **IPM**: Fix $\mathcal{R}(\varphi(X), Y) = Y\varphi(X)$; vary $\mathcal{F}$.

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$$\begin{cases} f^*(t) = t & t \in [-1, 1] & \text{TV} \\ f^*(t) = e^{t-1} & t \in \mathbb{R} & \text{KL} \\ f^*(t) = {}^{t}/_{1-t} & t < 1 & \text{Hellinger}^2 \\ f^*(t) = -\log(1 - e^t) & t < \log 2 & \text{JS} \end{cases}$$

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- **Restricted *f*-divergences**: Vary both $\mathcal{R}$ & $\mathcal{F}$.

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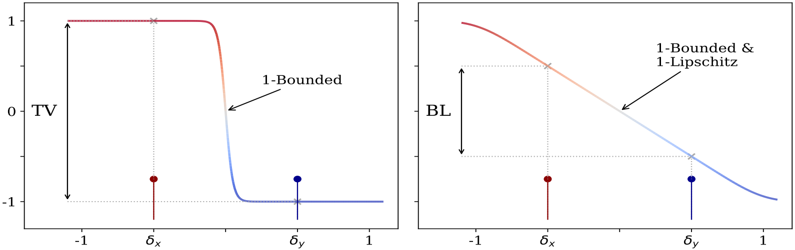

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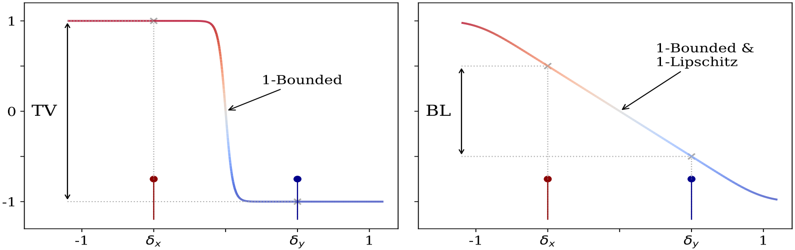

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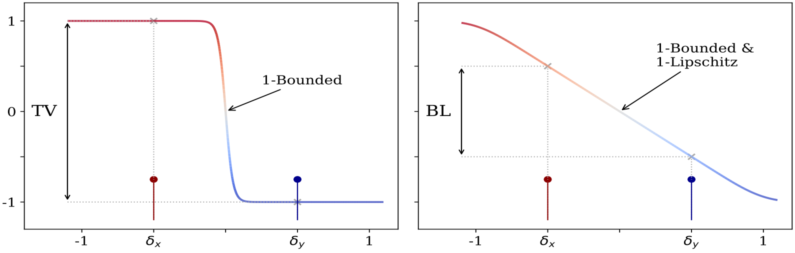

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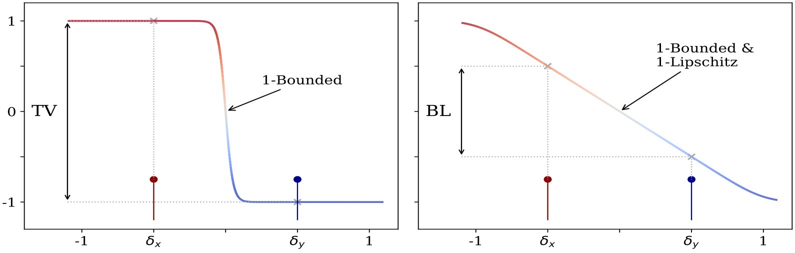

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3. Real-world examples with too high capacity?

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Joint work with

Bernhard Schölkopf

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$\mathscr{F}$	$\mathscr{F}'$	
$\mathscr{C}_0$	$\mathcal{M}_f$	
$\mathscr{C}$	$\mathcal{M}_c$	
$\mathrm{L}^p(\mu)$	$\mathrm{L}^q(\mu)$	
$\mathbb{C}^{\mathcal{X}}$	$\mathcal{M}_\delta$	

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Theorem (Answer to 1: Perfect discrimination [SS18])

If $\mathcal{H}_k \hookrightarrow \mathcal{F}$, the following is equivalent:

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$\mathcal{F}$	$\mathcal{F}'$	
$\mathscr{C}_0$	$\mathcal{M}_f$	c_0-universal
$\mathscr{C}$	$\mathcal{M}_c$	c-universal (or cc-universal)
$\mathrm{L}^p(\mu)$	$\mathrm{L}^q(\mu)$	
$\mathbb{C}^{\mathcal{X}}$	$\mathcal{M}_\delta$	
$((\mathscr{C}_b)_c)/\mathbb{1}$	$\mathscr{P}$ (or $\mathcal{M}_f^0$)	characteristic
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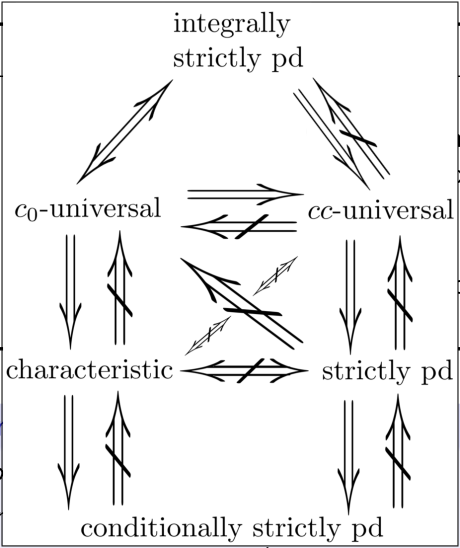

Based on Fig.1.1 [SFL11]

Theorem (Answer

If $\mathcal{H}_k \hookrightarrow \mathcal{F}$, the fo

(i) *$\mathcal{H}_k$ is dense i*

(ii) *MMD_k is perf. discr. over $\mathcal{M} := \mathcal{F}'$*

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- With $\mathcal{M} = \mathscr{P}$: mass can diffuse to infinity $\rightsquigarrow$ Kernel Stein Discrepancies
- If $\mathscr{H}_k \not\subset \mathscr{C}_0$, anything can happen: (i) without (ii) and (ii) without (i)

Conclusion on MMDs

For MMDs, we characterized

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- use other notions of capacity (VC dim, Rademacher complexity, ...)
- what differences/invariances are classifiers sensitive to?

Outline

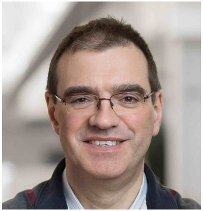
1. Introduction: classifier-based distribution-dissimilarities

2. Maximum Mean Discrepancies (MMD)

3. Adversarial Vulnerability of Neural Networks

Joint work with:

Yann Ollivier



Léon Bottou

Bernhard Schölkopf

David Lopez-Paz

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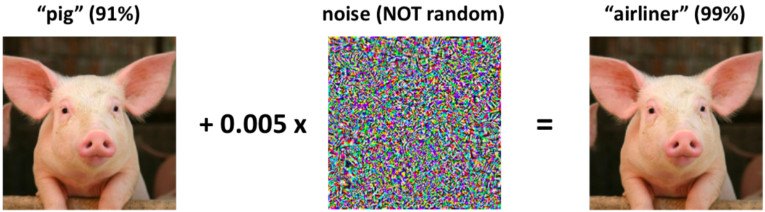

Figure: Madry, NIPS 2018, Adversarial Robustness Workshop

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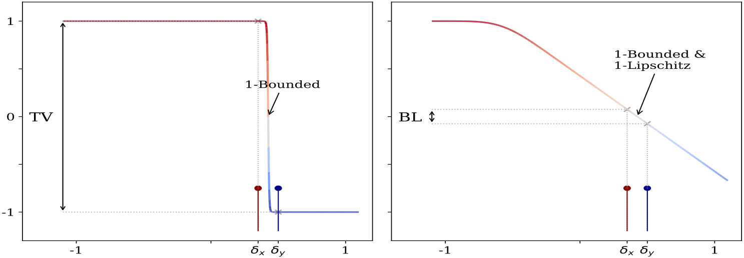

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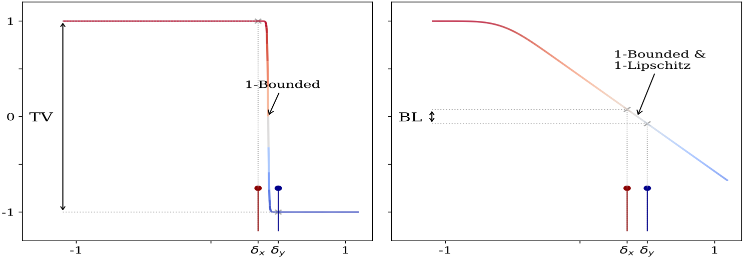

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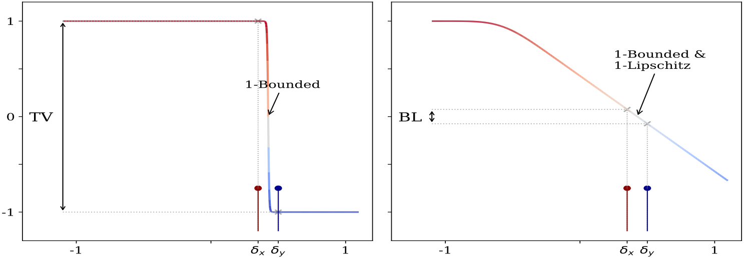

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Goal

Understand why neural networks are adversarially vulnerable.
Can we quantify & predict this vulnerability?

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Adversarially vulnerability increases with dimension

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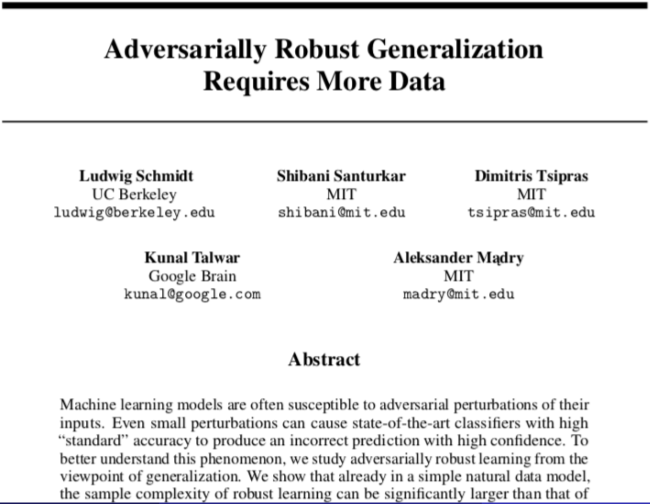
Adversarially Robust Generalization Requires More Data

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Abstract

Machine learning models are often susceptible to adversarial perturbations of their inputs. Even small perturbations can cause state-of-the-art classifiers with high "standard" accuracy to produce an incorrect prediction with high confidence. To better understand this phenomenon, we study adversarially robust learning from the viewpoint of generalization. We show that already in a simple natural data model, the sample complexity of robust learning can be significantly larger than that of

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1. Without data-assumptions, adv. robustness can be hard to get.
2. With structured data, model assumptions can alleviate vulnerability.

For images, higher resolutions should help, not hurt

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Question

What properties of neural nets are not enough adapted to data?

Adversarial Damage and Gradients

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Adversarial Damage and Gradients

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- $\epsilon, \|\cdot\|$-ATTACK: perturbed sample $\boldsymbol{x} + \boldsymbol{\delta}$ s.t. $\|\boldsymbol{\delta}\| \leq \epsilon$.
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$$\mathrm{Adv\,Dam}_{\epsilon,\|\cdot\|} := \mathbb{E}_{\boldsymbol{x}\sim P}\left[\sup_{\|\boldsymbol{\delta}\|\leq\epsilon} \mathcal{L}(\boldsymbol{x}+\boldsymbol{\delta}) - \mathcal{L}(\boldsymbol{x})\right]$$

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&\approx \mathbb{E}_{\boldsymbol{x}\sim P}\left[\sup_{\|\boldsymbol{\delta}\|\leq\epsilon} \partial_{\boldsymbol{x}}\mathcal{L}\cdot\boldsymbol{\delta}\right]
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Assuming that the Taylor-expansion is legit, question:

- How big is $\mathbb{E}_{\boldsymbol{x}} \left[|||\boldsymbol{\partial}_{\boldsymbol{x}} \mathcal{L}||| \right]$ in practice?

Size of $\mathbb{E}_{\boldsymbol{x}}\left[\|\partial_{\boldsymbol{x}}\mathcal{L}\|\right]$ for at initialization

Back to linear layer:

$$\underbrace{\boldsymbol{w}^T(\boldsymbol{x}+\boldsymbol{\delta})}_{\text{perturbed output}} - \underbrace{\boldsymbol{w}^T\boldsymbol{x}}_{\text{unperturbed output}} = \underbrace{\sum_{i=1}^{d} \underbrace{w_i\delta_i}_{+|w_i||\delta|}}_{\text{everything adds up! } \propto d|w||\delta|}$$

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Theorem (Gradient norms of NNs at initialization [SOBS+19])

At (He-)initialization, the adversarial damage of almost any usual feedforward network grows with the input-dimension d as

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Dimension-dependence is independent of network topology.

Gradient norms and vulnerability after training

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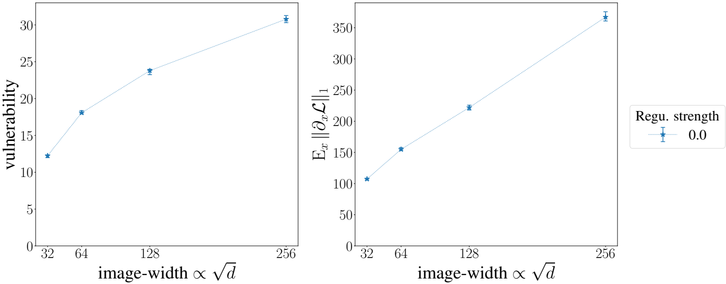

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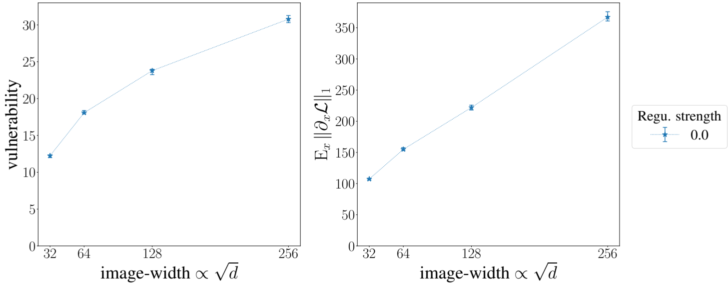
After usual training? After robust training?



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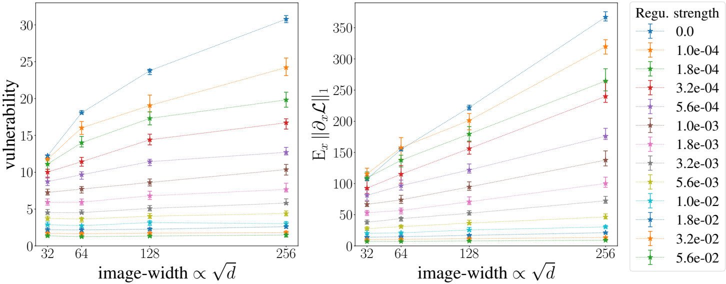

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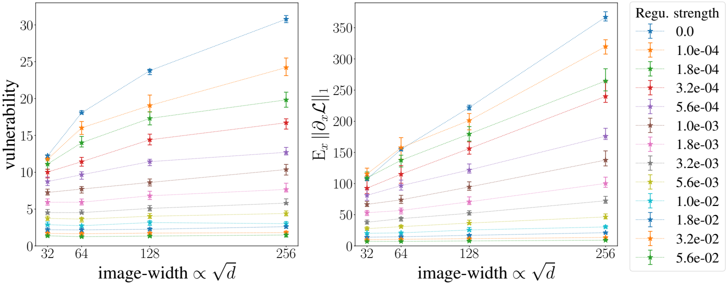

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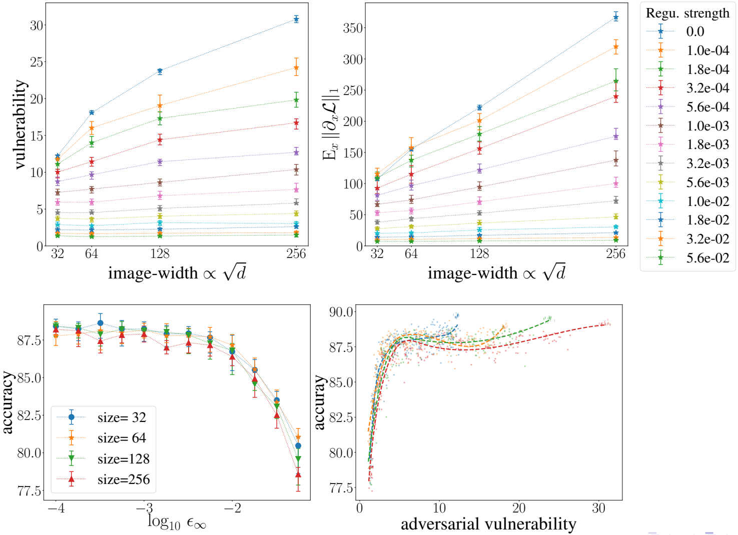

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Questons for future:

- Why does robust training not remove dimension-depence: training algo or function class problem?
- Design networks that incorporate more data-assumptions

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Collaborators and audience: THANKS! QUESTIONS?

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