Characterizing optimization bias in terms of optimization geometry

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Call it squared loss vs logistic loss talk

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Deep learning

very large neural networks + large scale datasets

loss minimization over examples using variations of gradient descent (GD)

$$\min_{\mathbf{w}} \sum_{(\mathbf{x},y) \text{ in } D} \text{loss}\left(f(\mathbf{w}, \mathbf{x}), y \right)$$

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- multiple functions $f(\mathbf{w}, .)$ *globally* minimize the loss over D
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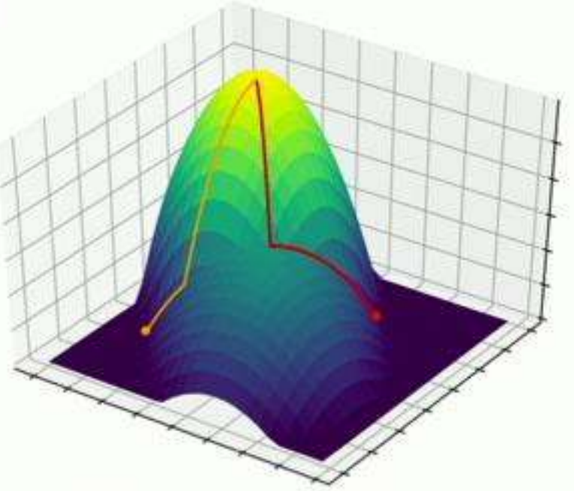

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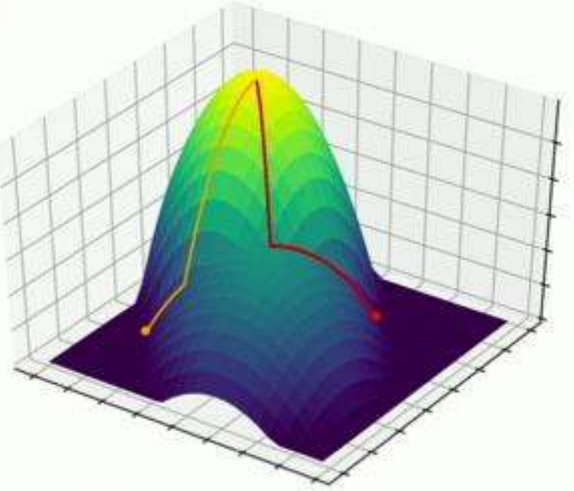

different algorithms
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What does (stochastic) gradient descent converge to in overparamterized learning?

Back to basics: linear models

$$f_{\mathbf{w}}(\mathbf{x}) = \text{linear-function}(\mathbf{x})$$

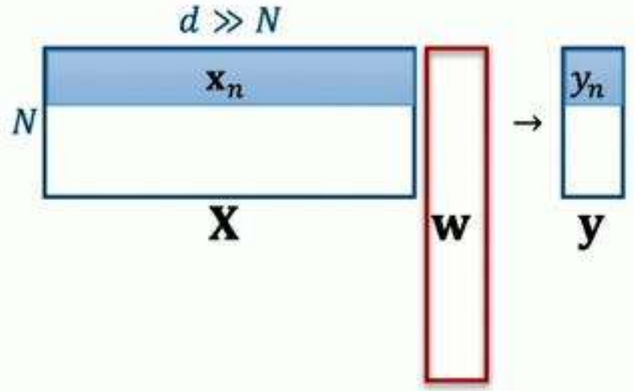
- Simple and natural starting point to build analytical tools
- Interesting and surprising results even in learning linear models
- Intuitions and empirical guidelines for neural networks

Linear regression

$$f(\mathbf{w}, \mathbf{x}) = \langle \mathbf{x}, \mathbf{w} \rangle$$

$$\min_{\mathbf{w}} L(\mathbf{w}) = \sum_{n=1}^{N} (\langle \mathbf{x}_n, \mathbf{w} \rangle - y_n)^2 = \|X\mathbf{w} - y\|_2^2$$

Many minimizers with zero loss



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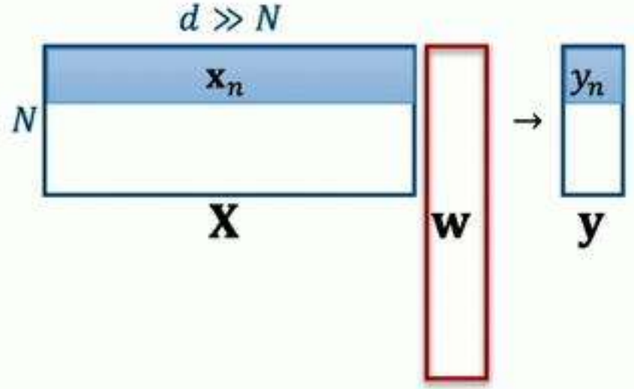

Gradient descent implicitly
minimizes the Euclidean norm of parameters

$$\mathbf{w}(t) \rightarrow \underset{X\mathbf{w}=y}{\operatorname{argmin}} \|\mathbf{w}\|_2 \quad \text{when } \mathbf{w}(0) = 0$$

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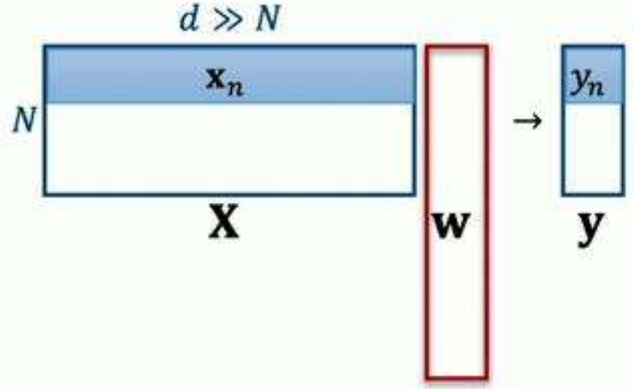

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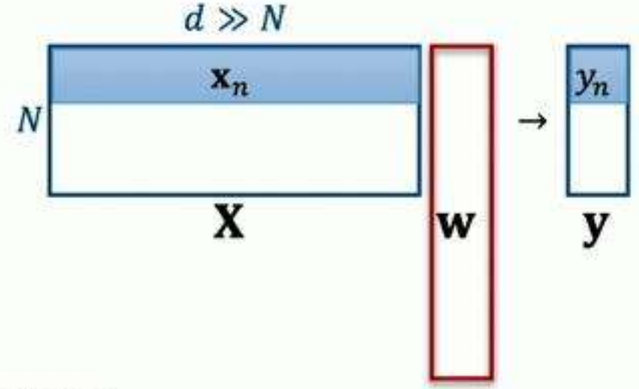

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Proof sketch:

$$\mathbf{w}(t+1) = \mathbf{w}(t) - \eta_t \nabla L(\mathbf{w}(t))$$

$$\nabla L(\mathbf{w}(t)) = \sum_{n=1}^{N} (\langle \mathbf{x}_n, \mathbf{w}(t) \rangle - y_n)\mathbf{x}_n$$

updates lie on a low-dim. manifold
$\Delta \mathbf{w}(t) \in span(\mathbf{x}_n)$

Geometry induced by algorithms

GRADIENT DESCENT

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Can we relate optimization bias to optimization geometry?

Algorithms in non-Euclidean geometry

- Mirror descent

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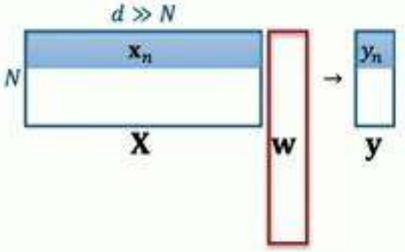

Gunasekar, Lee, Soudry, Srebro, (ICML 2018)

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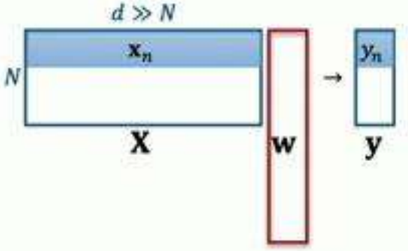

Theorem: for any step-size, instancewise SGD

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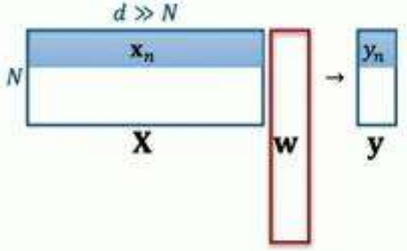

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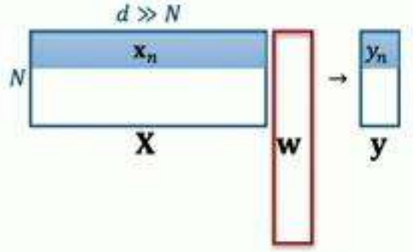

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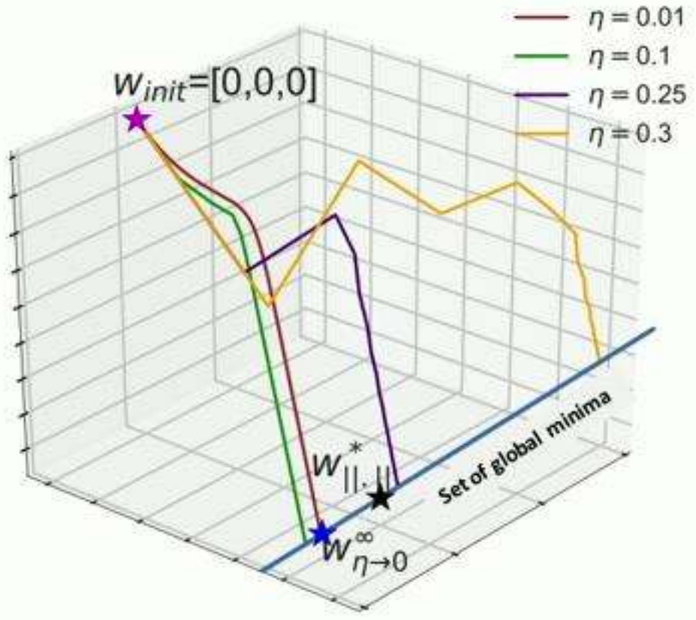

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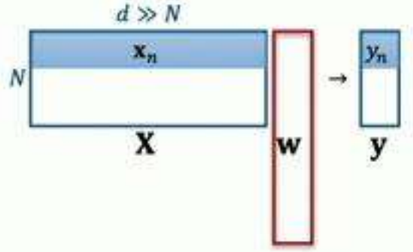

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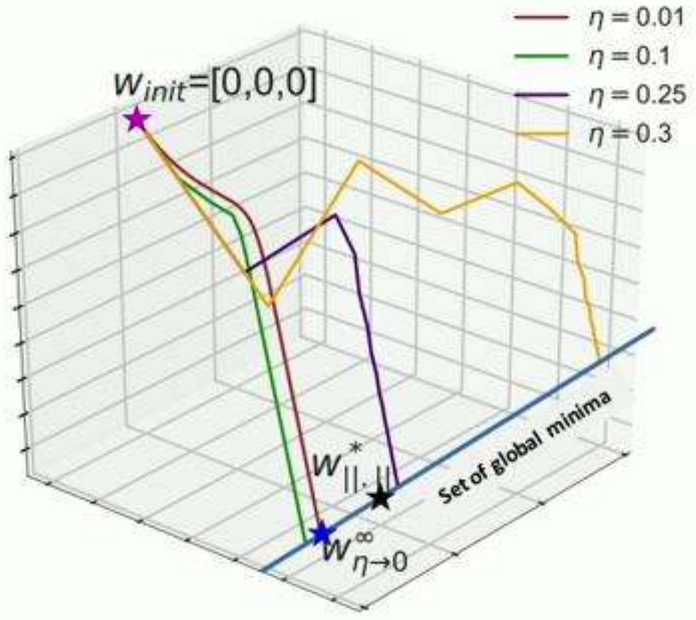

Previously: ϵ-boosting traces ℓ_1 reg. path when the reg. path is monotone in each coordinate Efron, Hastie, Johnstone, Tibshirani, 2004

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Geometry induced by parameters

- Many ways to parameterize a function class $\mathcal{F}$
  - e.g., standard parameterization of linear functions is $\mathbf{w} \in \mathbb{R}^d$
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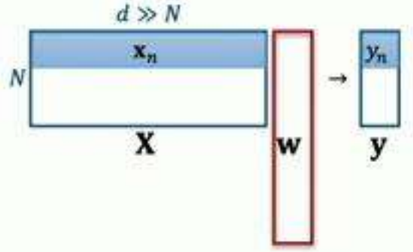

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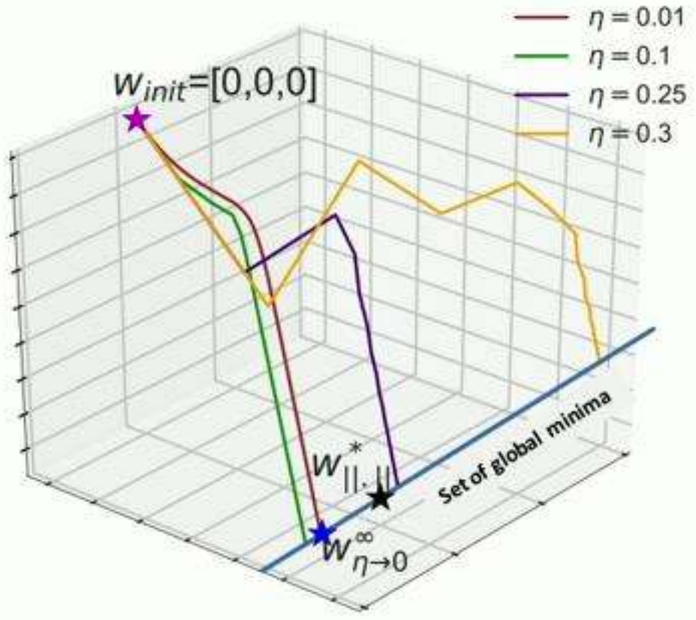

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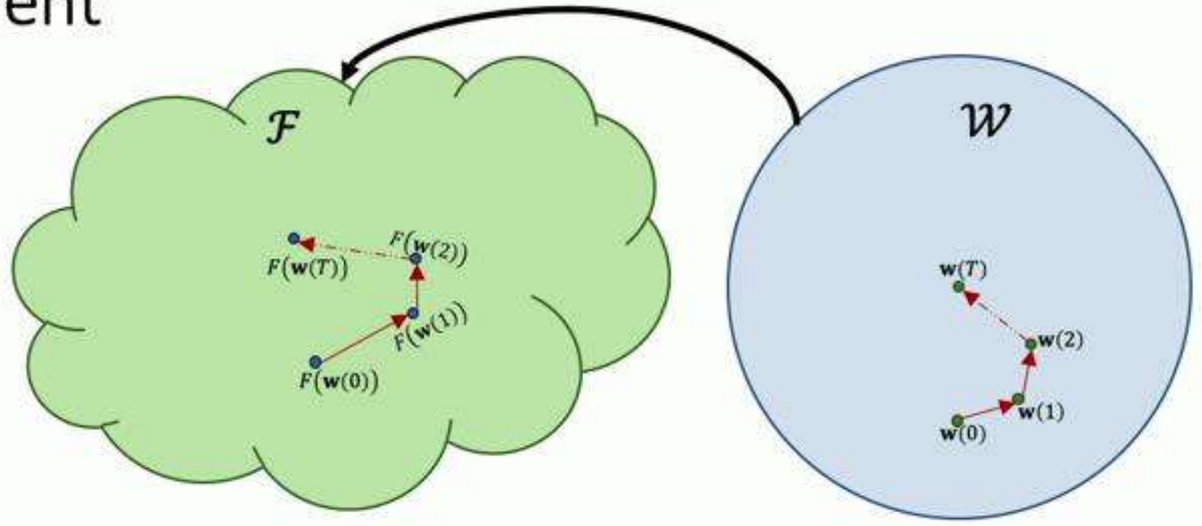

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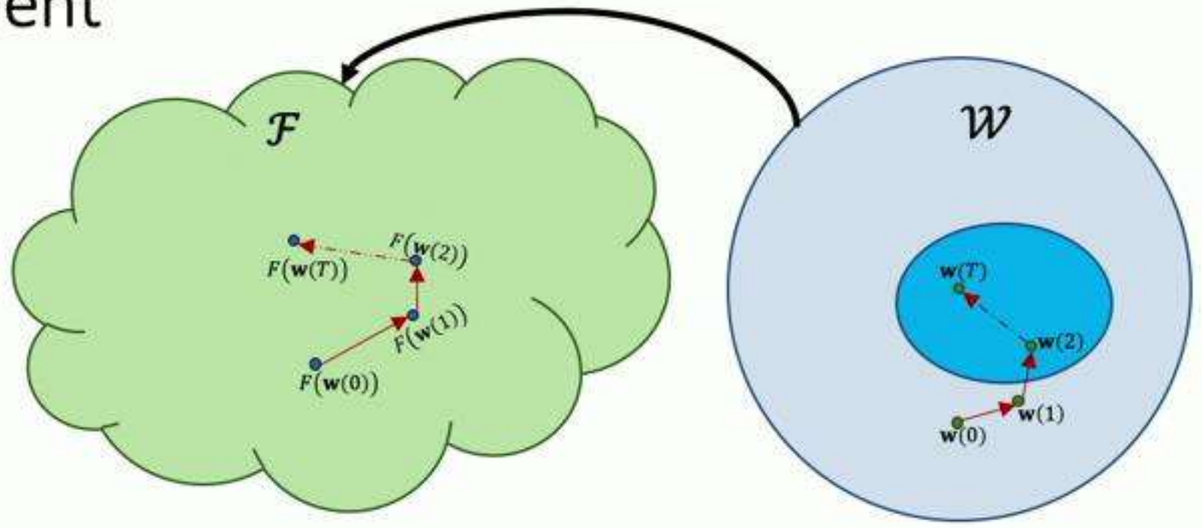

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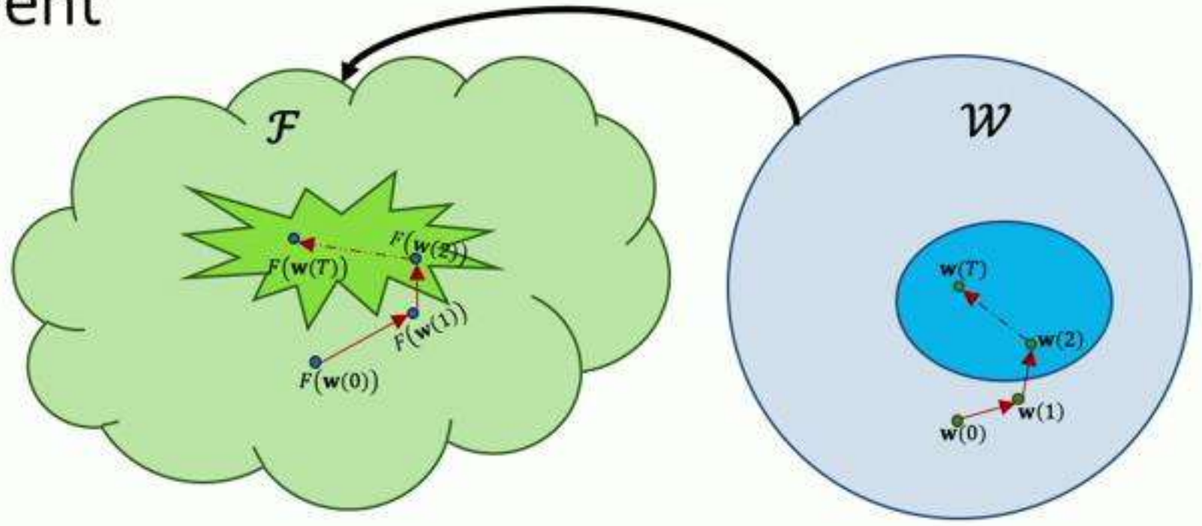

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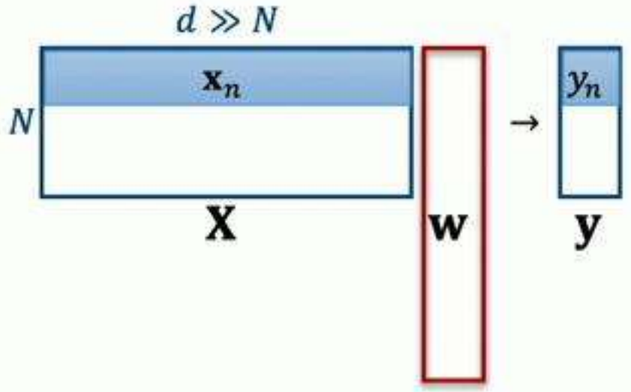
GD converges to the **minimum Euclidean norm** solution



Gunasekar, Woodworth, Bhojanapalli, Neyshabur, Srebro, (NIPS 2017)

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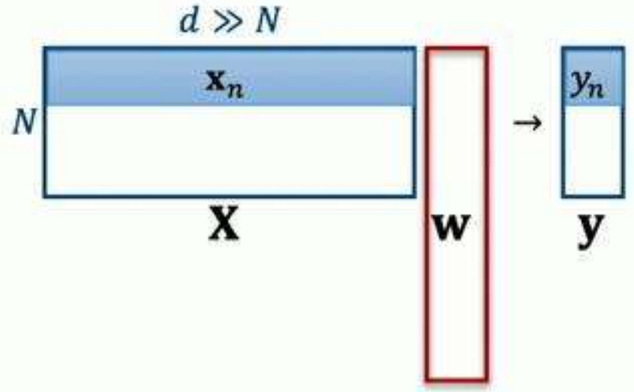

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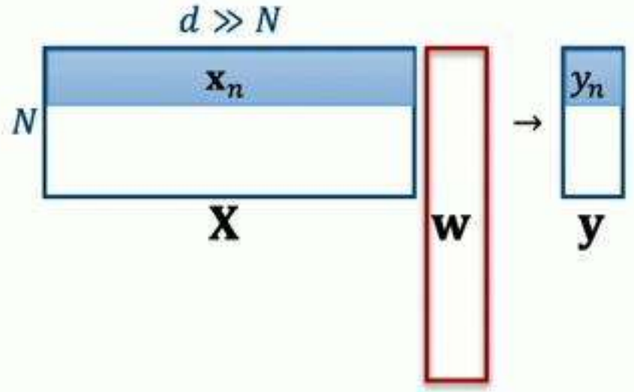

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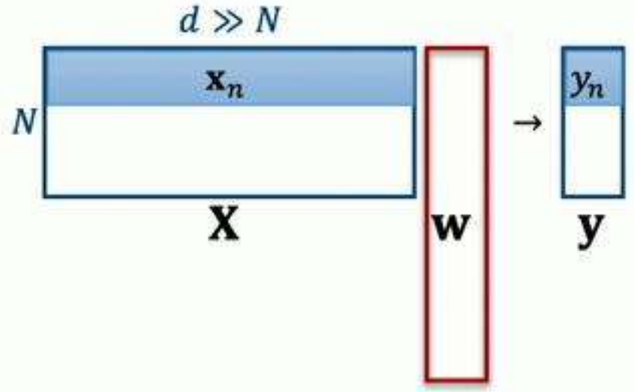

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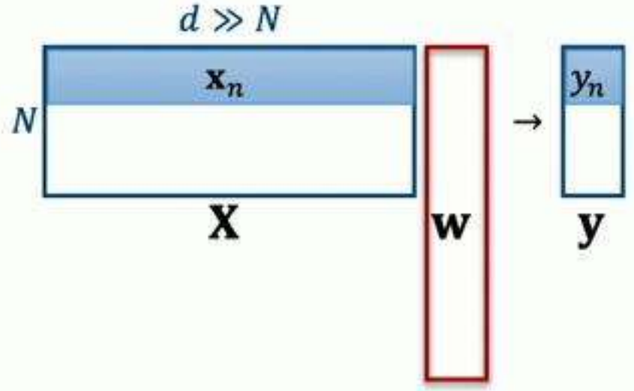
$$\min_{\mathbf{w}} L(\mathbf{w}) := \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2$$

GD converges to the **minimum Euclidean norm** solution



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$$\text{GD on } (\mathbf{u},\mathbf{v}) \to \operatorname*{argmin}_{\mathbf{X}\mathbf{w}=\mathbf{y}} \|\mathbf{w}\|_1$$

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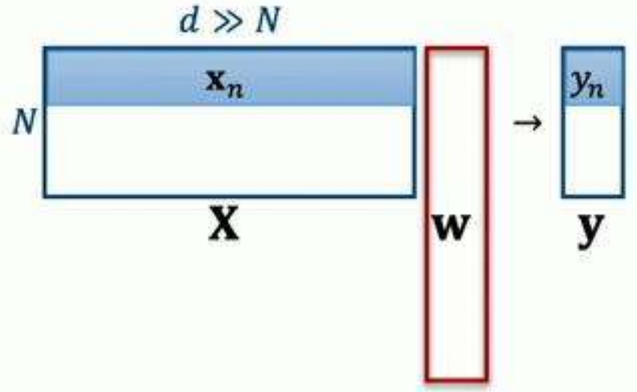

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- updates still in low dimensional manifold but a non-affine manifold

Gunasekar, Woodworth, Bhojanapalli, Neyshabur, Srebro, (NIPS 2017)

Implicit bias for squared loss

- General mirror descent: characterization for all initializations $\mathbf{w}(t) \to \underset{X\mathbf{w}=y}{\operatorname{argmin}} D_\psi(\mathbf{w}, \mathbf{w}(0))$
  - ⇢ for any step-size, dual momentum, instancewise SGD

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  - ⇢ Follow up: get minimum ℓ_1 norm solution even for $\mathbf{w} = \mathbf{u_1}.\mathbf{u_2}.\ldots\mathbf{u_k}$ - implicit bias is not directly related to Euclidean norm of parameters (Arora, Cohen, Hu, Luo 2019)

Implicit bias for squared loss

Optimization geometry directs optimization bias, but expected characterization does not always hold

- ⇢ initialization and step size crucially influence the optimization bias
- ⇢ precise characterization of the nature of implicit bias is elusive even in simple linear models

New tools required to analyze the nature of optimization bias

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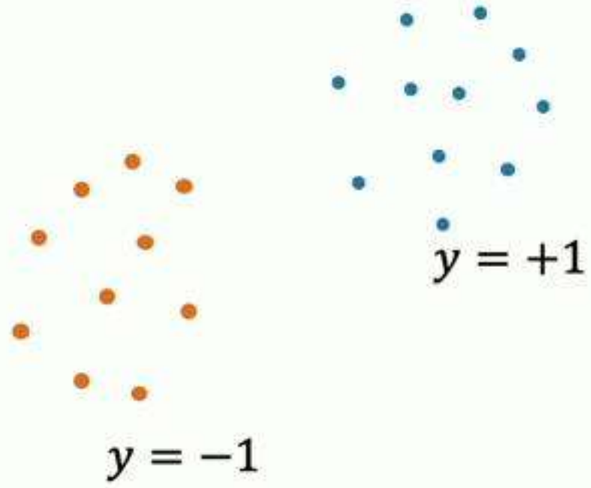
But why are we not looking at logistic loss?

Part II. Nature of optimization bias is very different for some classification losses

Linear classification using logistic loss



Linear classification using logistic loss

$$\min_{\mathbf{w}} \sum_{(\mathbf{x},y) \text{ in } D} \text{loss}\big(\langle \mathbf{w}, \mathbf{x} \rangle, y\big)$$

$\log(1 + \exp(-y\langle \mathbf{w}, \mathbf{x} \rangle))$

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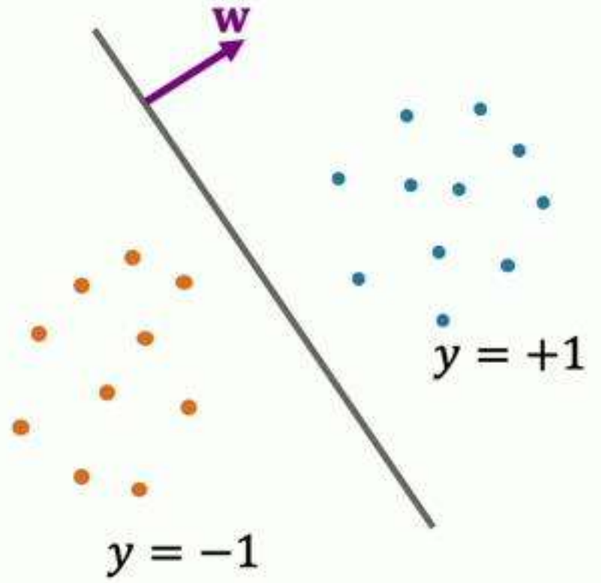
$$\text{prediction} = \text{sign}\left(\langle \mathbf{w}, \mathbf{x} \rangle\right)$$



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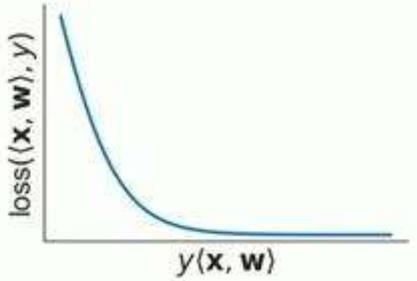

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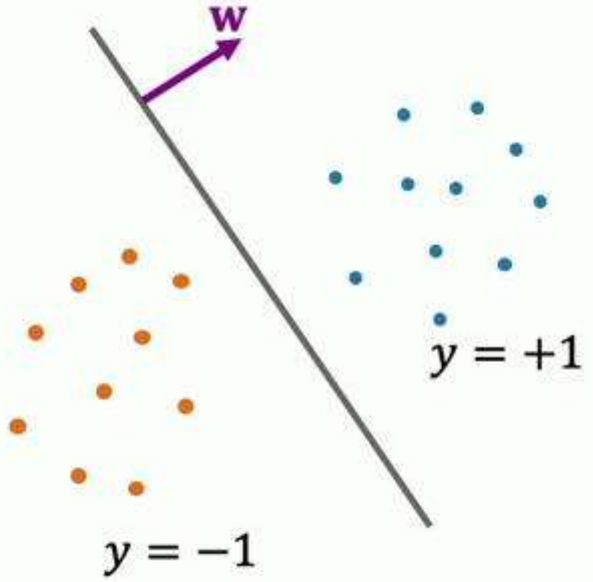

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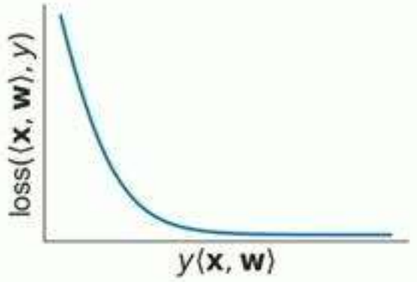

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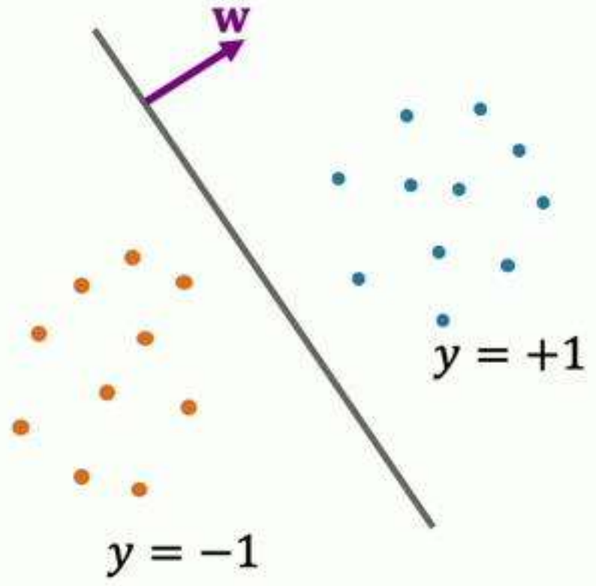

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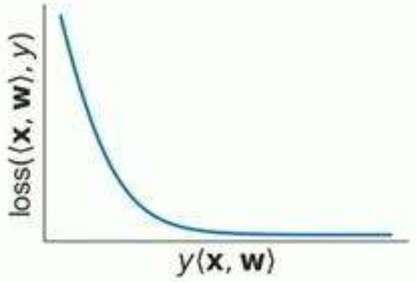

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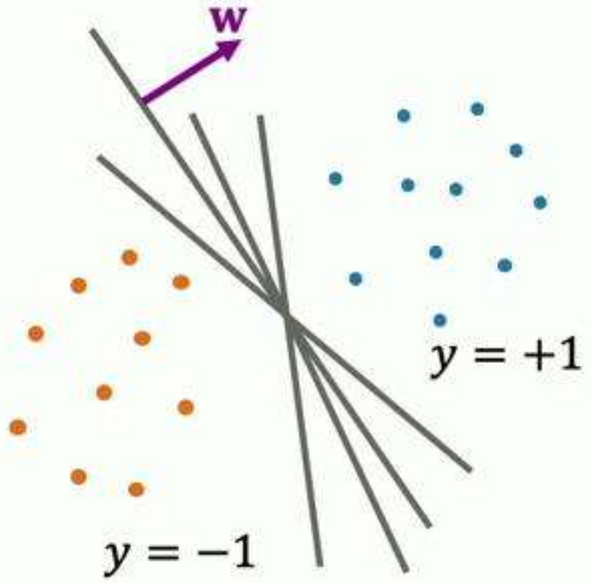

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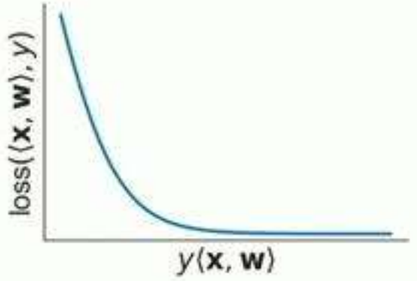

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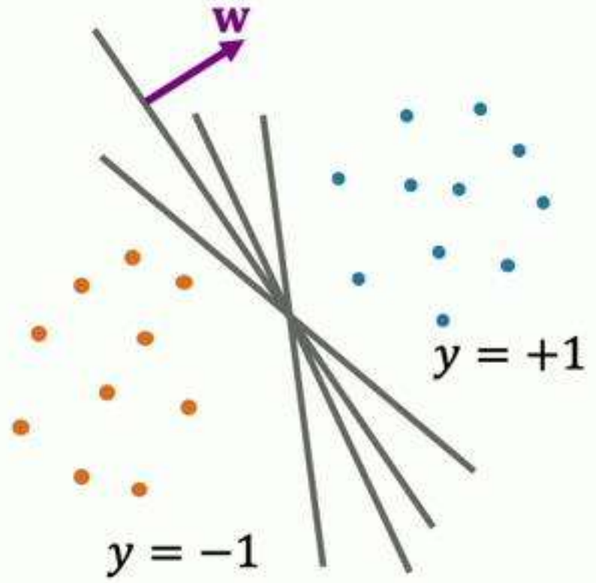

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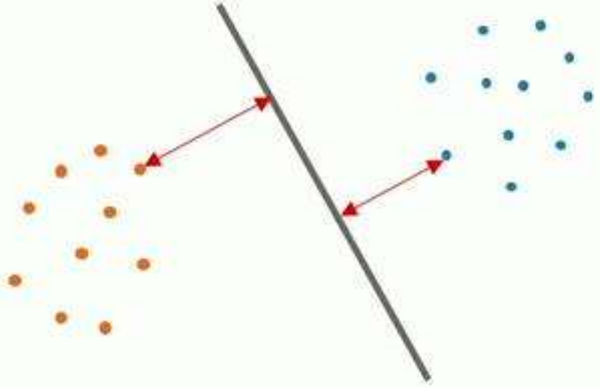
Which classifier/direction does gradient descent converge to?

Gradient descent for logistic regression

Theorem: Gradient descent returns the **Euclidean maximum margin classifier** aka hard margin support vector machine



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$$\underset{\mathbf{w}}{\operatorname{argmin}} \|\mathbf{w}\|_2^2 \quad \text{s.t.} \quad y\langle \mathbf{w}, \mathbf{x} \rangle \geq 1 \quad \forall\, (\mathbf{x}, y) \text{ in } D$$

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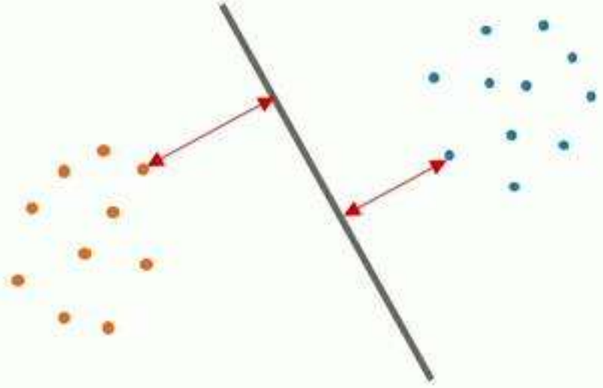

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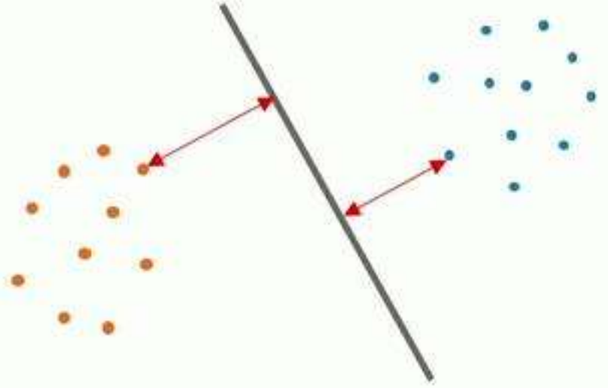

Previously: ℓ_1 maximum margin from boosting (coordinate descent) Telgarsky 2013

Follow up: Ji & Telgarsky 2018 **prove generalization guarantees and convergence rates of (S)GD with non-separable data**

Optimization bias with exp-tail losses

$$-\nabla L(\mathbf{w}(t)) \approx \sum_{n=1}^{N} \exp(-y_n \langle \mathbf{w}(t), \mathbf{x}_n \rangle)\, y_n \mathbf{x}_n$$

Soudry, Hoeffer, Schpigel, Gunasekar, Srebro, (JMLR 2018)

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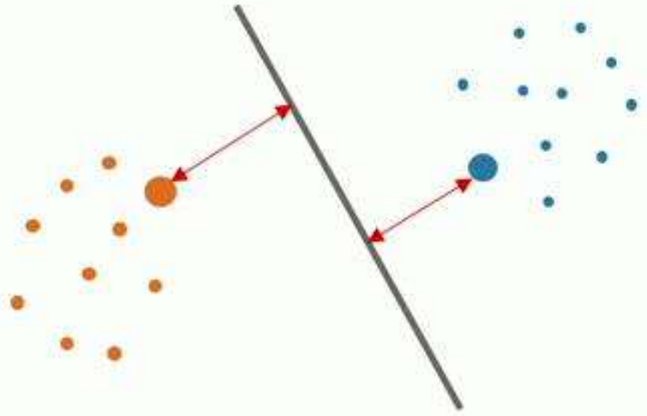
large for data points closest to the separator – "support vectors"



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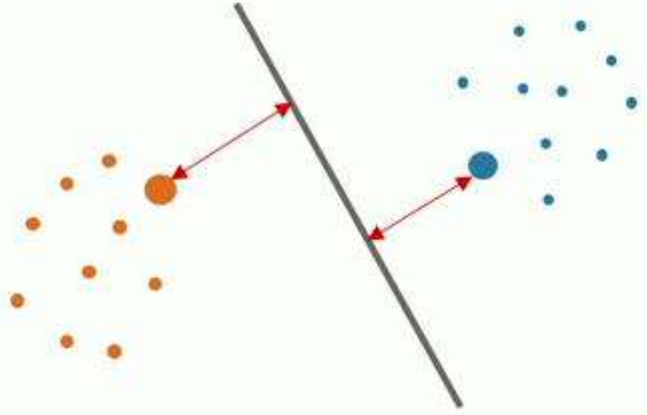

$$\mathbf{w}(t) = \mathbf{w}(0) - \textstyle\sum_{t'<t} \nabla L(\mathbf{w}(t'))$$

dominated by positive span of support vectors
→ sufficient condition for Euclidean max-margin separator

Soudry, Hoeffer, Schpigel, Gunasekar, Srebro, (JMLR 2018)

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Steepest descent w.r.t. general norms

$$\mathbf{w}(t+1) = \underset{\mathbf{w}}{\text{argmin}} \ \langle \mathbf{w}, \nabla L(\mathbf{w}(t)) \rangle + \frac{1}{2\eta_t} \|\mathbf{w} - \mathbf{w}(t)\|^2$$

Theorem: steepest descent returns maximum margin solution w.r.t. norm of optimization geometry

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Generalization of analysis in **Telgarsky (2013)**

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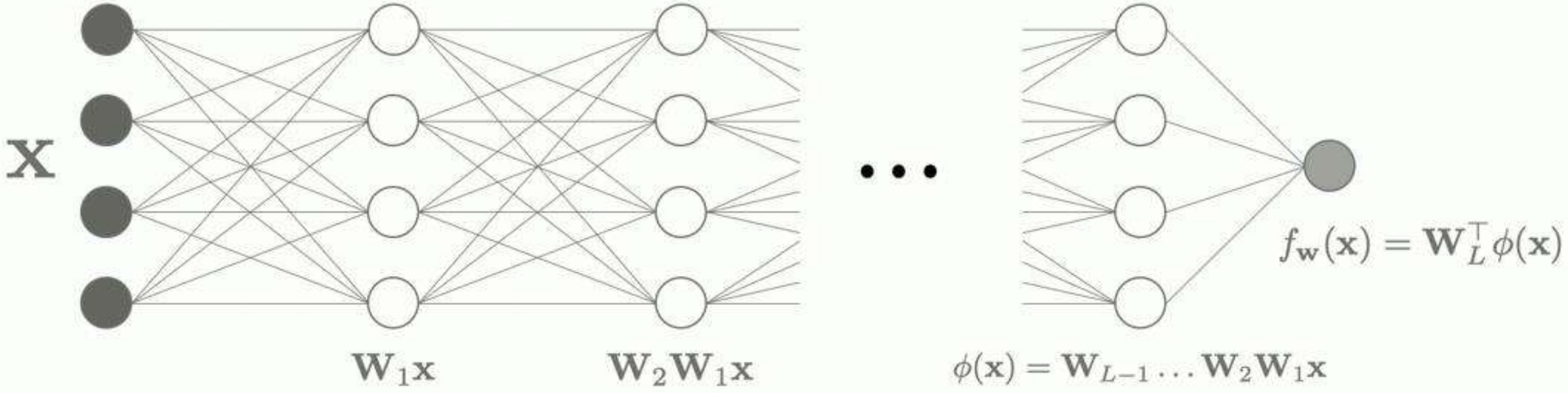
For non-homogeneous ψ, margin of 1 is not special

For some potentials, MD converges to limit of margin path

$$\lim_{\gamma \to \infty} \frac{\operatorname*{argmin}_{\mathbf{w}} \psi(\mathbf{w}) \quad \text{s.t.} \quad \forall n, y_n \langle \mathbf{w}, \mathbf{x}_n \rangle \geq \gamma}{\gamma}$$

Gunasekar, Lee, Soudry, Srebro (ICML 2018)

Multilayer linear network



Gunasekar, Lee, Soudry, Srebro (NeurIPS 2018)

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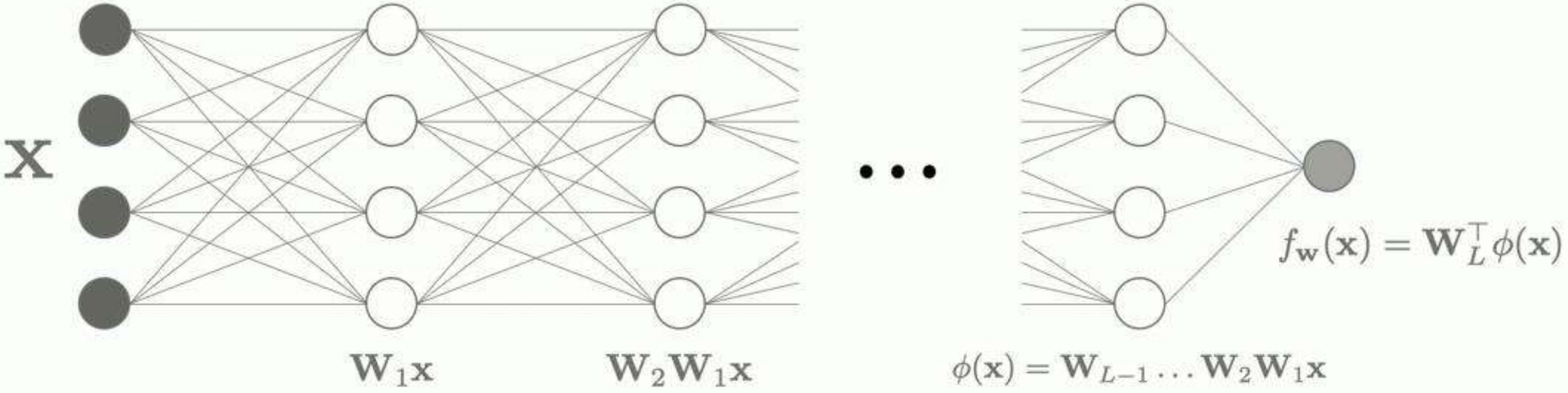
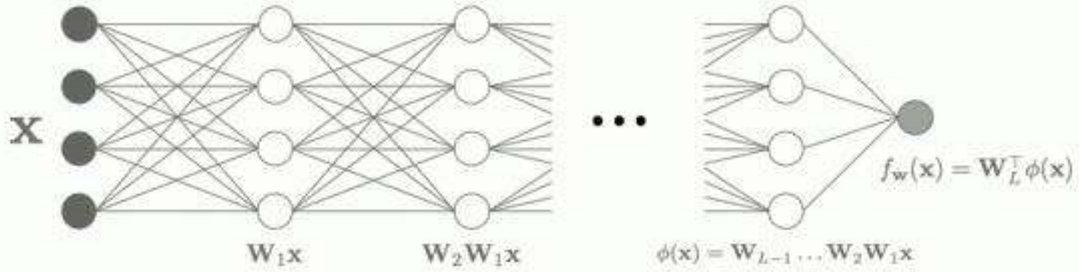


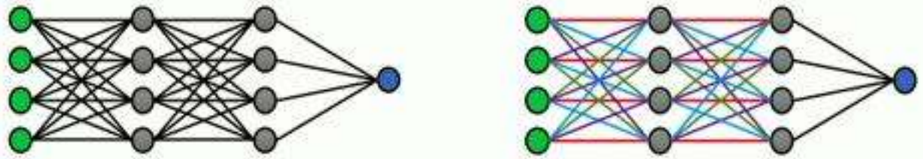
different constraints on $\mathbf{w} = [\mathbf{W}_1, \mathbf{W}_2, \ldots, \mathbf{W}_{L+1}]$ $\longrightarrow$ different architectures

e.g., fully connected networks,

convolutional networks

Gunasekar, Lee, Soudry, Srebro (NeurIPS 2018)





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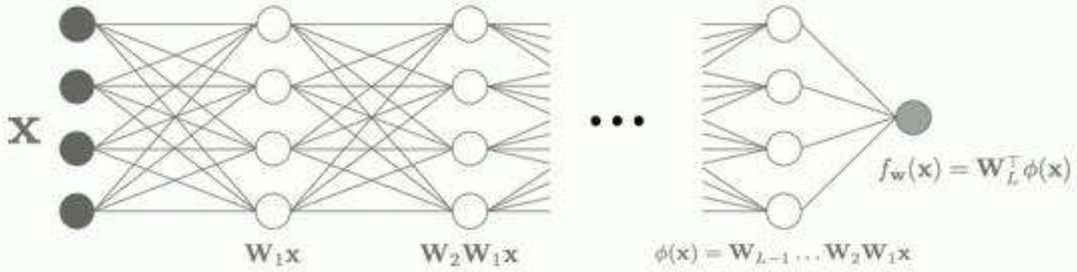

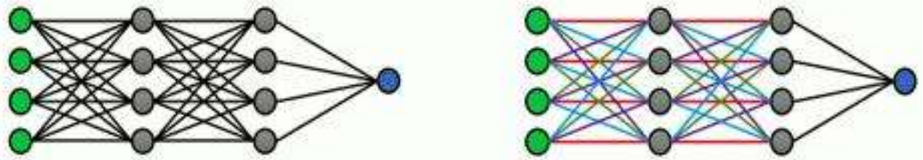

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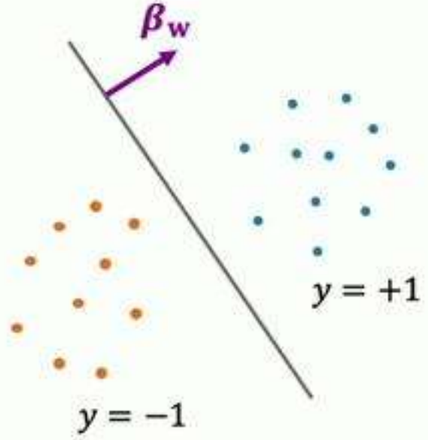
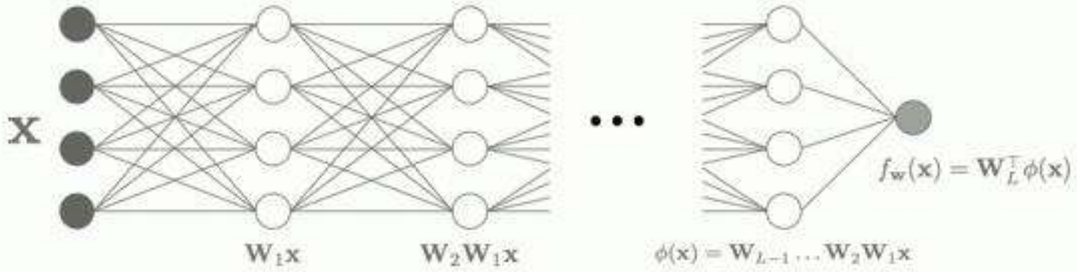
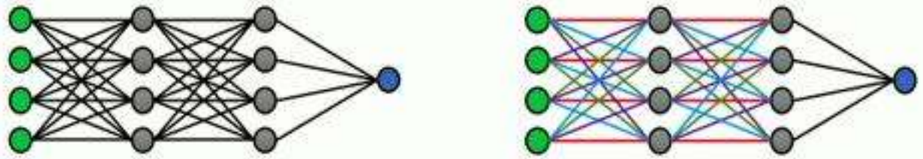


Gunasekar, Lee, Soudry, Srebro (NeurIPS 2018)





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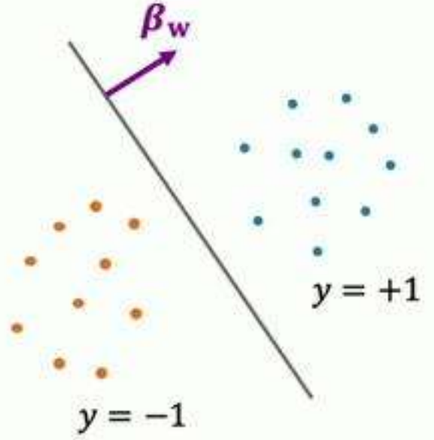
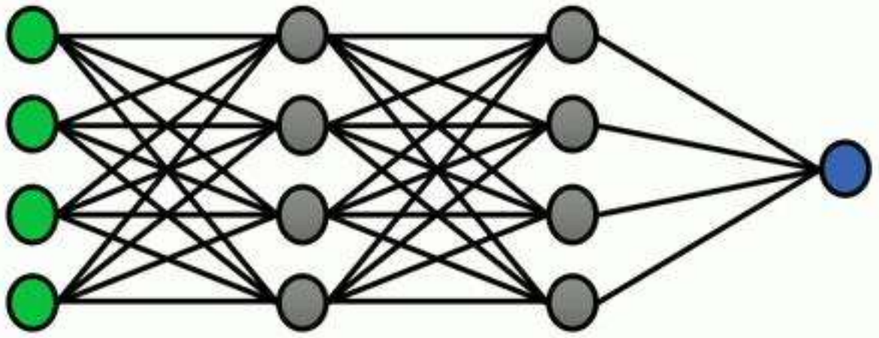


What classifier does gradient descent on $L(\mathbf{w})$ return for different architectures?

Gunasekar, Lee, Soudry, Srebro (NeurIPS 2018)

Linear fully connected networks



Gunasekar, Lee, Soudry, Srebro NeurIPS 2018

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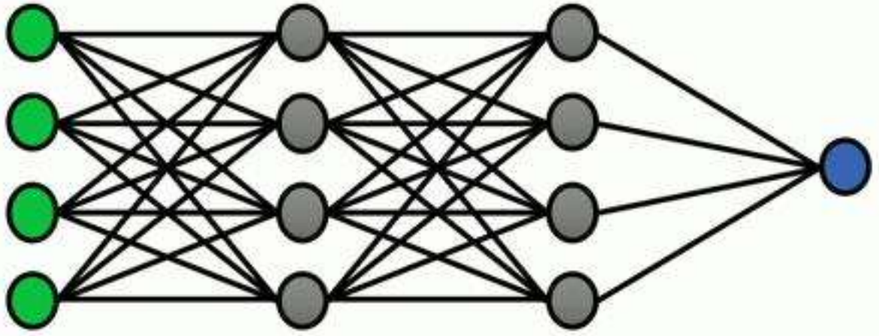

Theorem*: for any depth (#layers), gradient descent again returns the **Euclidean max-margin** classifier

$$\underset{\beta}{\text{argmin}} \|\beta\|_2^2 \quad \text{s.t.} \quad y\langle \beta, \mathbf{x} \rangle \geq 1 \quad \forall\, (\mathbf{x}, y) \text{ in } D$$

Gunasekar, Lee, Soudry, Srebro NeurIPS 2018

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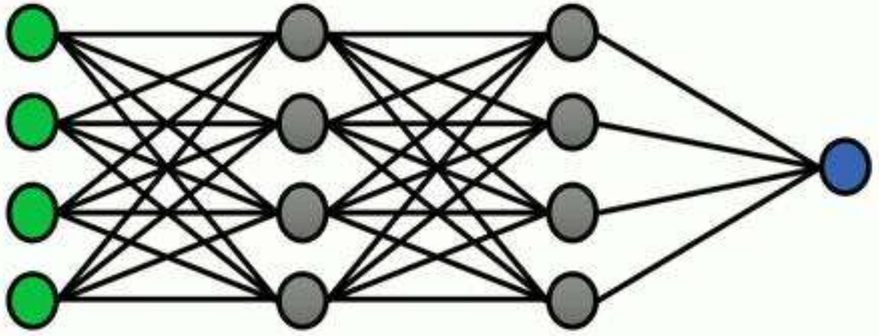

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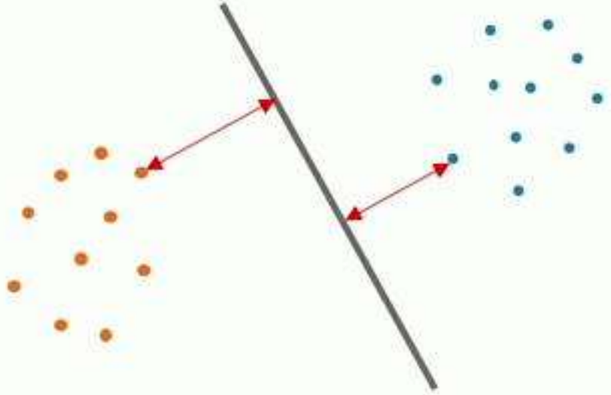
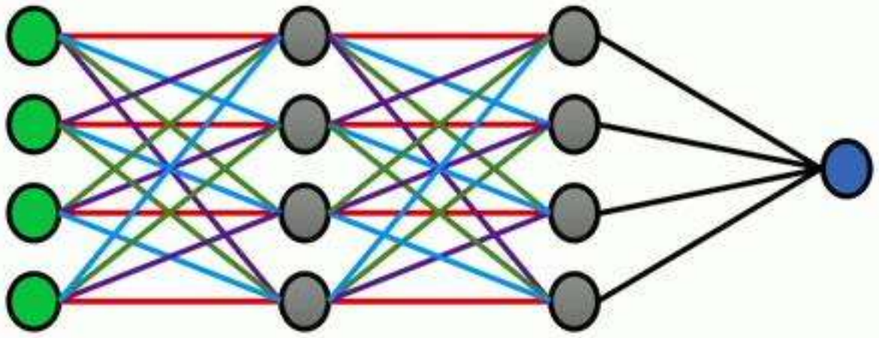


same solution as logistic regression!

Gunasekar, Lee, Soudry, Srebro NeurIPS 2018

Linear convolutional network



Theorem*: gradient descent implicitly introduces biases that

1. promote sparsity in the frequency domain (Fourier coefficients) → frequency filtering
2. changes with the depth/#layers of network

2 layers

$$\underset{\beta}{\text{argmin}} \; \|\text{DFT}(\beta)\|_1 \quad \text{s.t.} \quad y\langle \beta, \mathbf{x} \rangle \geq 1 \quad \forall\, (\mathbf{x}, y) \text{ in } D$$

Fourier coefficients/ frequency components

minimizing ℓ_1 norm is known to encourage sparse solutions

Gunasekar, Lee, Soudry, Srebro NeurIPS 2018

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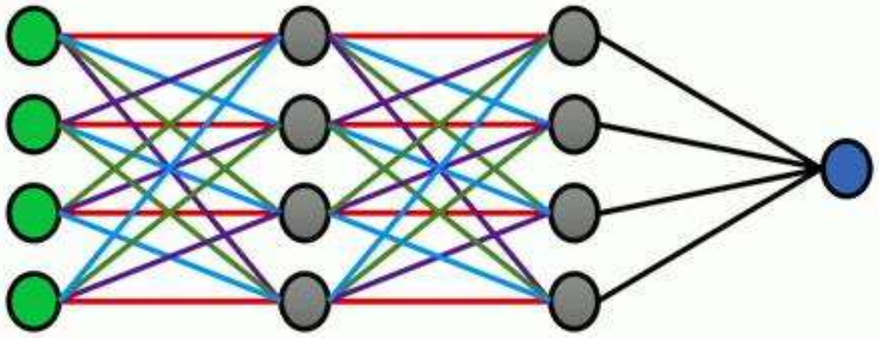

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L convolutional layers

stationary points of $\underset{\beta}{\text{argmin}} \|\text{DFT}(\beta)\|_{2/L} \quad \text{s.t.} \quad y\langle \beta, \mathbf{x}\rangle \geq 1 \quad \forall\, (\mathbf{x}, y) \text{ in } D$

Gunasekar, Lee, Soudry, Srebro NeurIPS 2018

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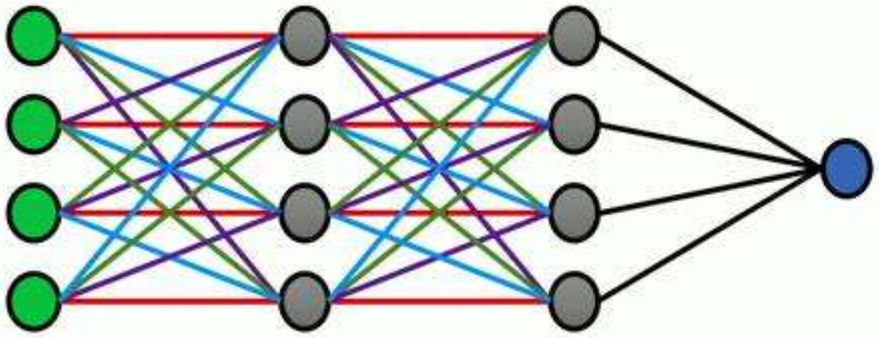

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Bias not simply because of convolutional architecture

but from gradient descent on convolutional parameterization

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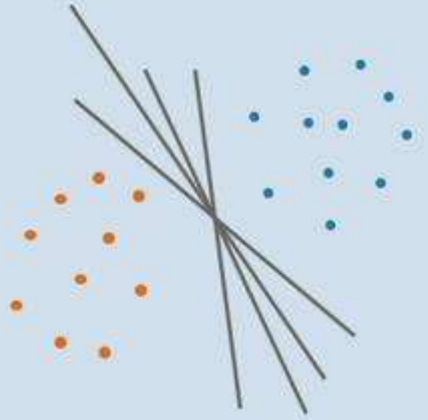
Gunasekar, Lee, Soudry, Srebro NeurIPS 2018

Theorem details and assumptions

Gradient descent on exp-loss for separable datasets

- Many directions/classifiers separate the data

  ⇢ **which classifier does gradient descent return? ← our work!**



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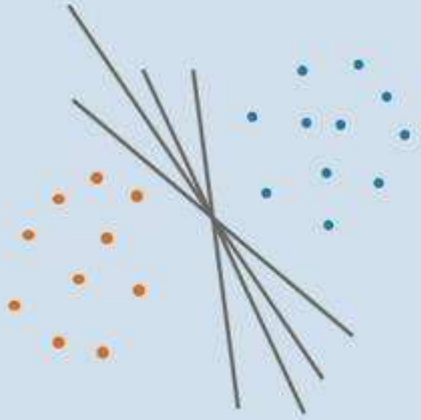

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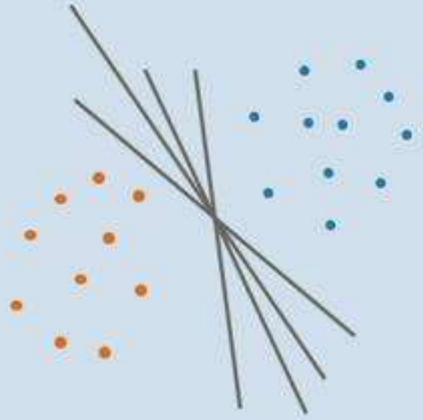

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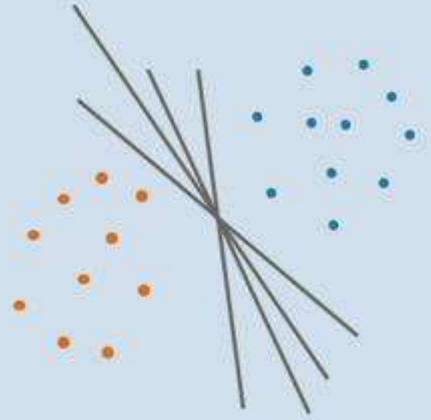

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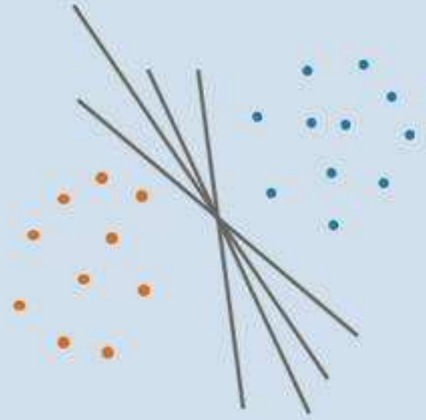
Follow up work:

- **Ji & Telgarsky 2018 – prove the result for linear fully connected networks without assumptions on convergence of loss and update direction**



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Homogeneous linear models

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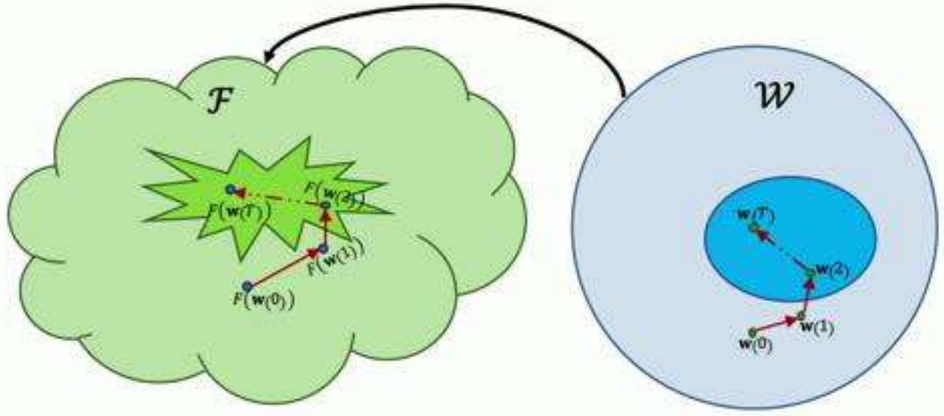

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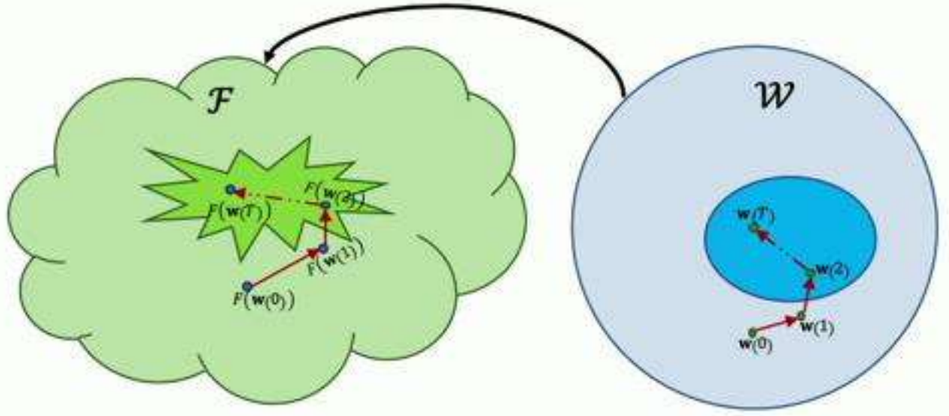

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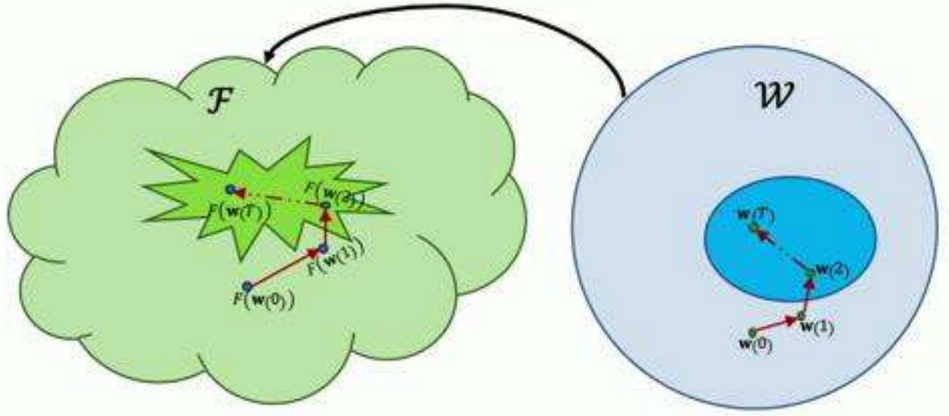

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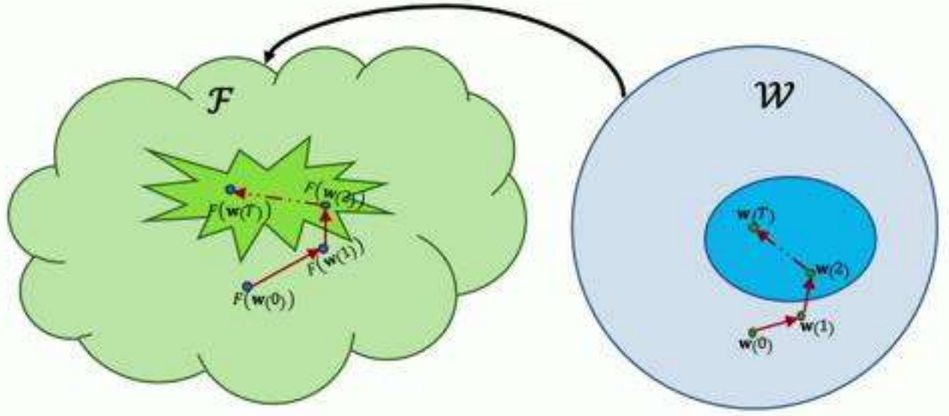
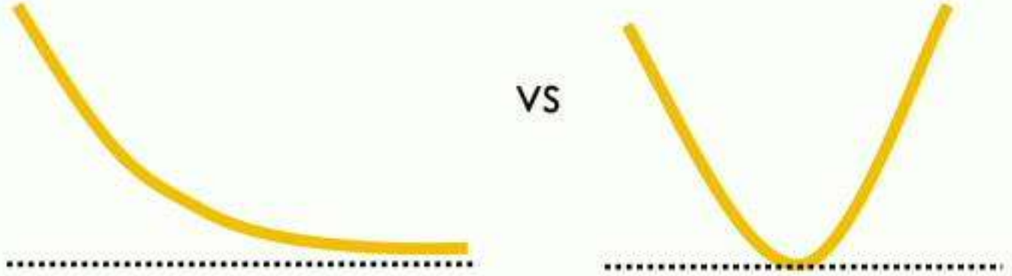
Follow up: [Lyu & LI 2019][Nacson, Gunasekar, Lee, Soudry, Srebro 2019] – generalization to homogeneous models



Gunasekar, Lee, Soudry, Srebro NeurIPS 2018

Optimization bias with exponential loss

Nature of optimization bias is very different from squared loss



Exp-tailed losses on separable data

optimization path has infinite arc length

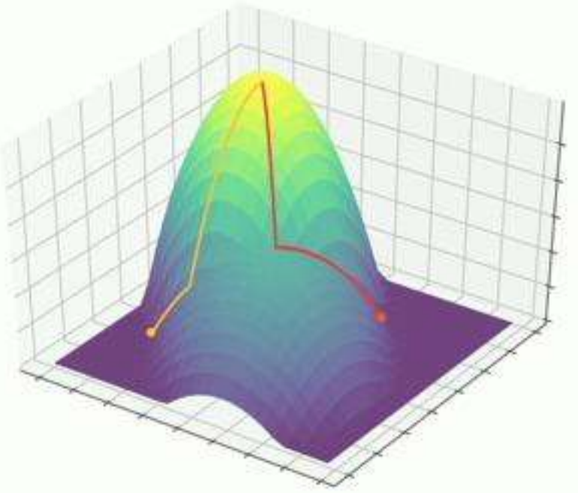
→ max-margin vs min-norm solutions

→ initialization and step size independent characterizations

- Interesting non-RKHS biases independent of step-size and initialization (as long as they are finite)
  e.g. max margin w.r.t $\|\mathrm{DFT}(\beta)\|_1$ for convolutional networks
- WIP: reconciling with NTK type analysis

→ simple asymptotic characterizations for many complicated models

Role of optimization in ML extends beyond reaching any global minimum



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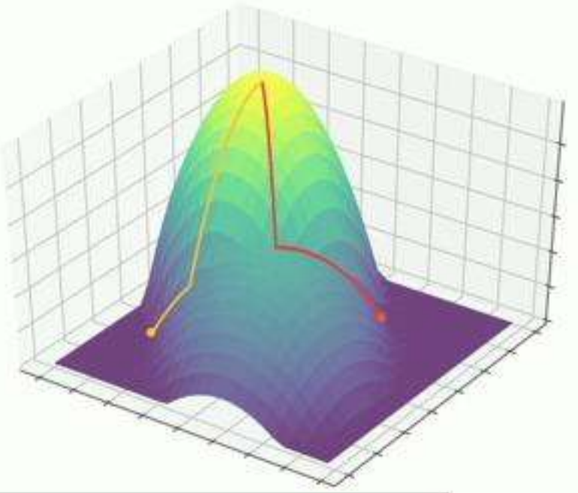

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- characterization of bias and its dependence on hyperparameters are very different for regression and classification tasks

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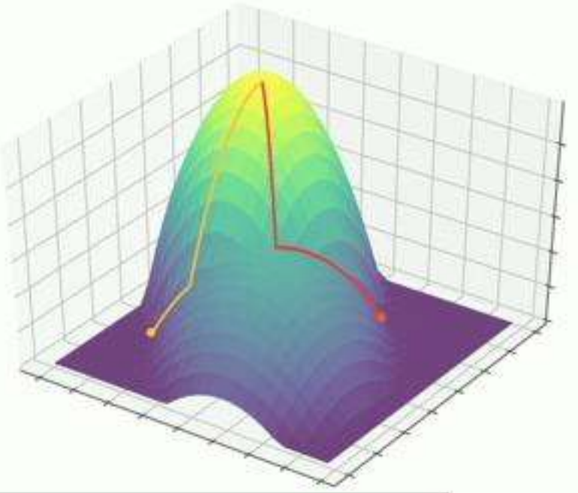

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Thank
you!

A New Perspective on Adversarial Perturbations

Aleksander Mądry

Based on joint works with:

Logan Engstrom

Andrew Ilyas

Shibani Santurkar

Brandon Tran

Dimitris Tsipras

Alexander Turner

gradientscience.org

Why do we love deep learning?

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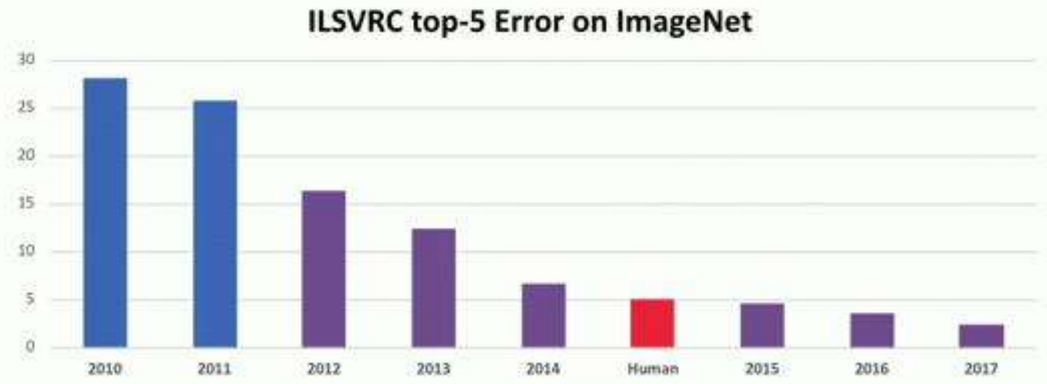

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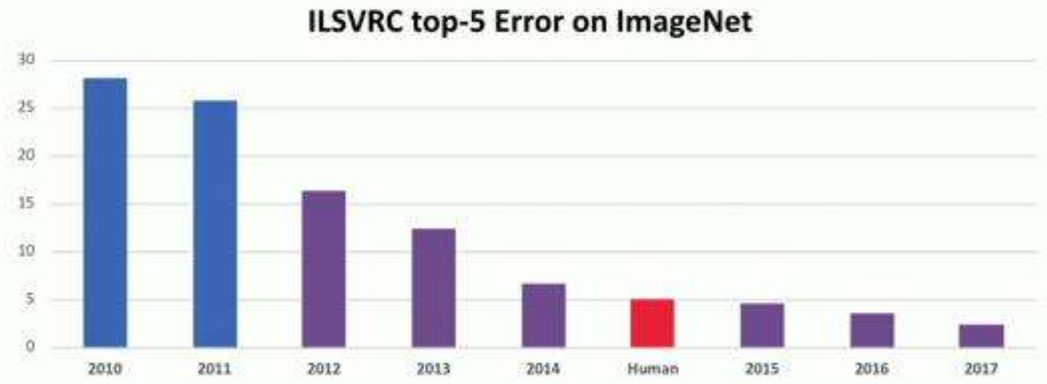

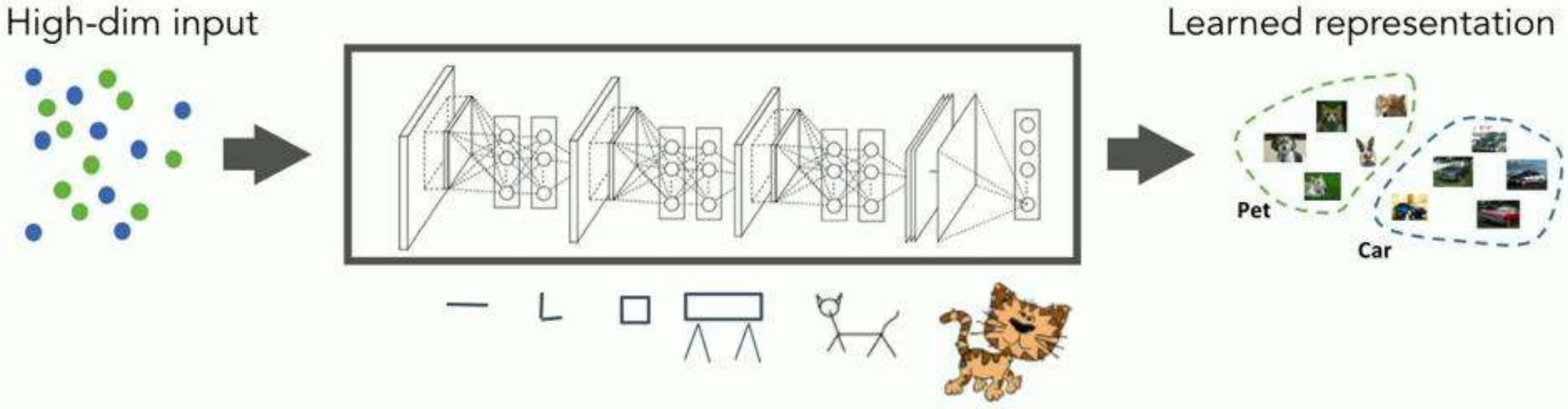

But...

But...

But...

But...

Correct label: insect

But...

Correct label: insect
Predicted label: dog

But...

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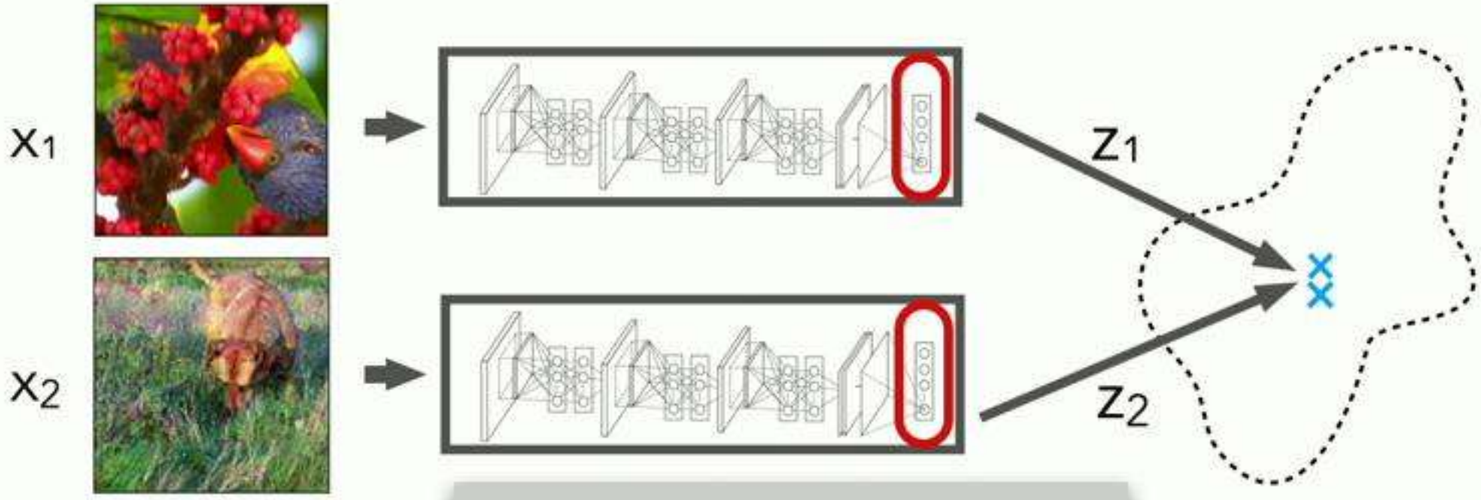


$x_1 \neq x_2$ but $z_1 \approx z_2$

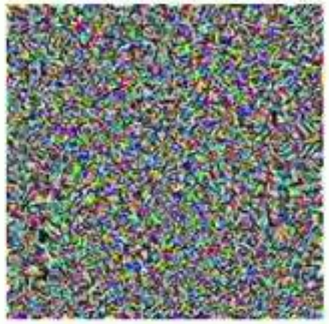
What's going on?

Key Problem: Adversarial Perturbations

[Szegedy et al 2013] [Biggio et al 2013]

“pig” (91%)

+ 0.005 x



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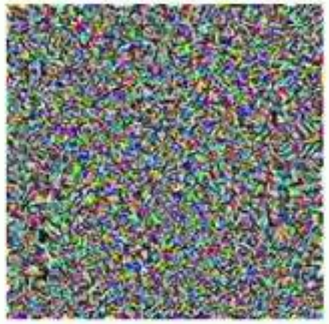

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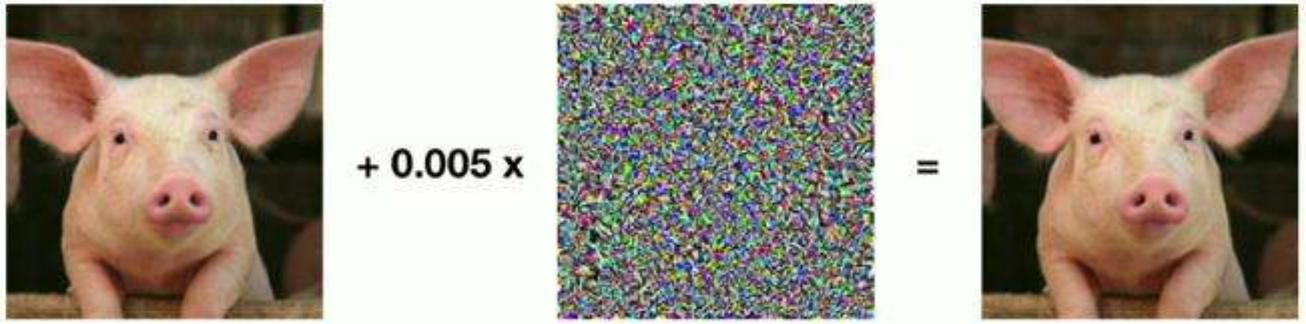
Emerging goal: (Adversarially) robust generalization

$$\min_{\theta} \mathbb{E}_{(x,y)\sim D}[\max_{\delta\in\Delta} \ell(\theta; x+\delta, y)]$$

Desired invariance

Key Problem: Adversarial Perturbations

[Szegedy et al 2013] [Biggio et al 2013]



"pig" (91%) **noise (NOT random)** **"airliner" (99%)**

Emerging goal: (Adversarially) robust generalization

$$\min_{\theta} \mathbb{E}_{(x,y)\sim D}[\max_{\delta\in\Delta} \ell(\theta; x+\delta, y)]$$

→ We are (finally) succeeding in achieving this goal

ML via Adversarial Robustness Lens

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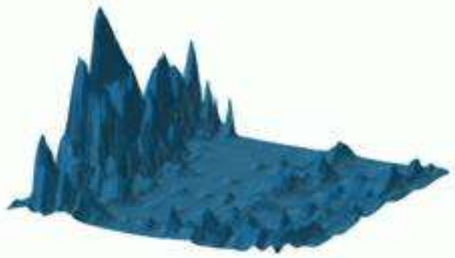
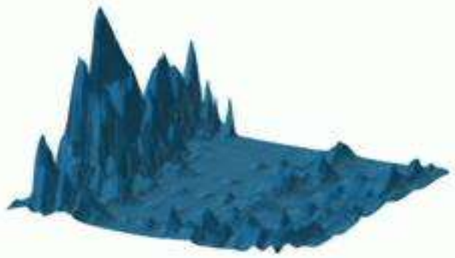


- Training is harder and models need to be more complex

[M Makelov Schmidt Tsipras Vladu 2018]

ML via Adversarial Robustness Lens



- Training is harder and models need to be more complex

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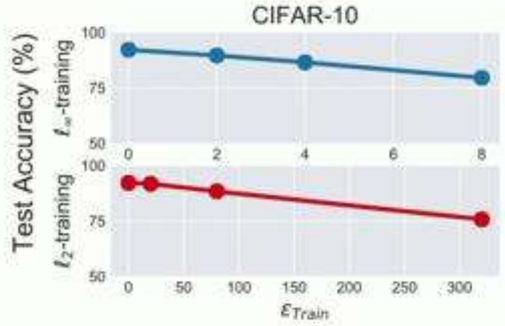
- Models may <u>have</u> to be less accurate

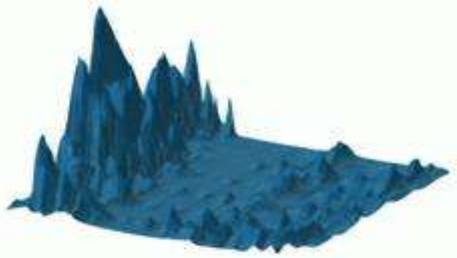
  [Tsipras Santurkar Engstrom Turner M 2018]

  [Bubeck Price Razenshteyn 2018]

  [Degwekar Nakkiran Vaikunatanathan 2018]



ML via Adversarial Robustness Lens



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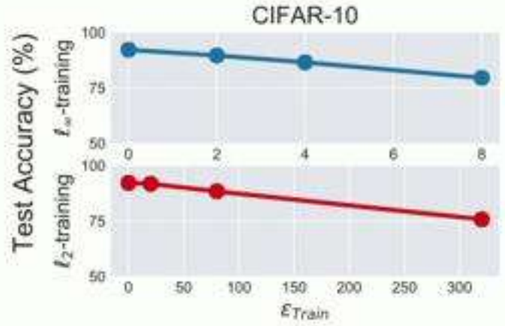

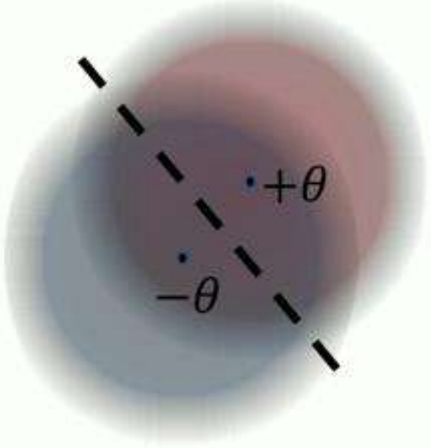

- We might need more training data

  [Schmidt Santurkar Tsipras Talwar M 2018]

But: “How”/“what” does not tell us “why”

But: "How"/"what" does not tell us "why"

Why adversarial perturbations **exist**
(and **are so widespread**)?

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Why are our models brittle?

$$d \to \infty$$

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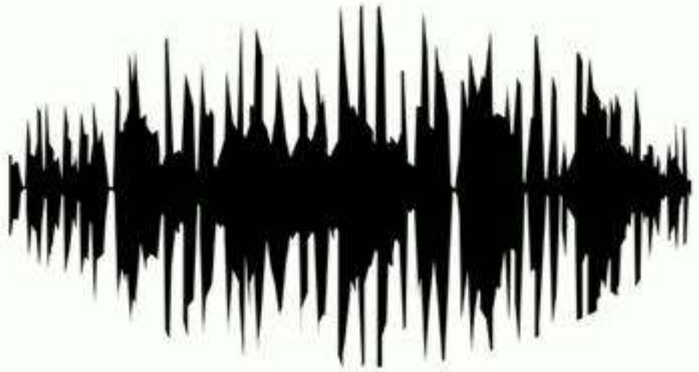

Why are our models brittle?

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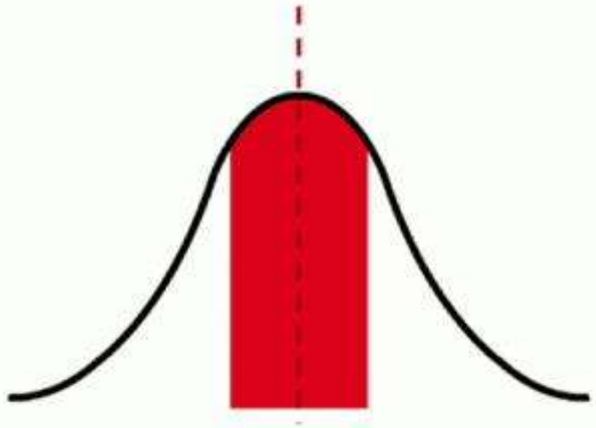

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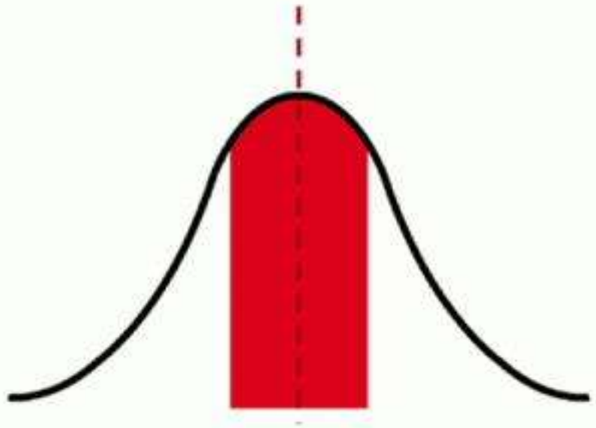

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Why are our models brittle?

Unifying theme: Adversarial examples are aberrations

Why Are Adv. Perturbations Bad?

Why Are Adv. Perturbations Bad?

dog

Why Are Adv. Perturbations Bad?

dog

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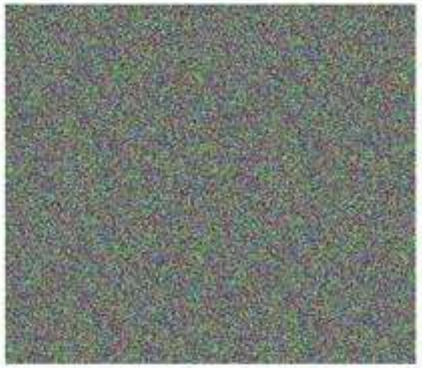

meaningless
perturbation

Why Are Adv. Perturbations Bad?

dog

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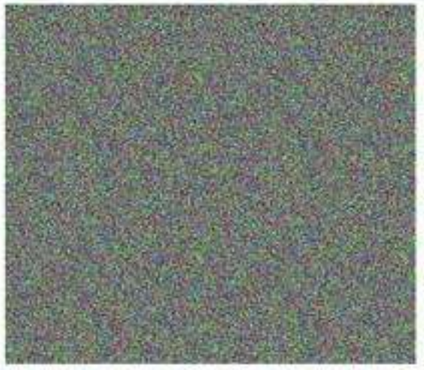

meaningless
perturbation

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cat

Why Are Adv. Perturbations Bad?

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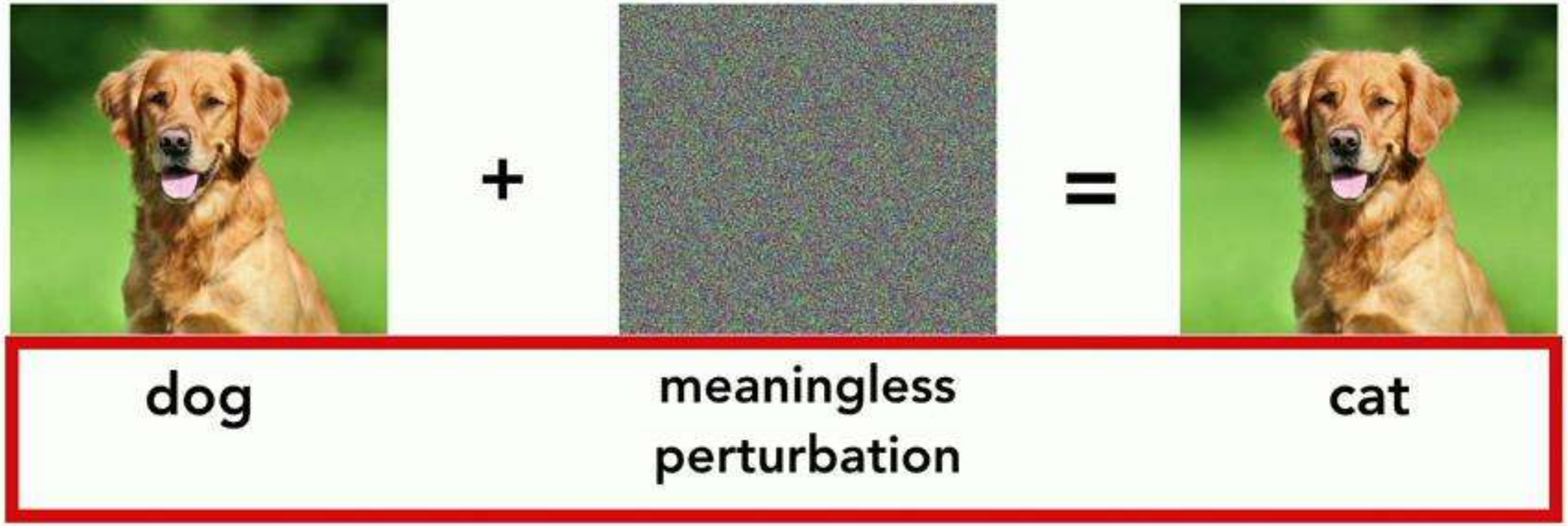


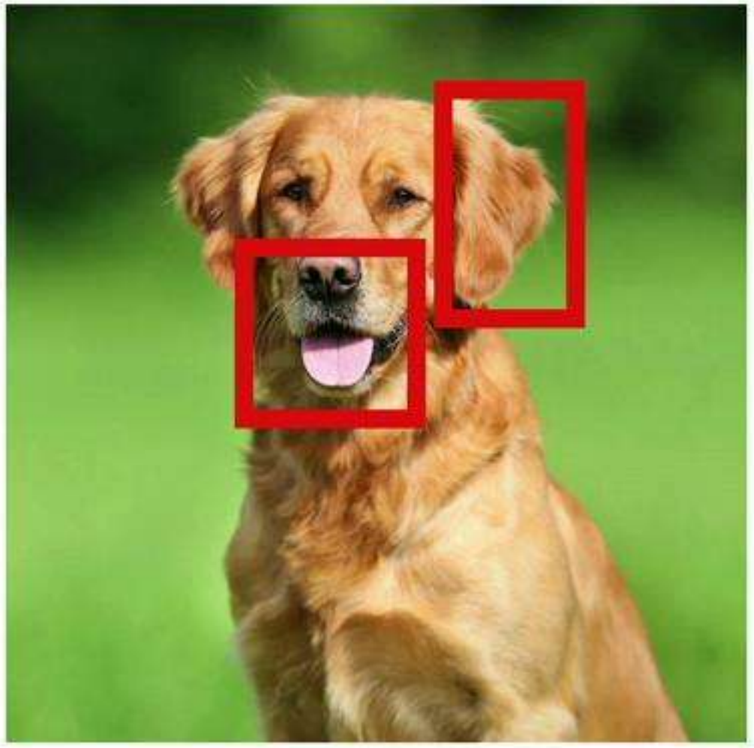
But: This is only a "human" perspective

Human Perspective

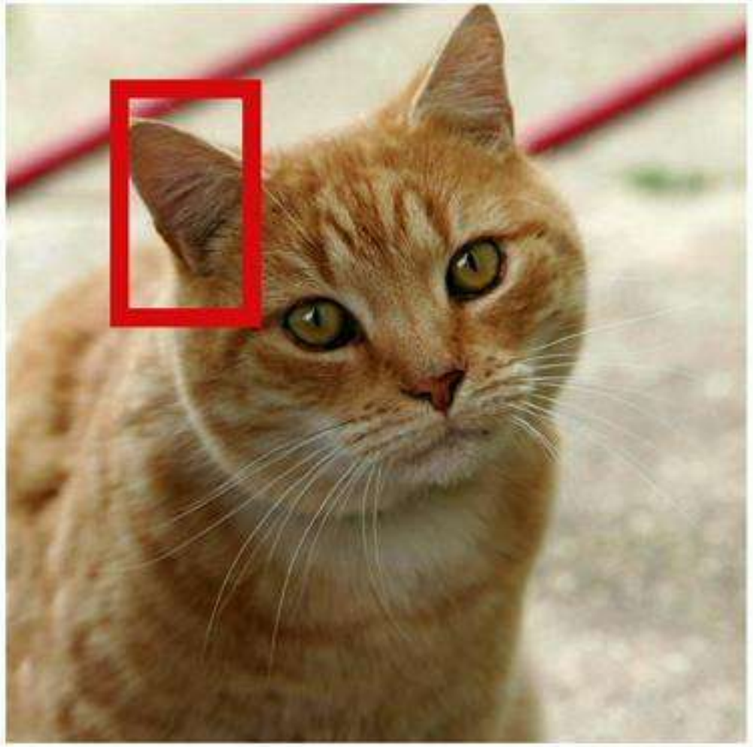
dog

cat

Human Perspective



dog



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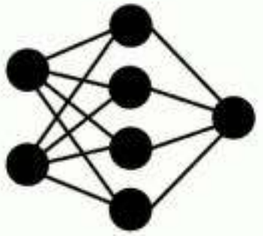
ML Perspective

ML Perspective



dog

ML Perspective

dog

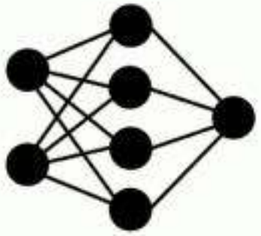


Image is meaningless

ML Perspective

dog

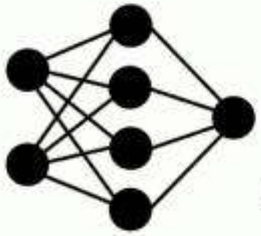


Image is meaningless

Classes are meaningless

ML Perspective

dog

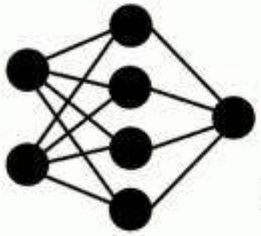


Image is meaningless

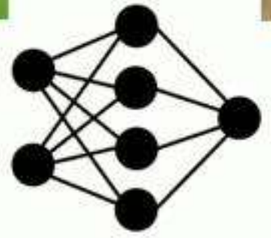
Classes are meaningless

Only goal:

Max (test) accuracy

ML Perspective

dog



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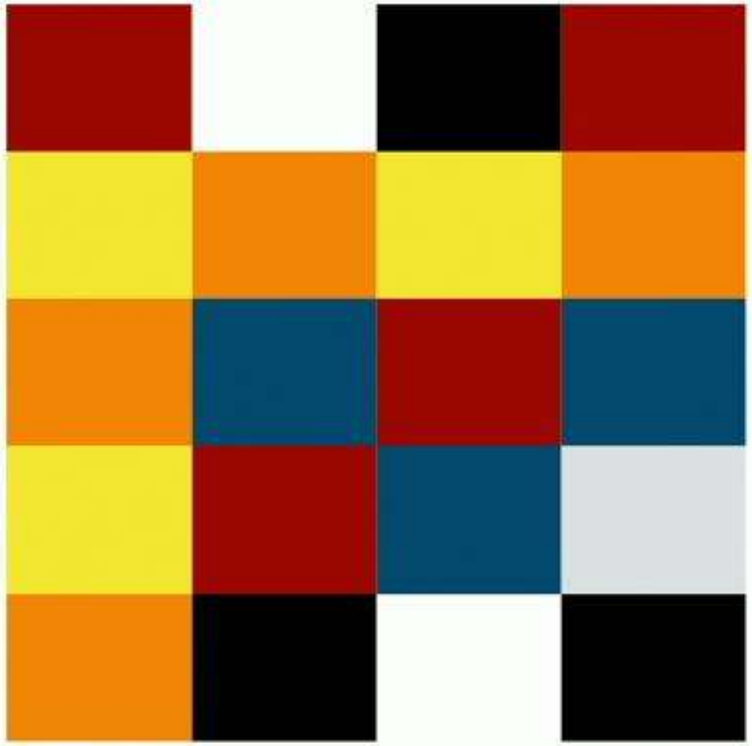
ML Perspective



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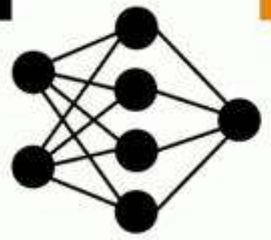

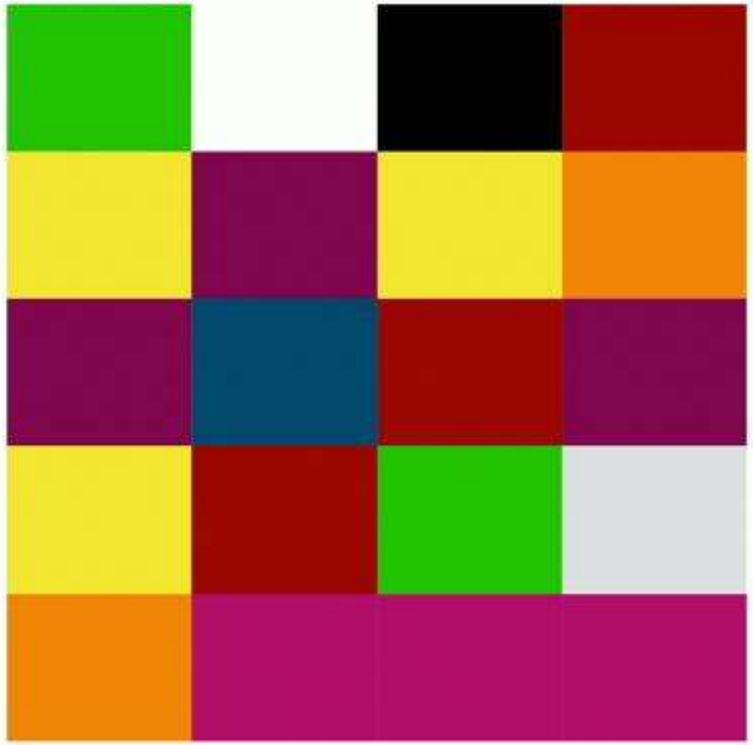

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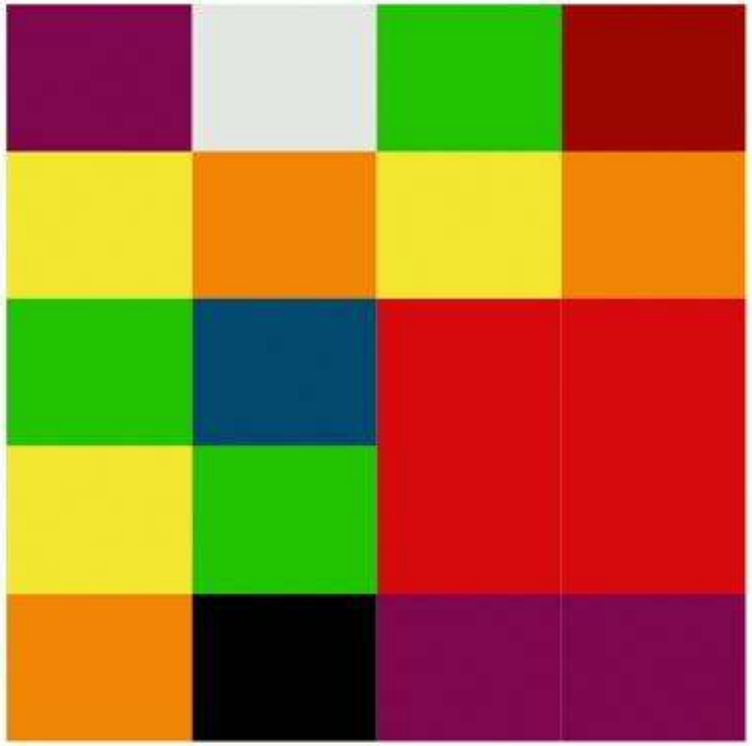
ML Perspective



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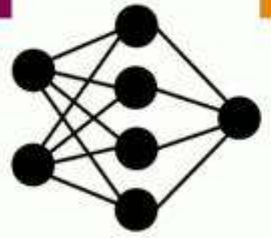

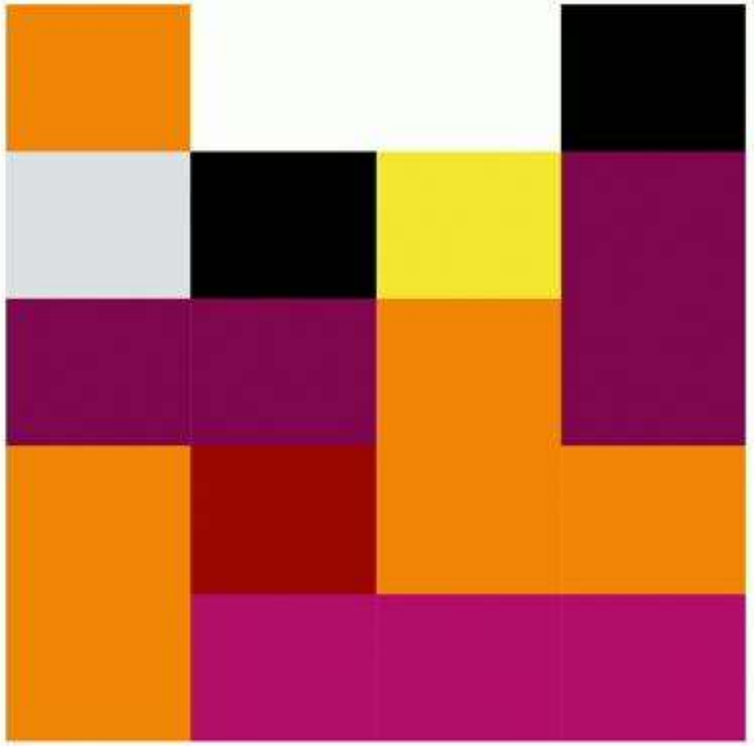

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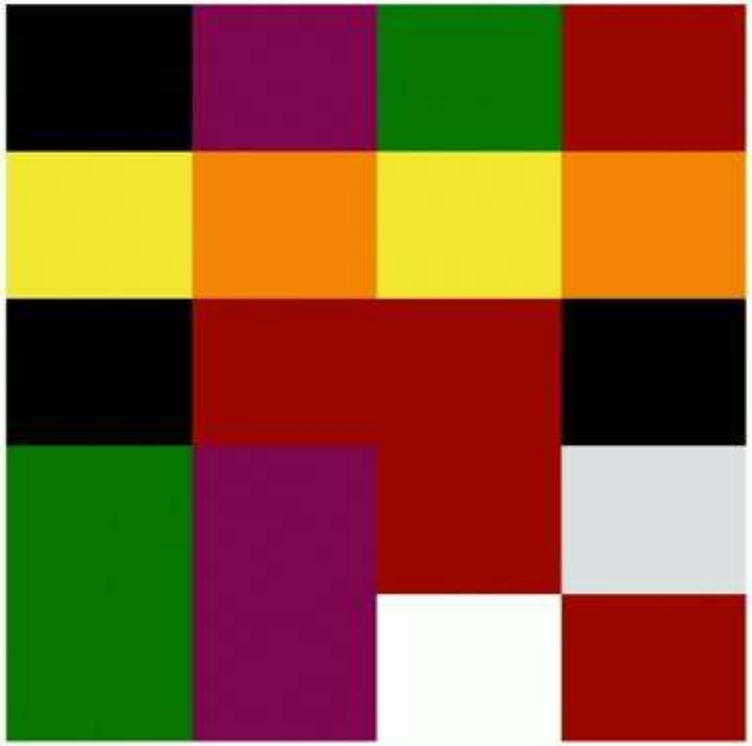

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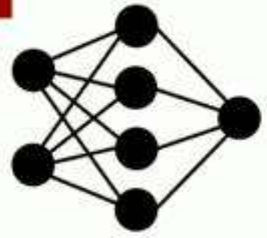

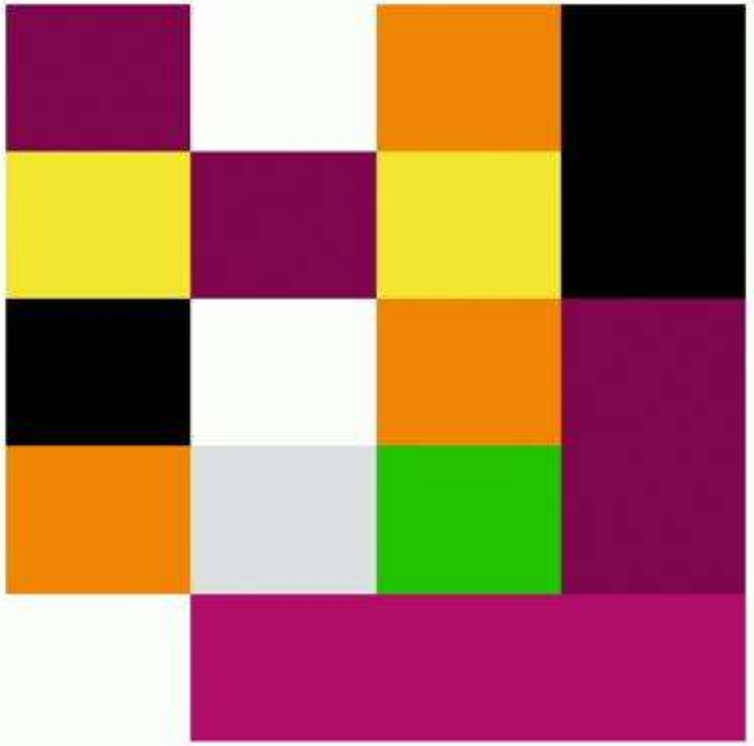

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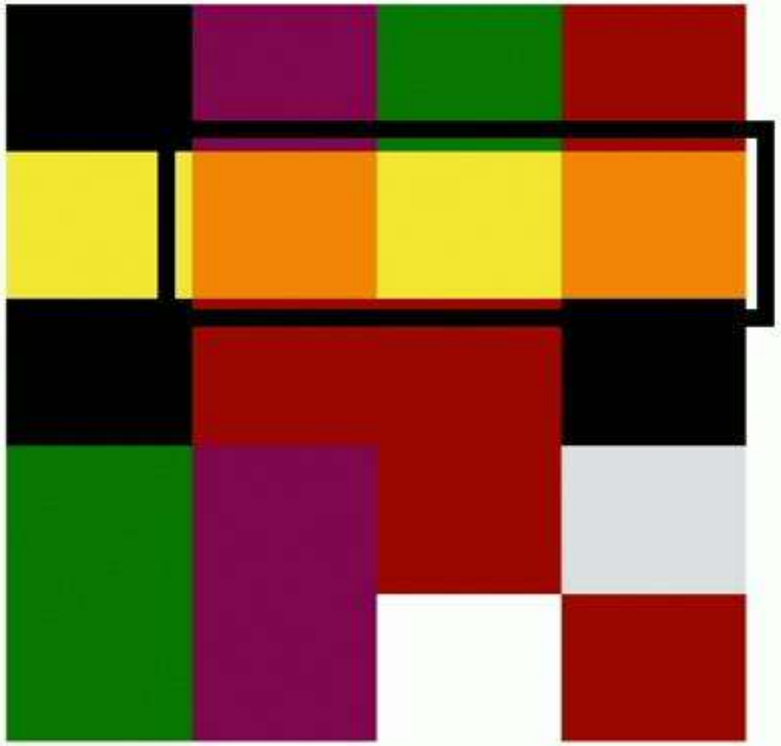

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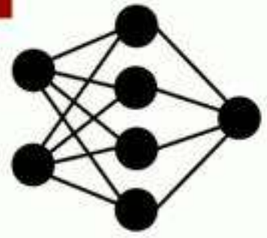

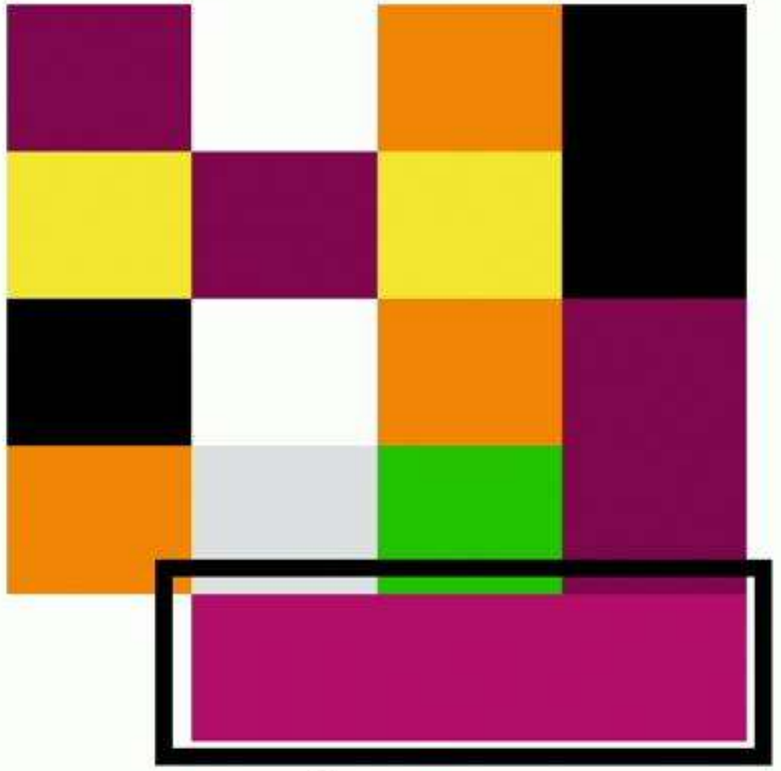

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ML Perspective

dog

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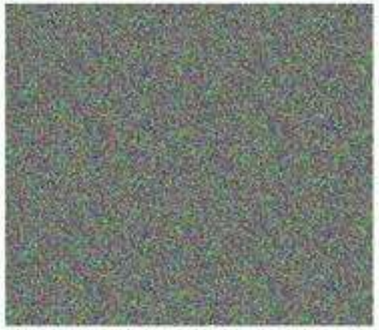

meaningless
perturbation

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cat

ML Perspective

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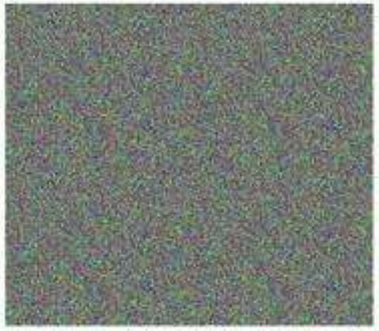

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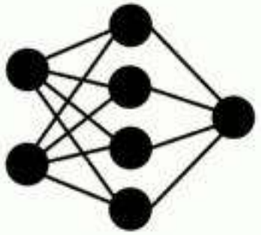

ML Perspective

dog

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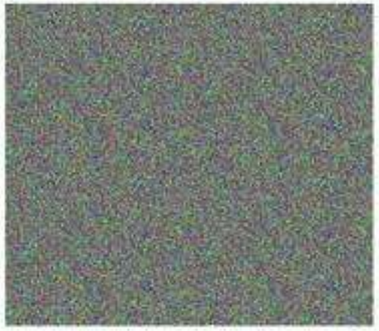

meaningless perturbation

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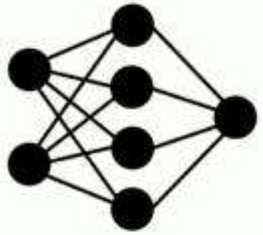

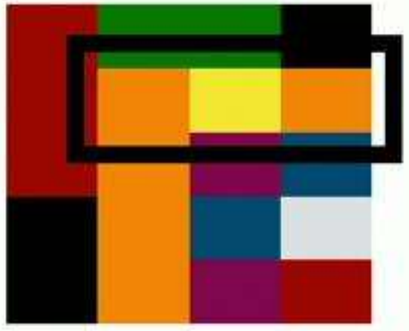

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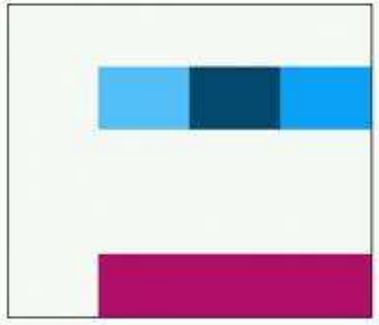

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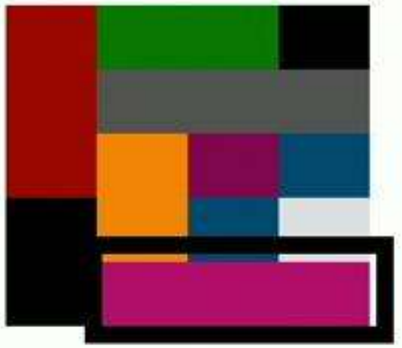

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ML Perspective

dog

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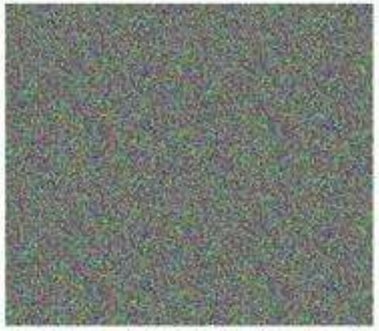

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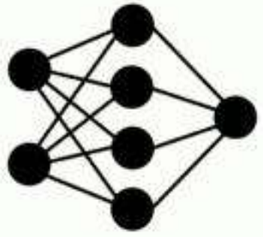

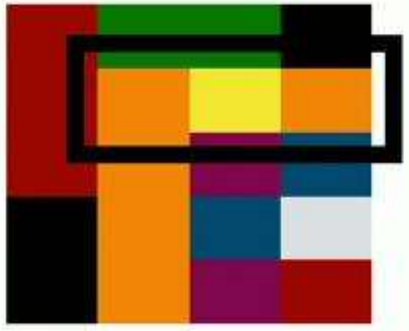

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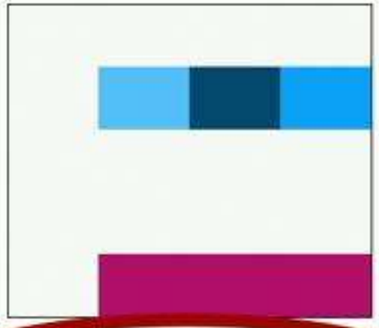

meaningless perturbation

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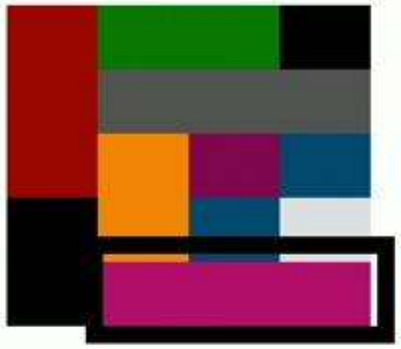

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Are adversarial perturbations just meaningless artifacts?

[Ilyas Santurkar Tsipras Engstrom Tran M '19]

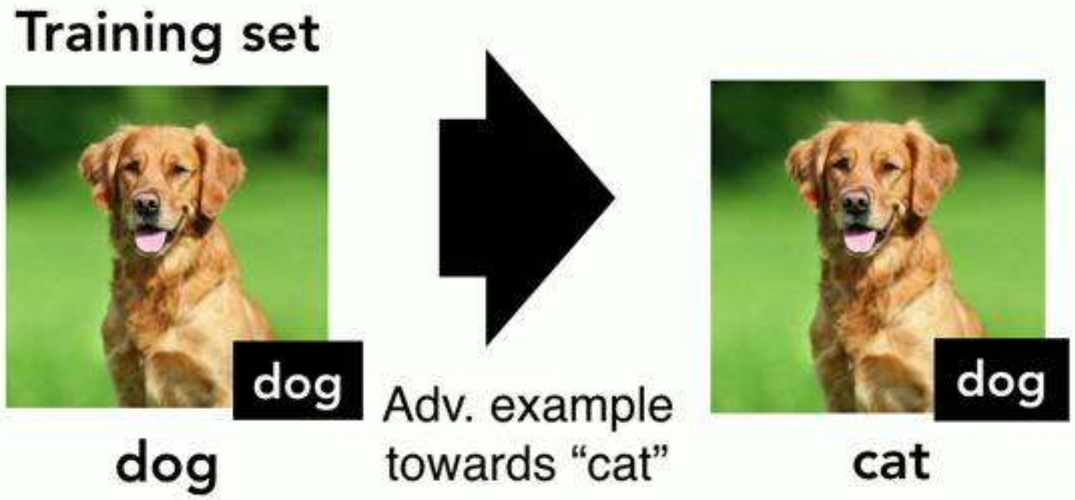
A Simple Experiment

A Simple Experiment

Training set

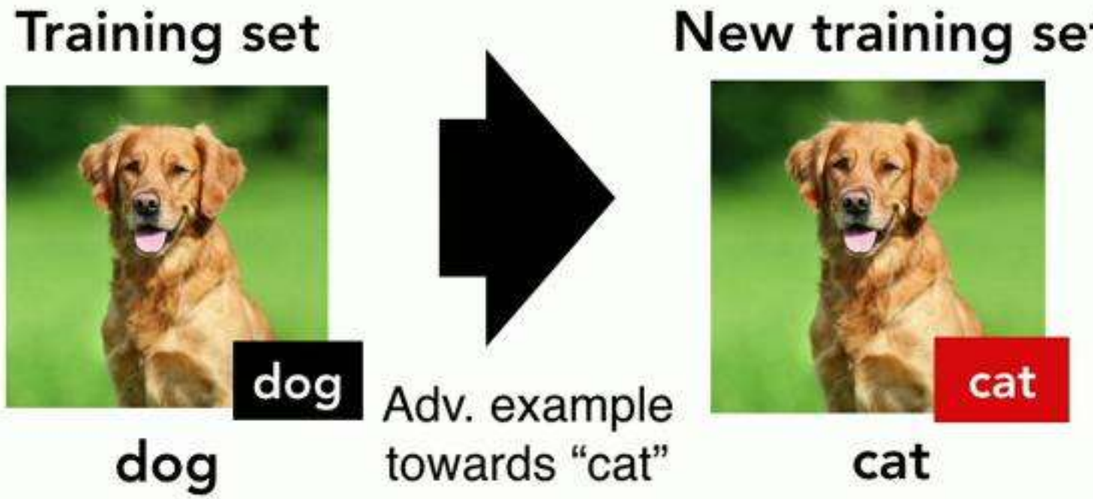
dog

A Simple Experiment



1. **Make adversarial example** towards the other class

A Simple Experiment



1. **Make adversarial example** towards the other class
2. **Relabel** the image as the target class

A Simple Experiment

1. **Make adversarial example** towards the other class
2. **Relabel** the image as the target class
3. Train with **new** dataset but test on the **original** test set

A Simple Experiment

So: We train on a “totally mislabeled” dataset but expect performance on a “correct” dataset

A Simple Experiment

So: We train on a “totally mislabeled” dataset but expect performance on a “correct” dataset

What will happen?

A Simple Experiment

Result: We get a **nontrivial accuracy** on the **original** classification task

A Simple Experiment

Result: We get a **nontrivial accuracy** on the **original** classification task

(For example, 78% on the CIFAR dog vs cat)

What's going on?

What's going on?

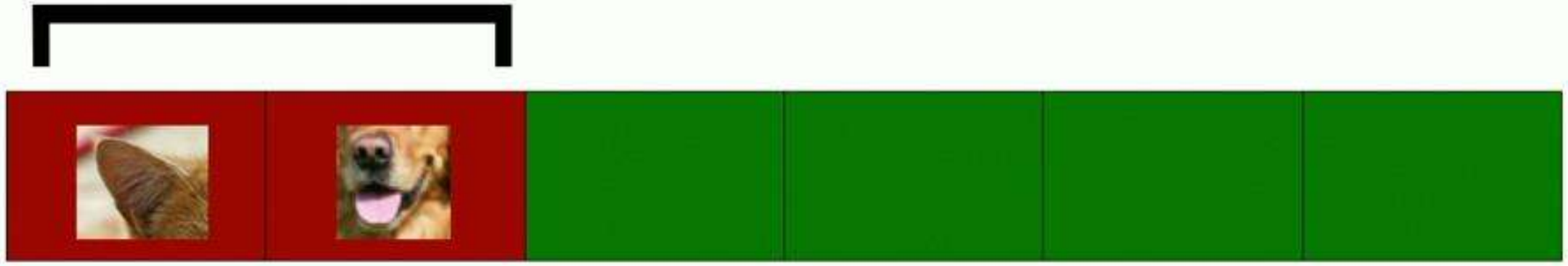
What if adversarial perturbations are **not** aberrations but **features**?

The Robust Features Model

The Robust Features Model

Robust features

Correlated with label
even with adversary



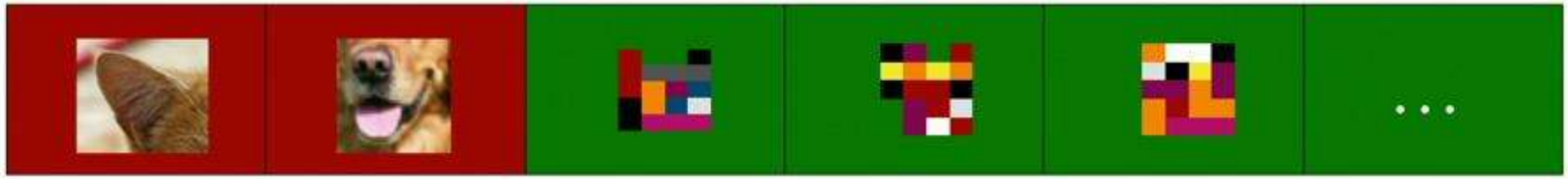
The Robust Features Model

Robust features

Correlated with label
even with adversary

Non-robust features

Correlated with label on average,
but can be flipped within, e.g., ℓ_2 ball



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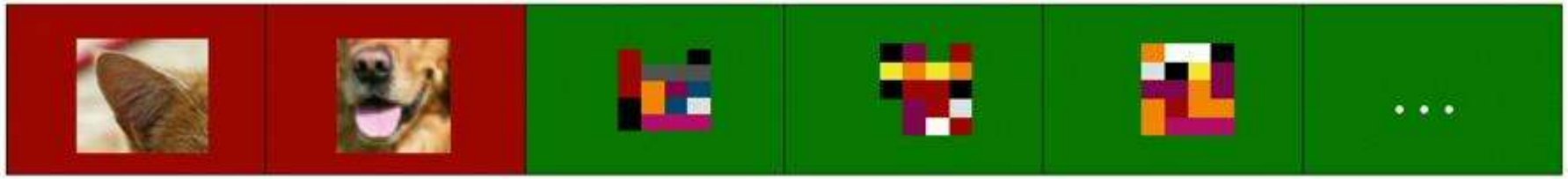
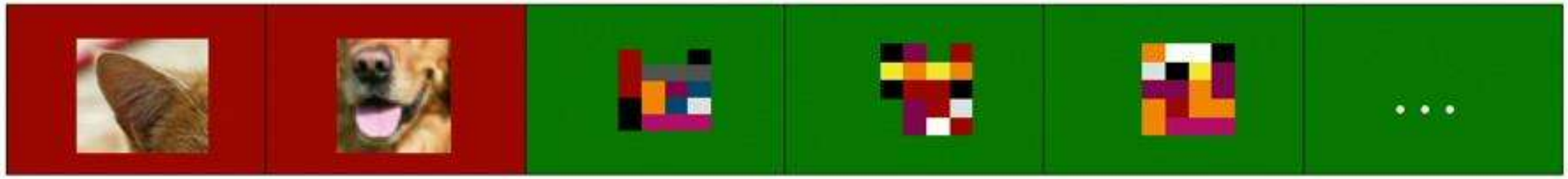


When maximizing (test) accuracy: All features are good

The Robust Features Model

Robust features
Correlated with label
even with adversary

Non-robust features
Correlated with label on average,
but can be flipped within, e.g., ℓ_2 ball



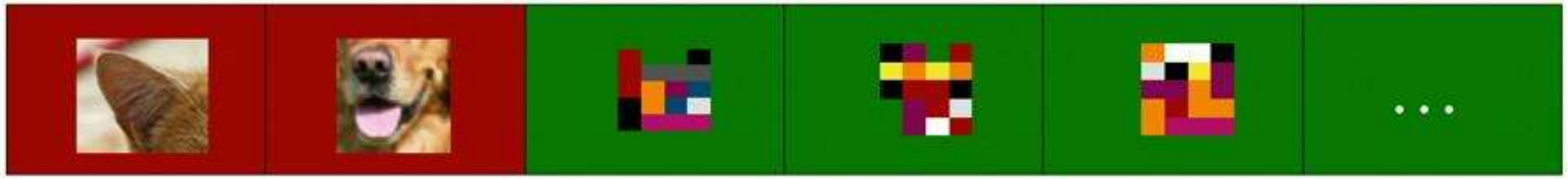
When maximizing (test) accuracy: All features are good

And: Non-robust features are often great!

The Robust Features Model

Robust features
Correlated with label
even with adversary

Non-robust features
Correlated with label on average,
but can be flipped within, e.g., ℓ_2 ball



When maximizing (test) accuracy: All features are good

And: Non-robust features are often great!

That's why our models pick on them
(and **become vulnerable to adversarial perturbations**)

The Simple Experiment: A Second Look

The Simple Experiment: A Second Look

Training set

dog

The Simple Experiment: A Second Look

Training set

dog

Robust features: dog

Non-robust features: dog

The Simple Experiment: A Second Look

Training set

dog

Adversarial example towards “cat”

New training set

cat

Robust features: dog
Non-robust features: dog

Robust features: dog
Non-robust features: cat

The Simple Experiment: A Second Look

Training set

New training set

All robust features are **misleading**

Robust features: dog
Non-robust features: dog

Robust features: dog
Non-robust features: cat

The Simple Experiment: A Second Look

Training set

New training set

All robust features are **misleading**

But: Non-robust features suffice for good generalization

The Simple Experiment: A Second Look

New training set

cat

Robust features: dog

Non-robust features: cat

The Simple Experiment: A Second Look

New training set

cat

Train

Test set

Robust features: dog

Non-robust features: cat

The Simple Experiment: A Second Look

New training set

cat

Train

Test set

Robust features: dog
Non-robust features: cat

Good test accuracy on original test set

Human vs ML Model Priors

Human vs ML Model Priors

dog

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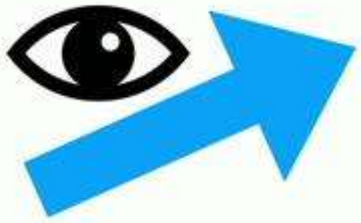

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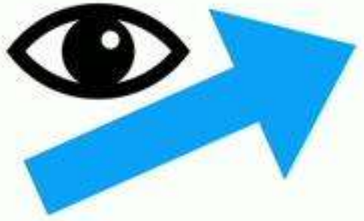

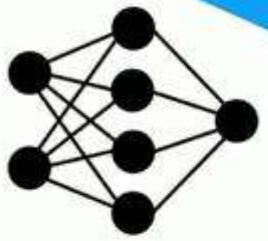

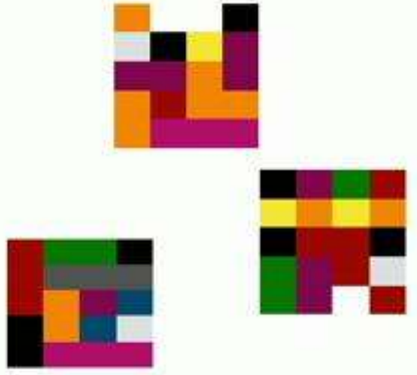

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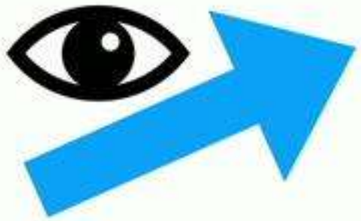
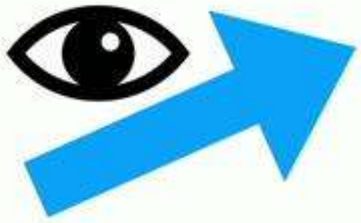
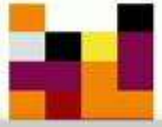


These are **equally valid** classification methods

dog

Human vs ML Model Priors





These are **equally valid** classification methods

No reason to expect our models to use the first one

Human vs ML Model Priors

Adversarial examples are a **human** phenomenon

Human vs ML Model Priors

Adversarial examples are a **human** phenomenon

No hope for interpretable models without intervention **at training time** (instead of post-hoc)

Human vs ML Model Priors

Adversarial examples are a **human** phenomenon

No hope for interpretable models without intervention **at training time** (instead of post-hoc)

Need **additional restrictions (priors)** on what features models should use to make predictions

What now?

What now?

A (new) perspective on adversarial robustness

What now?

A (new) perspective on adversarial robustness

(Provides insights into other questions too)

New capability: Robustification

New capability: Robustification

Training set

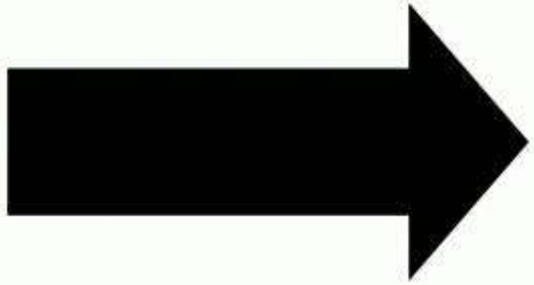
frog

New capability: Robustification

Training set

frog

Restrict to features
of robust model



New capability: Robustification

Training set

frog

Restrict to features of robust model

New training set

"robustified" frog

New capability: Robustification

Test set

Standard training

New training set

"robustified" frog

New capability: Robustification

Test set

Standard training

New training set

"robustified" frog

We get both standard and **robust** accuracy

New capability: Robustification

Test set

Standard training

New training set

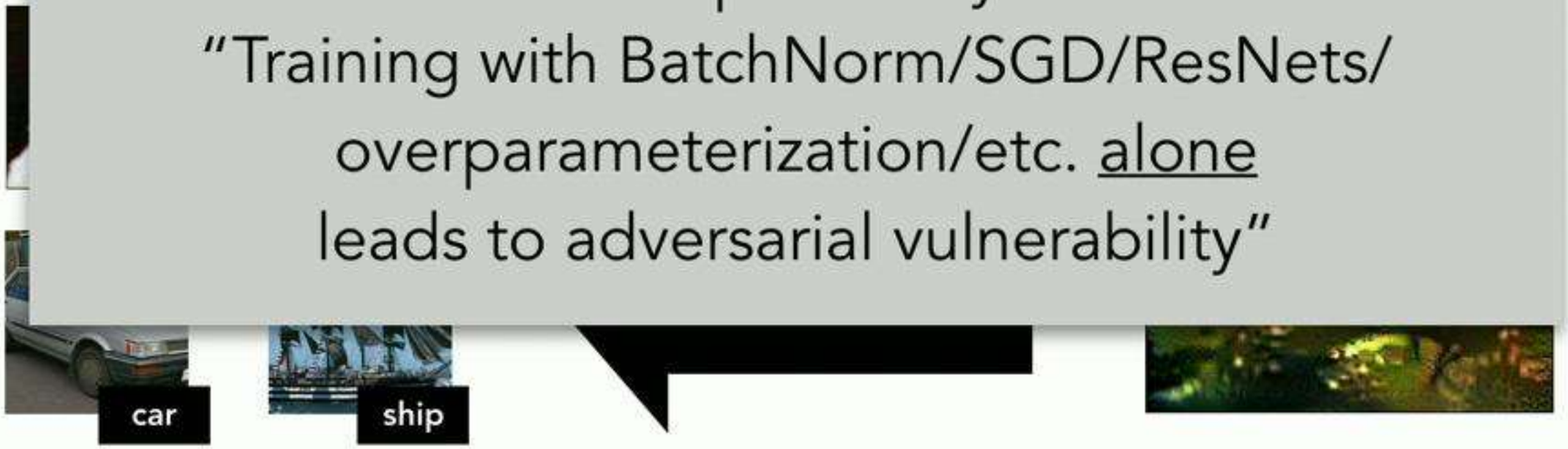
"robustified" frog

We get both standard and **robust** accuracy

So: It really is about features

New capability: Robustification

Also: Counterexample to any statement that "Training with BatchNorm/SGD/ResNets/ overparameterization/etc. alone leads to adversarial vulnerability"



"robustified" frog

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Some Direct Consequences

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Transferability: Features = property of **datasets** (not models)

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Makes features that are non-robust w.r.t. Δ **useless**

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Effectiveness of Randomized Smoothing:
Overwhelms non-robust (w.r.t. Δ) features with noise

Robustness and Data Efficiency

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Robust models can only leverage **robust** features

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A Simple Theoretical Setting:

Robust Max Likelihood Gaussian Classification

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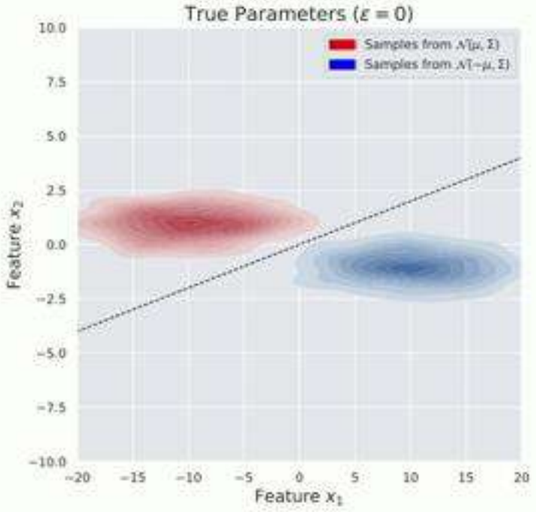

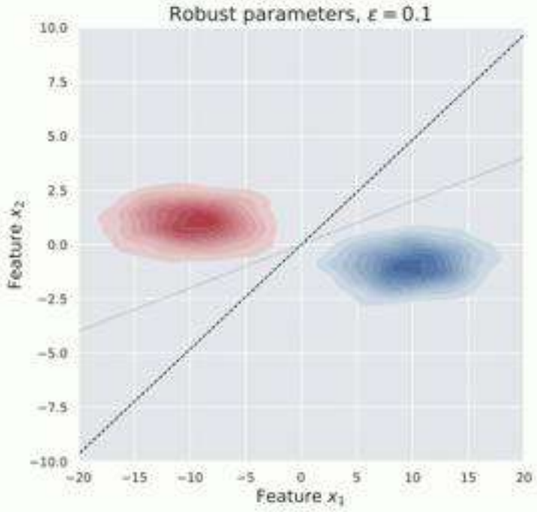

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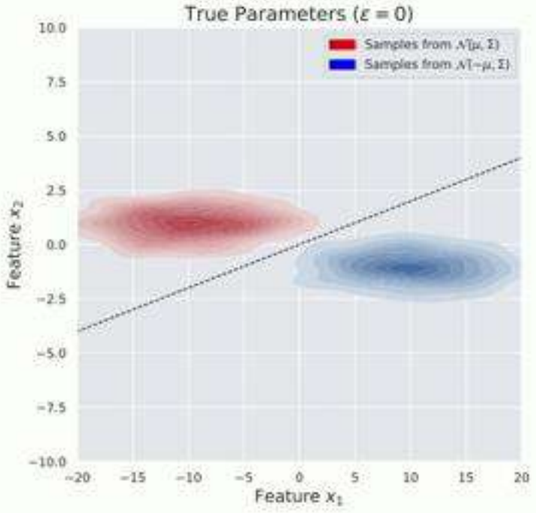

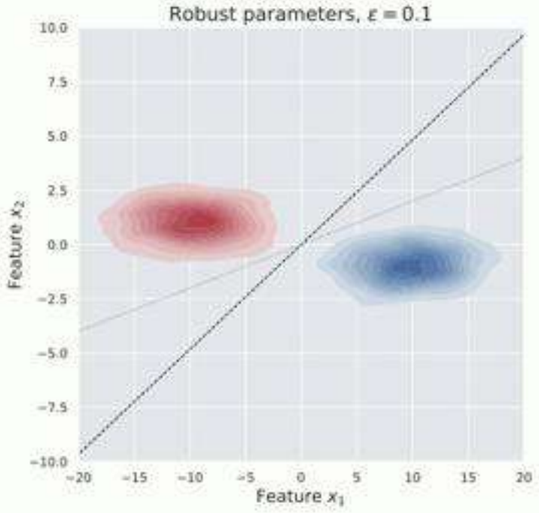

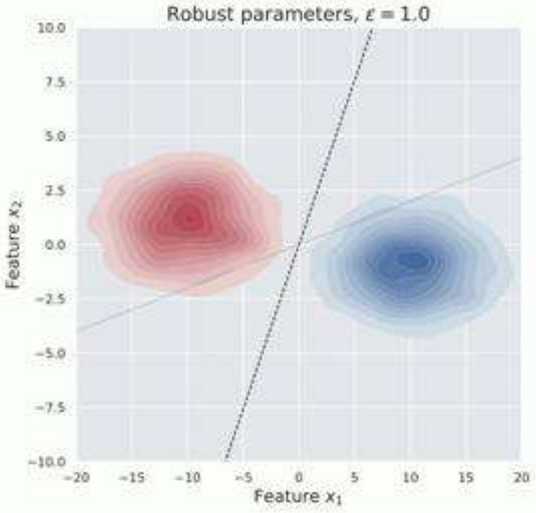

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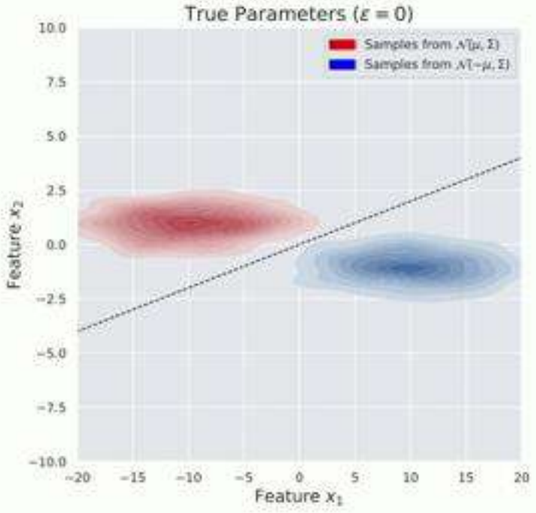

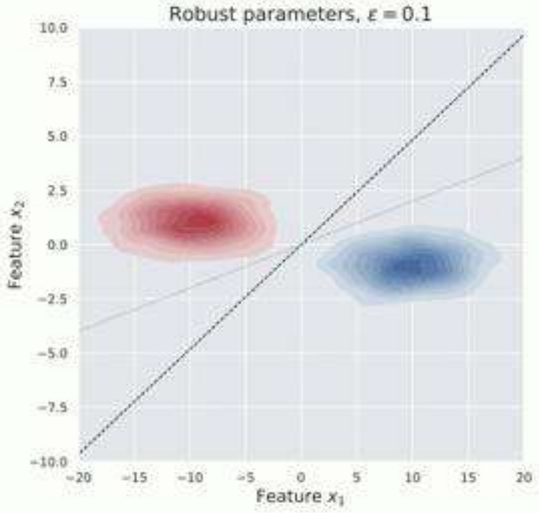

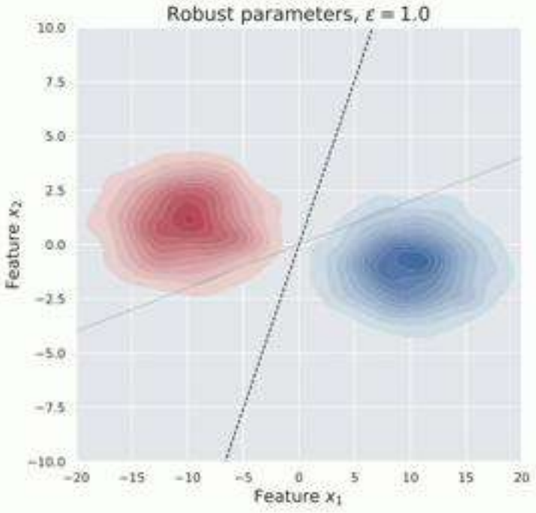

(Exact theorems in the paper)

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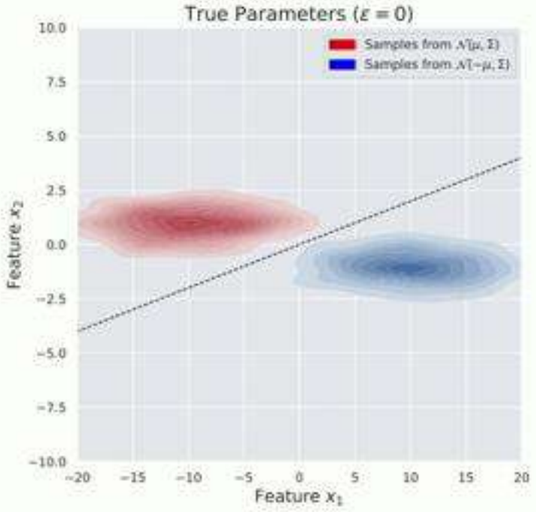

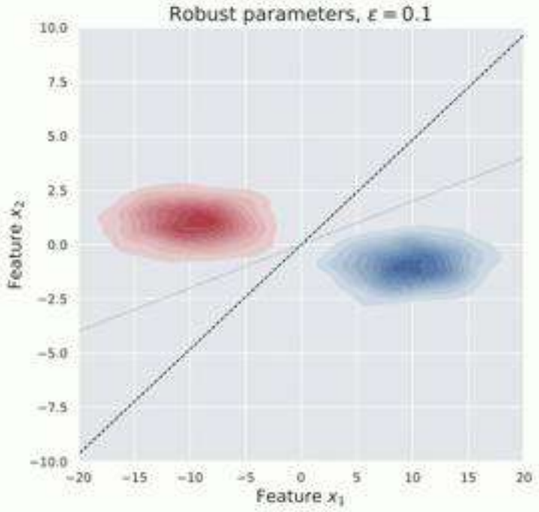

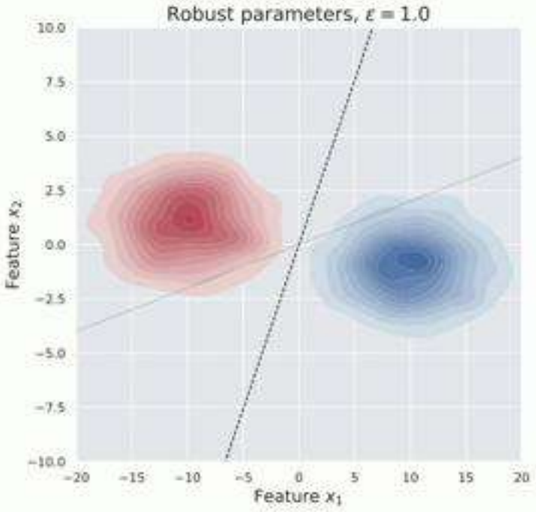

Things to observe:

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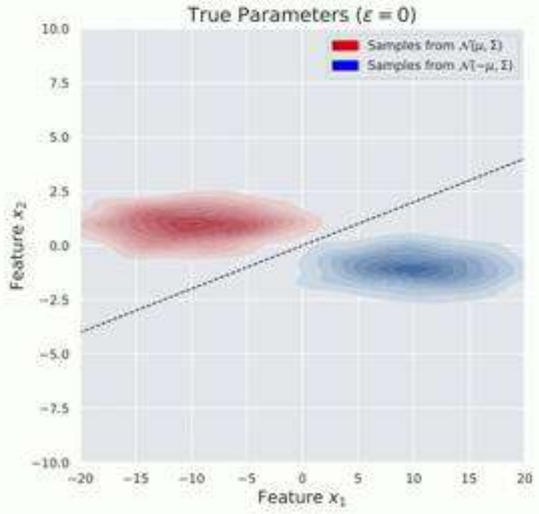

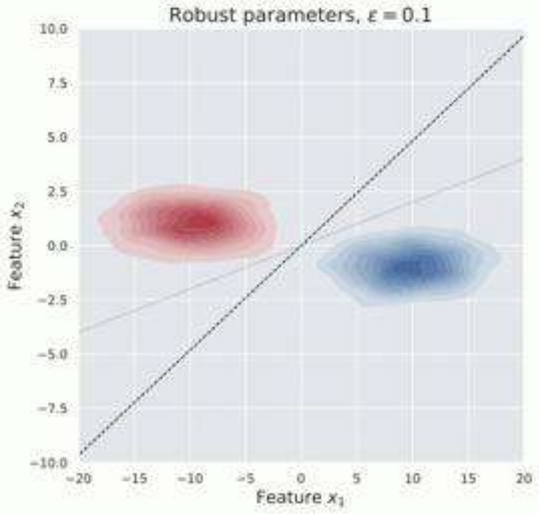

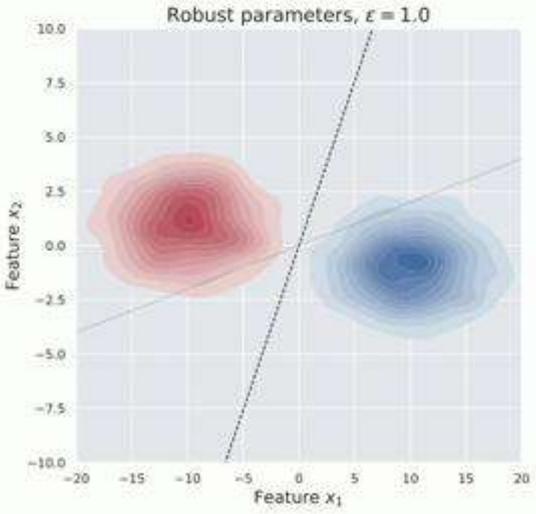

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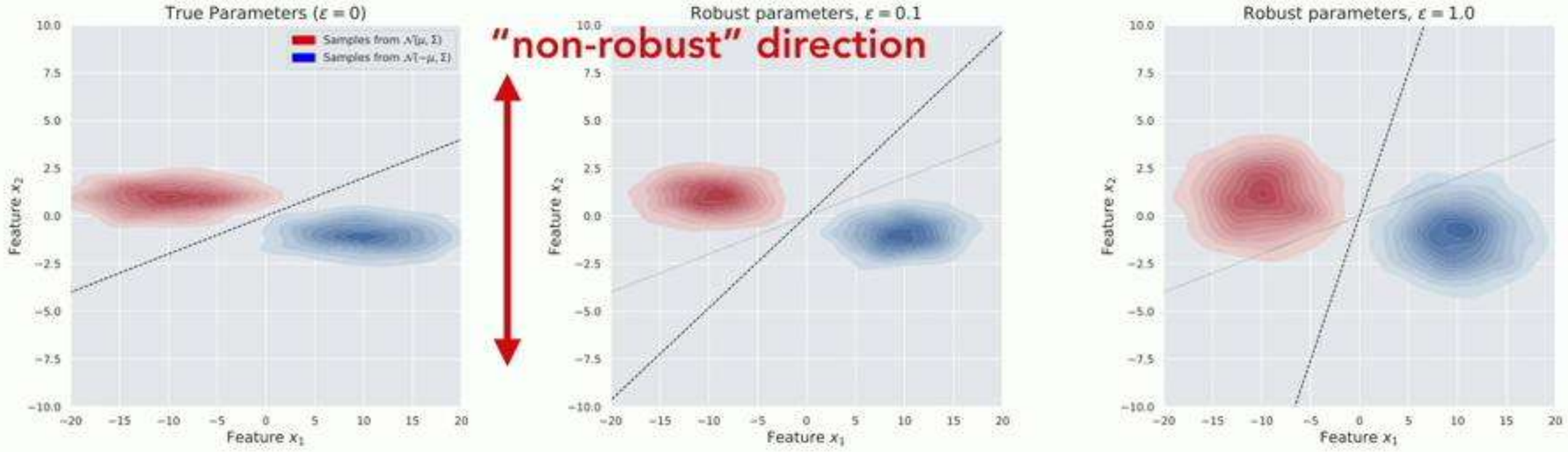

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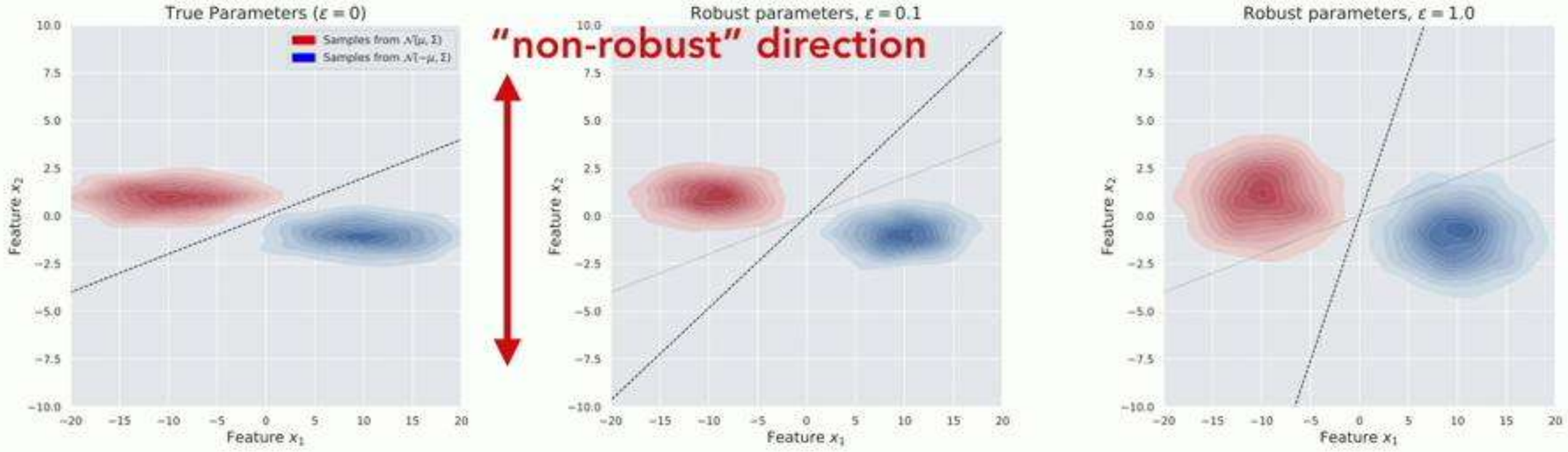

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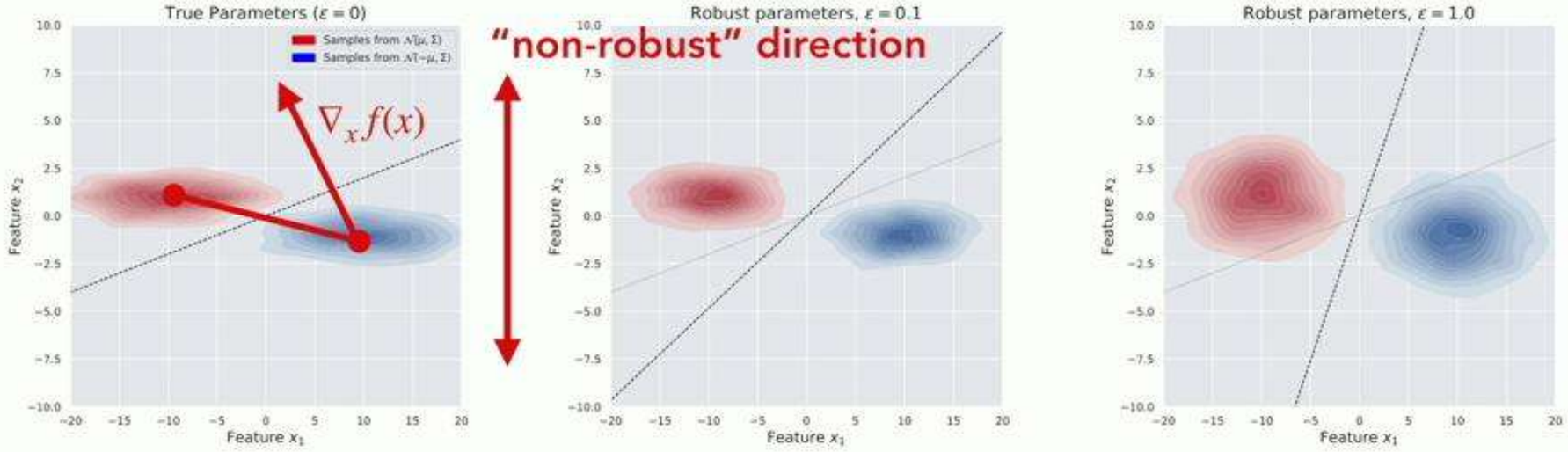

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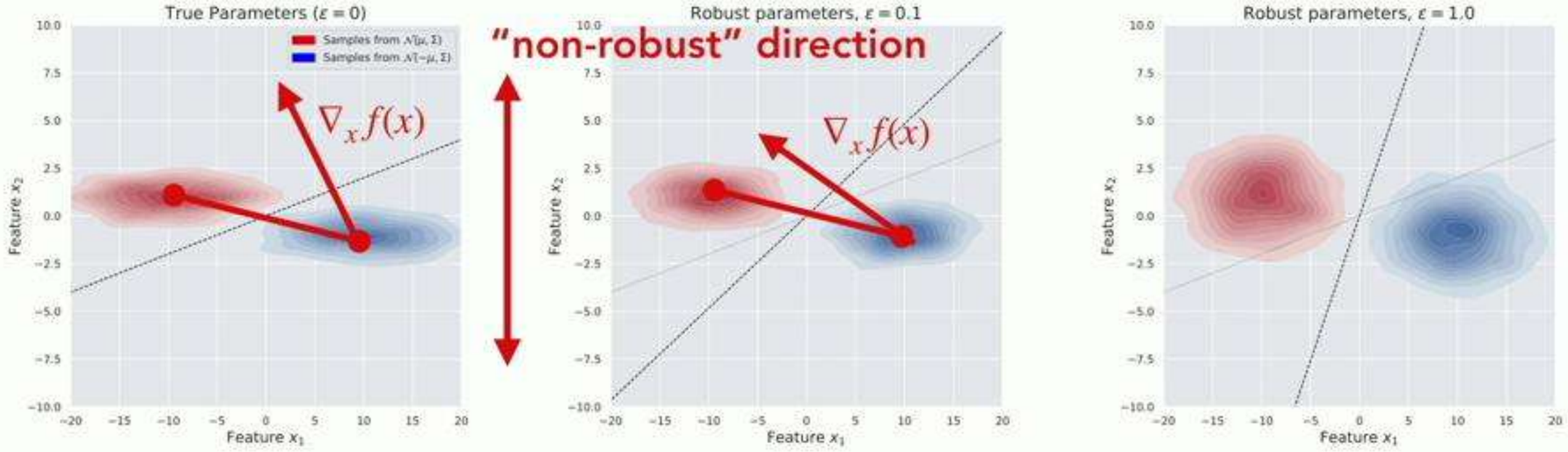

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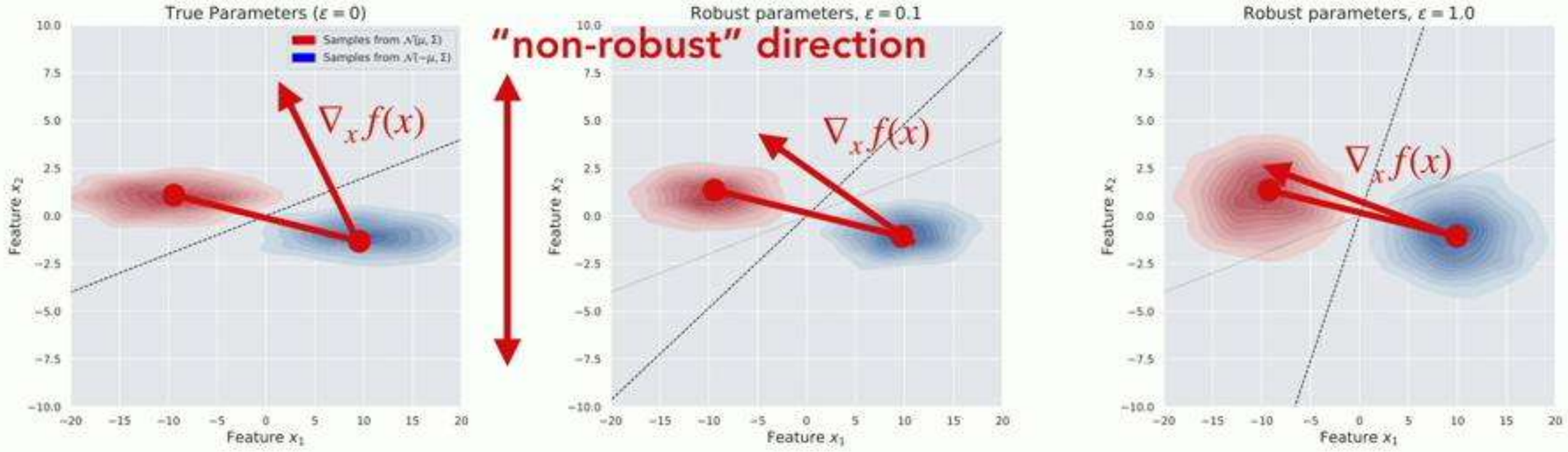

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What if we **prevent** models from learning **non-robust** features?

[Tsipras Santurkar Engstrom Turner M '18]

[Engstrom Ilyas Santurkar Tsipras Tran M '19]

Robustness → Perception Alignment

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Models become more (human) perception aligned

Robustness → Perception Alignment

Input

Models become more (human) perception aligned

Robustness → Perception Alignment

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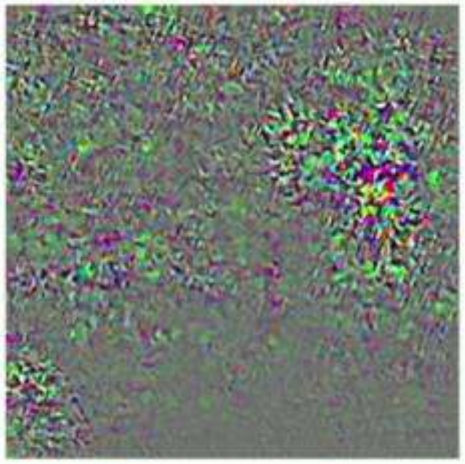
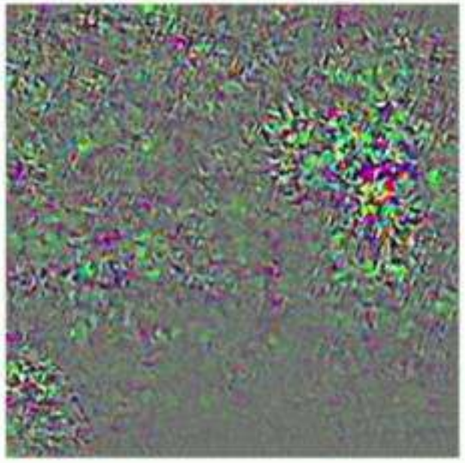


Gradient of
standard model

Models become more (human) perception aligned

Robustness → Perception Alignment

Input



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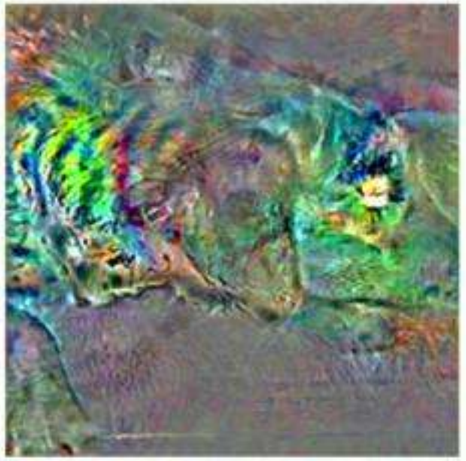

Gradient of
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Robustness → Perception Alignment

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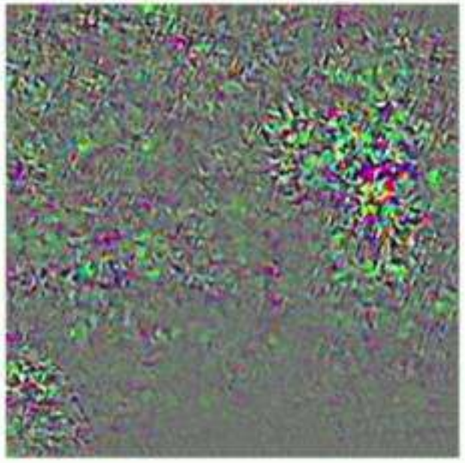

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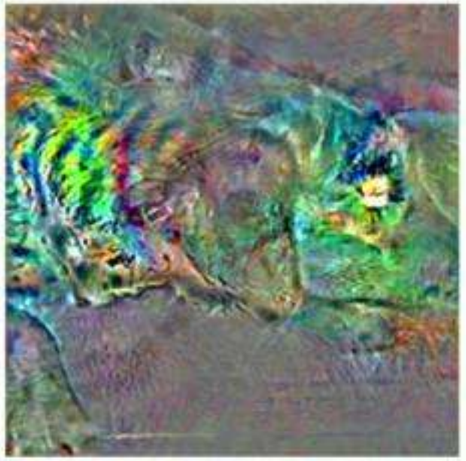

Gradient of
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Models become more (human) perception aligned

→ Robustness acts as a **prior** for "meaningful" features

Robustness → Better Representations

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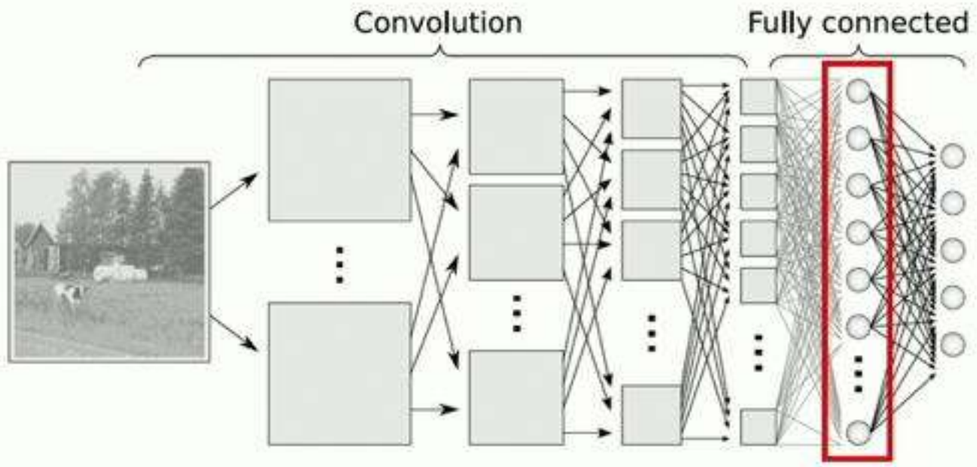

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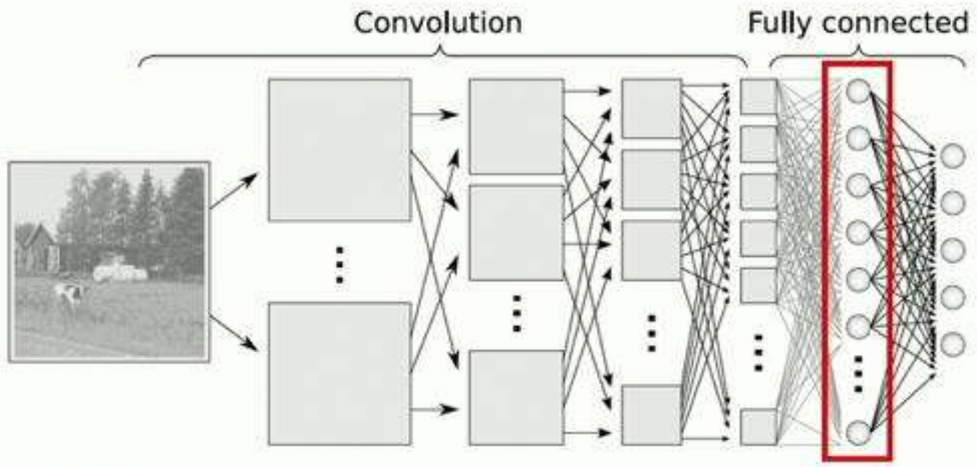
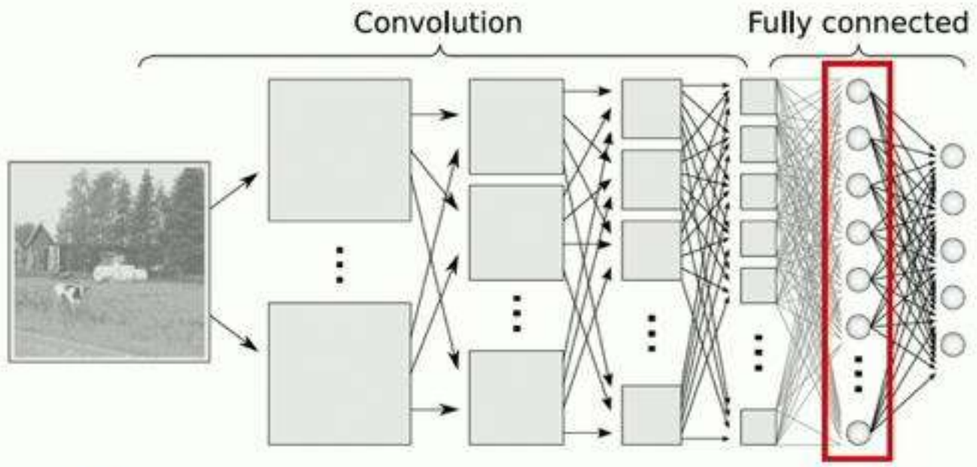


≈

Standard Representation

Robustness → Better Representations



≈

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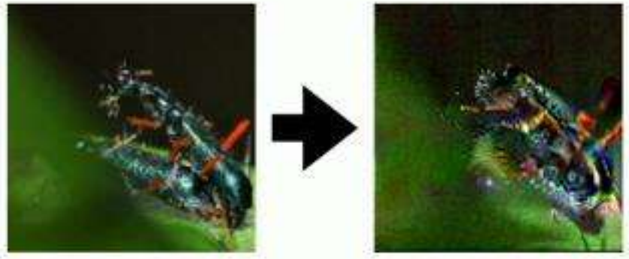


Robust Representation

Robustness → Better Representations

Robust representations enable a wide range of feature manipulations/visualizations in a **simple** way

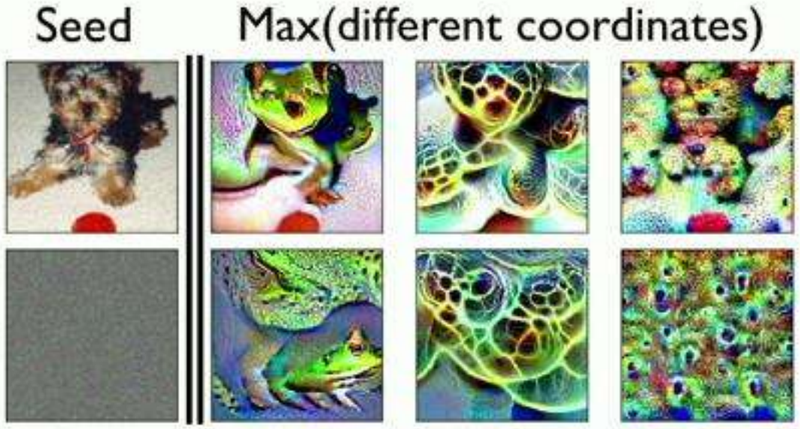
Robustness → Better Representations

Interpolation between **any** two inputs

Robustness → Better Representations

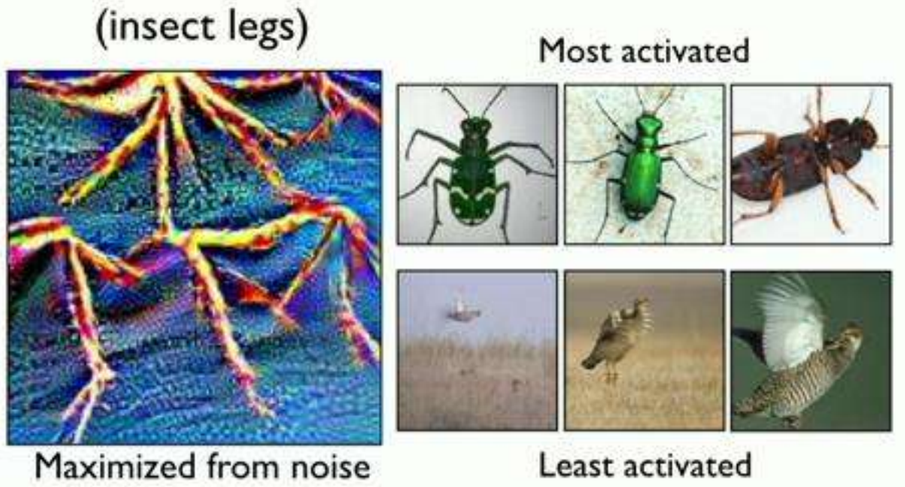
Direct feature visualization

Robustness → Better Representations



Direct feature visualization

Robustness → Better Representations



Direct feature visualization

Robustness → Better Representations

Add stripes

Direct feature manipulation

Robustness → Better Representations

Original image

label: “insect”; prediction: “dog”

Feature-level sensitivity analysis

Robustness → Better Representations

Original image

Top two features

label: "insect"; prediction: "dog"

Feature-level sensitivity analysis

Robustness → Better Representations

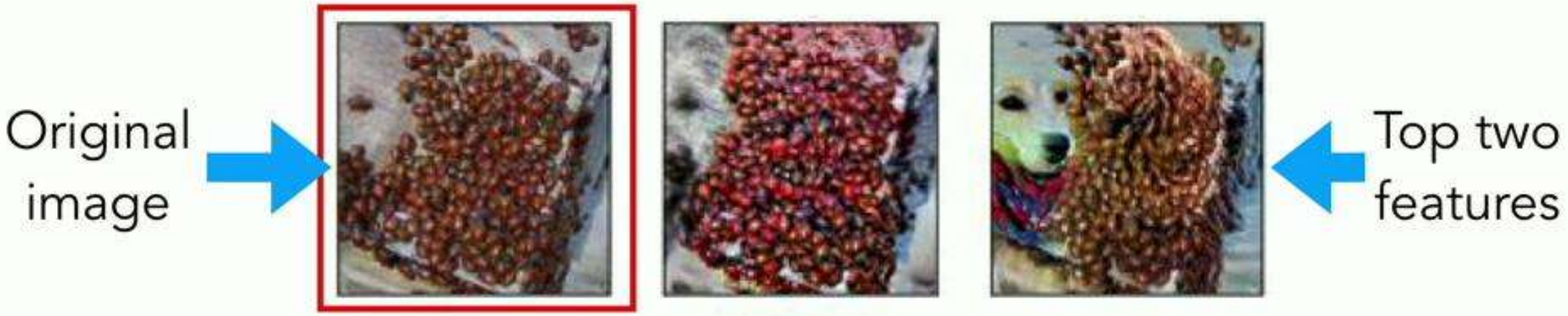
Original image

Top two features

label:“insect”; prediction:“dog”

Feature-level sensitivity analysis

Robustness → Better Representations



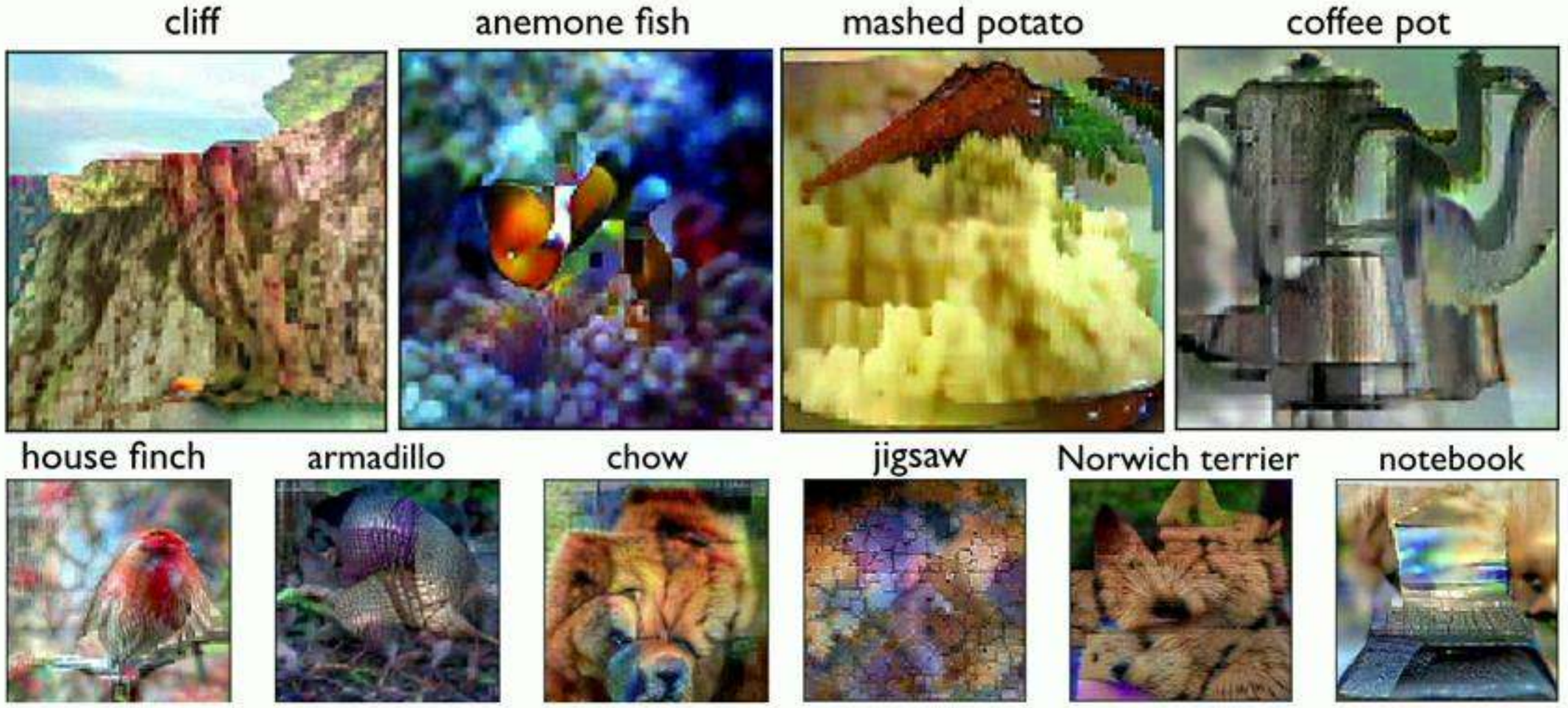
label: "insect"; prediction: "dog"

Feature-level sensitivity analysis

What else can we do?

[Santurkar Tsipras Tran Ilyas Engstrom M ’19]

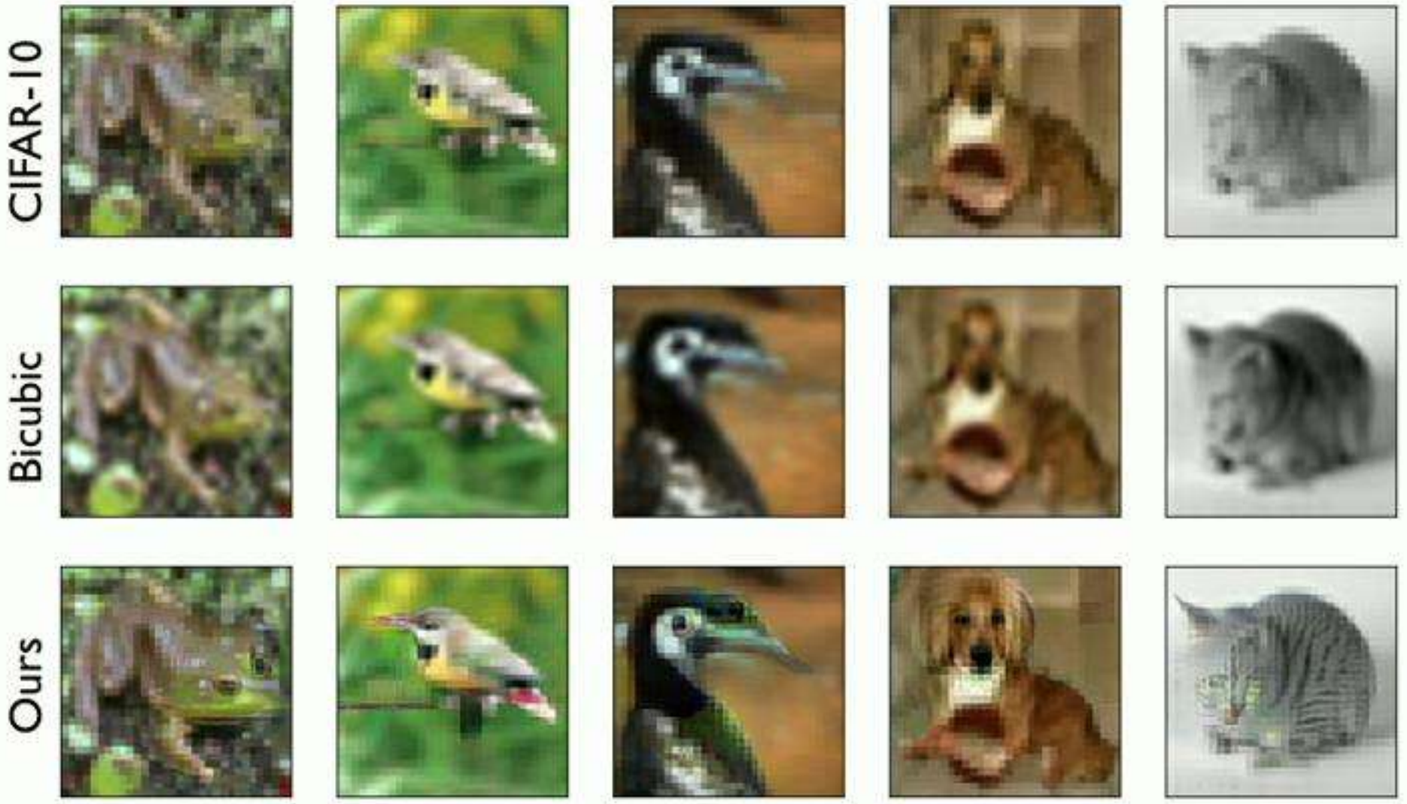
Robustness → CV Applications



(Random samples, 1K training images, no tuning)

Generative models (that work **better** on **large** datasets)

Robustness → CV Applications

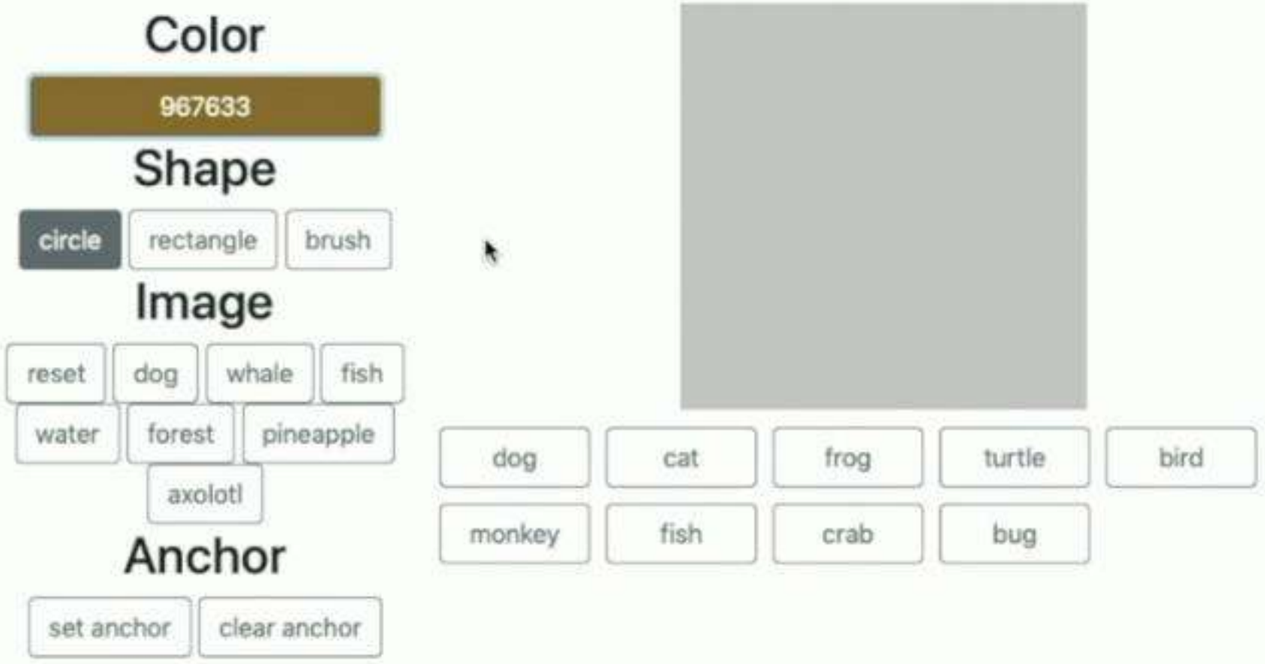


Super-Resolution

Robustness → CV Applications

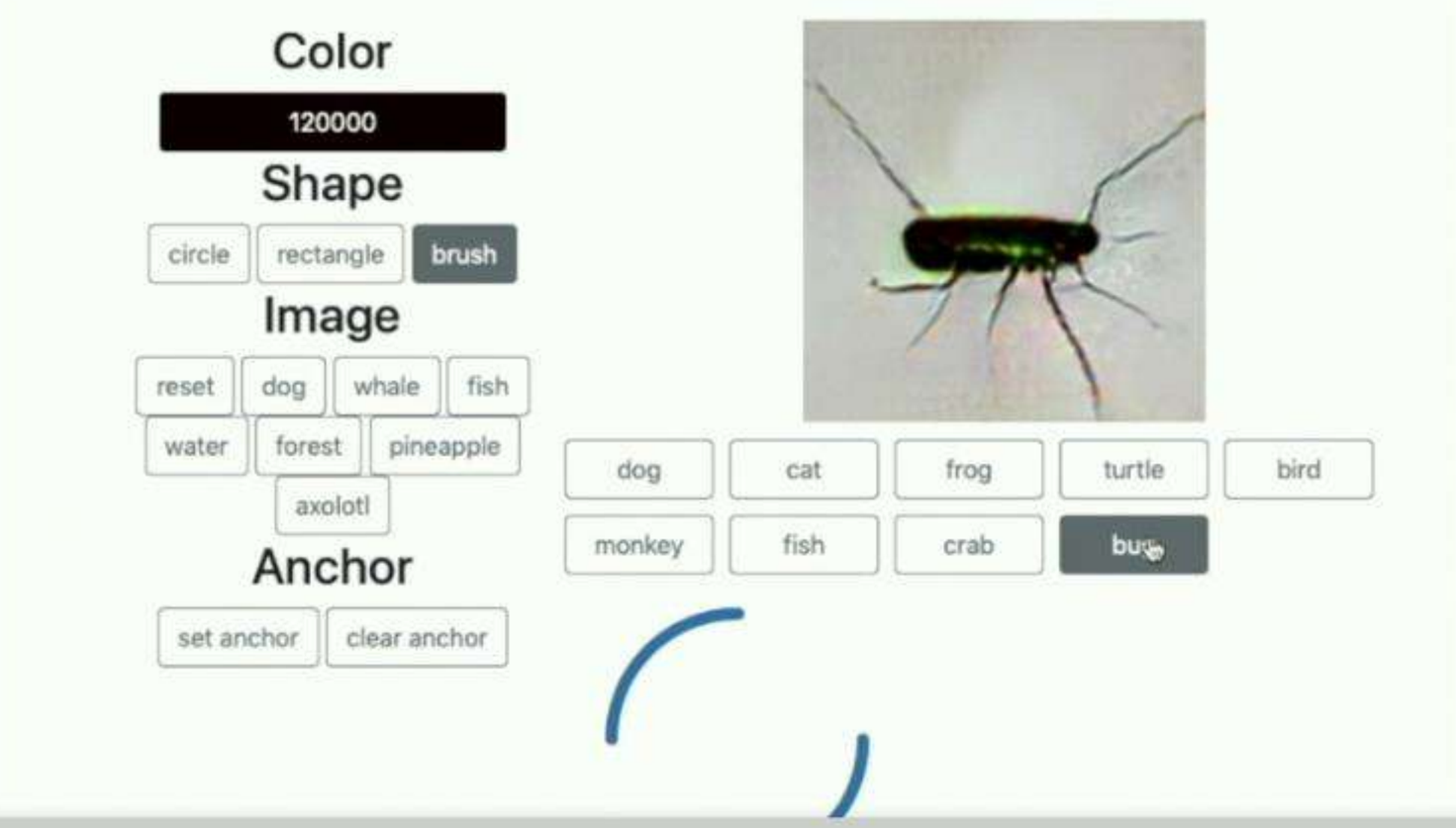
In-Painting

Robustness → CV Applications



Interactive **image class** manipulation

Robustness → CV Applications

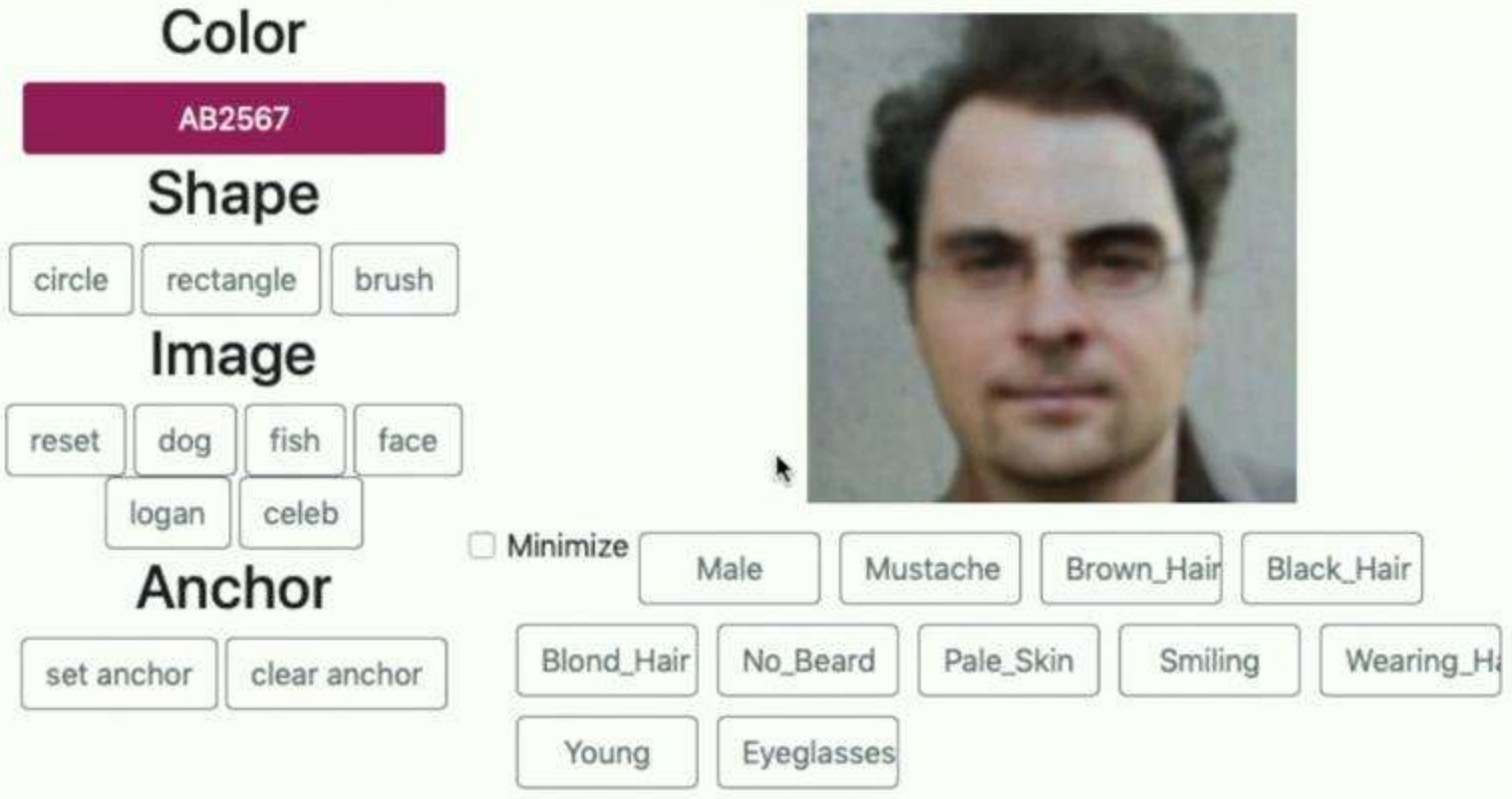


Interactive **image class** manipulation

Robustness → CV Applications

Enables exploration of data space

Robustness → CV Applications



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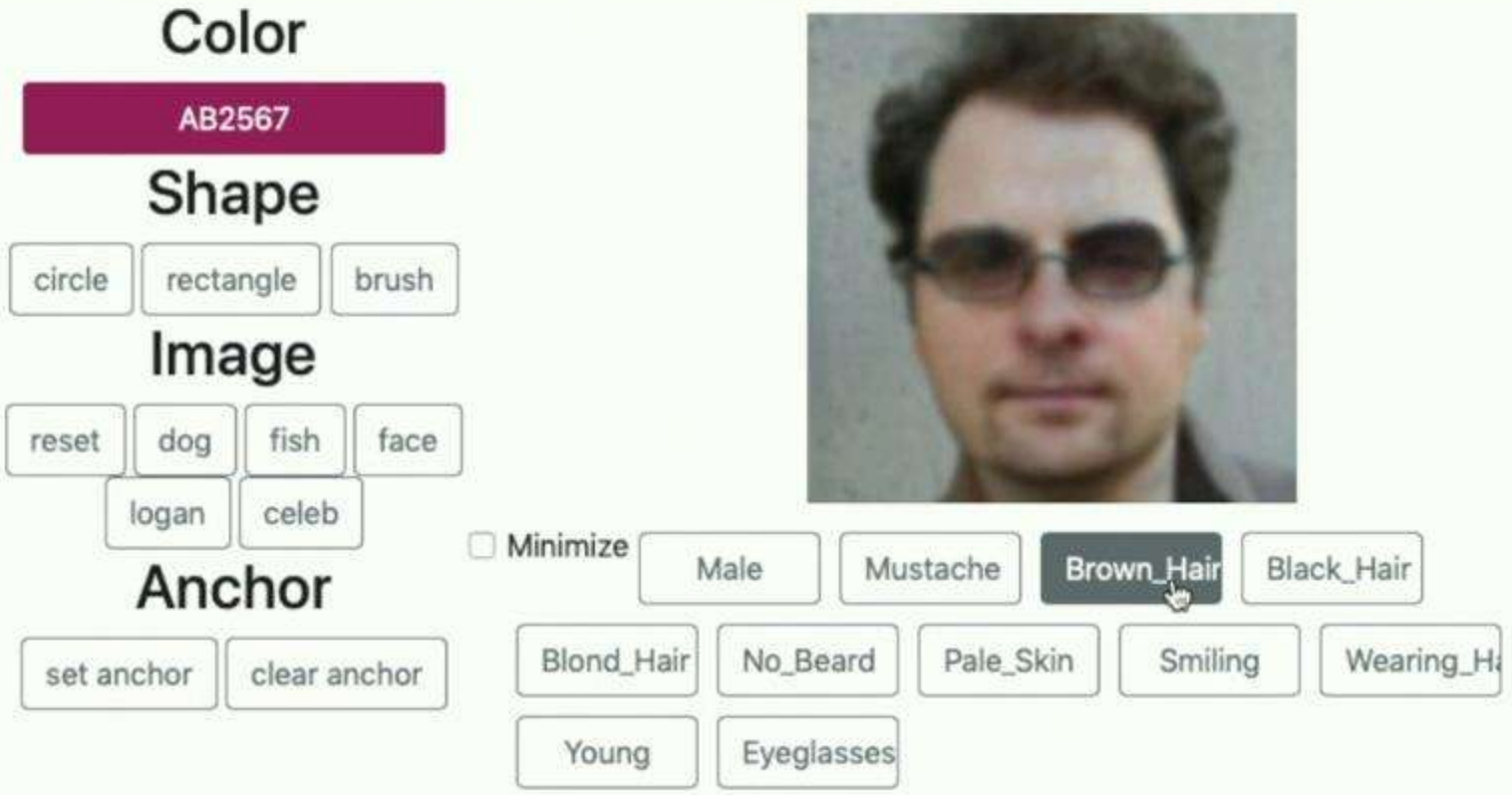

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See: http://bit.ly/robustness_demo

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Takeaways

But: Adv. robustness is not only about robustness to an adversary → it's about **how our models learn**

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→ What is the "right" notion of generalization?
Is it really about getting max accuracy possible?

→ How to measure distribution shift?
Shouldn't it be more about representations?

→ How much do we value human alignment/interpretability?

Adversarial robustness =
Framework for making our models better

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gradientscience.org

Graph neural networks and graph isomorphism

Soledad Villar

Center for Data Science
Courant Institute of Mathematical Sciences

NEW YORK UNIVERSITY

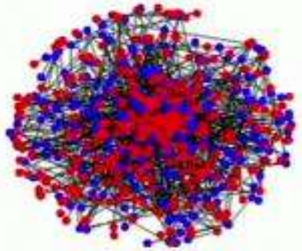
Geometry of Deep Learning
Microsoft, August 27 2019

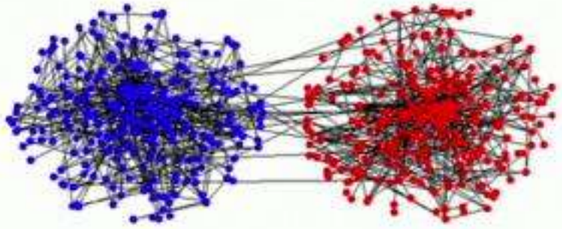
Motivating example 1

Clustering the stochastic block model

$A \sim SBM(p, q, n, 2)$ (two equal-sized communities):

$$\mathbb{P}(A_{ij} = 1) = \begin{cases} p & \text{if } i, j \text{ in the same community} \\ q & \text{if } i, j \text{ in different communities} \end{cases}$$





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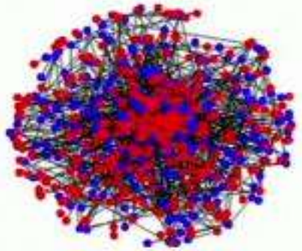
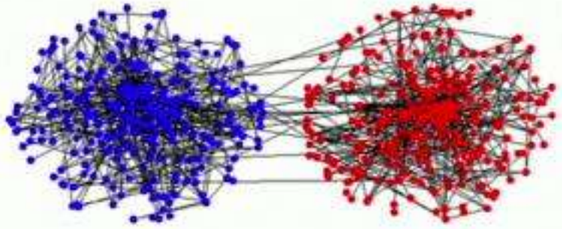
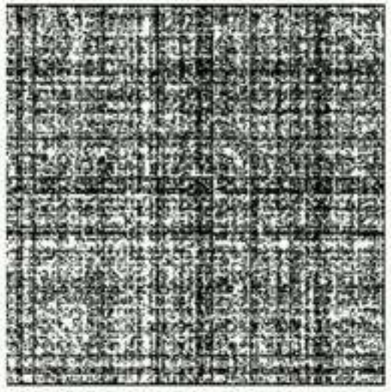
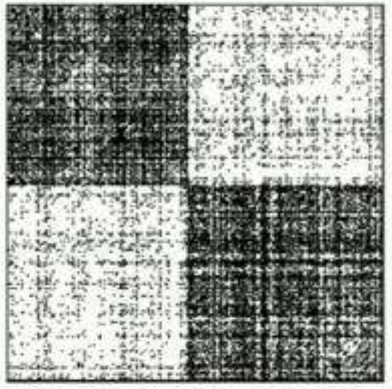




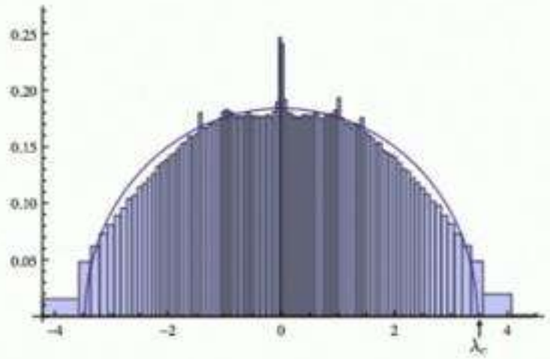




Clustering the stochastic block model

$A \sim SBM(a/n, b/n, n, 2)$ sparse.
Statistical threshold for detection: $(a-b)^2 > 2(a+b)$.

Spectrum doesn't concentrate (high degree vertices dominate it)
Laplacian is not useful for clustering



Other methods succeed. Example: semidefinite programming.

Krzakala, Moore, Mossel, Neeman, Sly, Zdeborová, Zhang, 2013

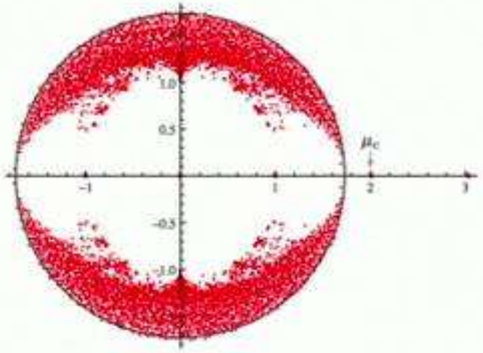
Deshpande, Abbe, Montanari, 2014

Abbe, Bandeira, Hall, 2014

Spectral redemption

Consider the non-backtracking operator (from linearized BP)

$$B_{(i\to j)(i'\to j')} = \begin{cases} 1 \text{ if } j = i' \text{ and } j' \neq i \\ 0 \text{ otherwise} \end{cases}$$



Second eigenvector of B reveals clustering structure

Krzakala, Moore, Mossel, Neeman, Sly, Zdeborová, Zhang, 2013

Bordenave, Lelarge, Massoulie, 2015

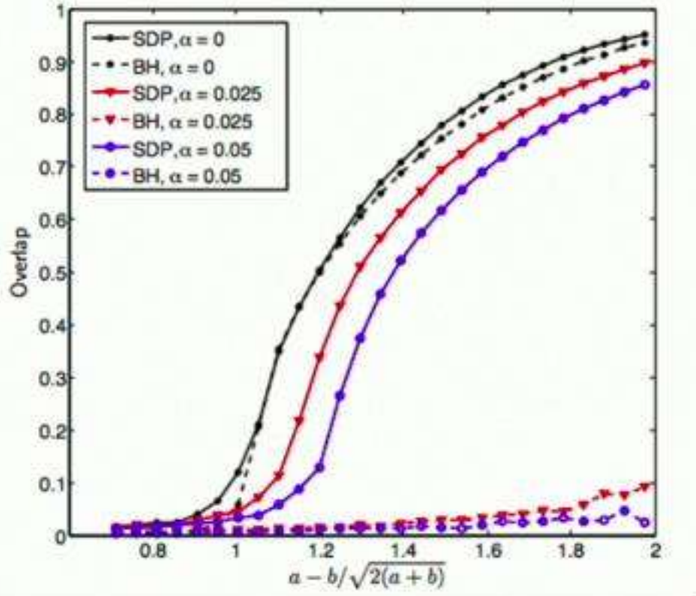
Bethe Hessian

$$BH(r) = (r^2 - 1)I - rA + D$$

Fixed points of BP $\longleftrightarrow$ Stationary points of Bethe free energy

Second eigenvector reveals clustering structure

Pitfall: highly dependent in the model.



Saade, Krzakala, Zdeborová, 2014

Javanmard, Montanari, Ricci-Tersenghi, 2015

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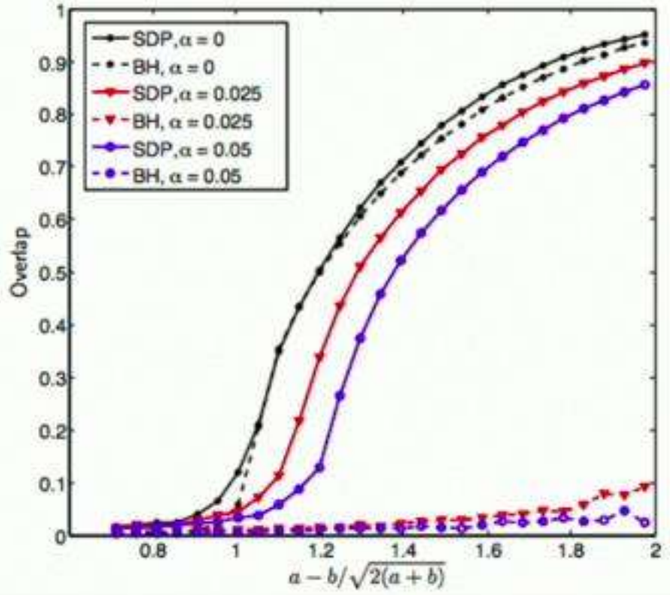

Saade, Krzakala, Zdeborová, 2014

Javanmard, Montanari, Ricci-Tersenghi, 2015

Goal: Combine graph operators $I, D, A, \ldots$ to generate robust "data-driven spectral methods" for problems in graphs

Graph neural networks

sGNN($\mathcal{M}$)

Power method: $v^{t+1} = Mv^t \qquad t = 1, \ldots, T.$

Scarselli, Tsoi, Hagenbuchner, Monfardini, 2009

Chen, Li, Bruna, 2017

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Graph with adjacency matrix A. Set $\mathcal{M} = \{I_n, D, A, A^2, \dots, A^{2^J}\}$,

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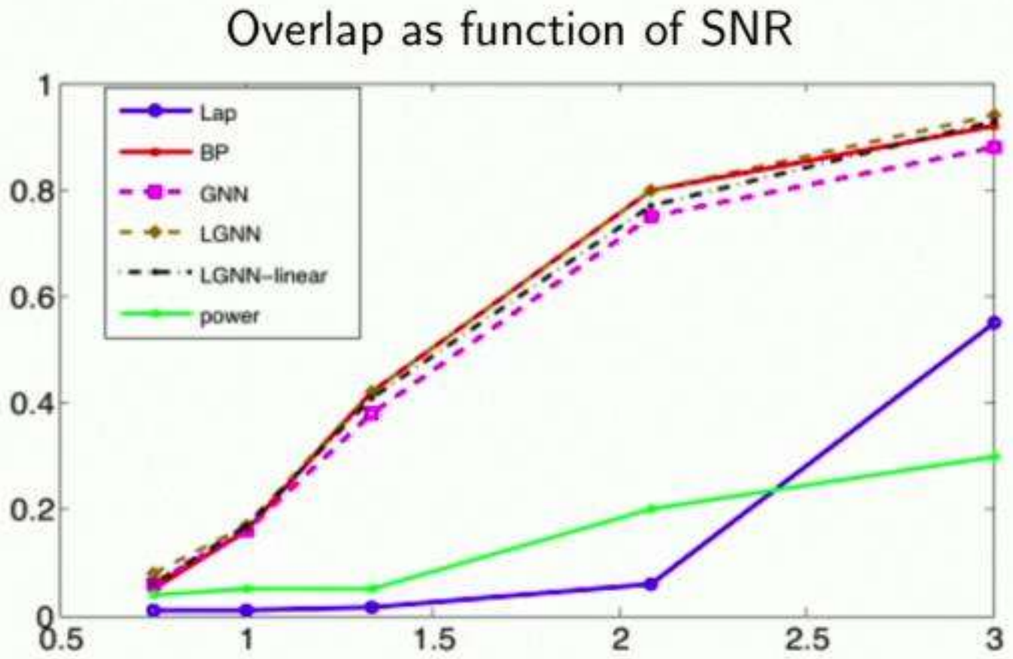
- Equivariant wrt permutations $G \mapsto \phi(G)$ then $G_\Pi \mapsto \Pi\phi(G)$.

Scarselli, Tsoi, Hagenbuchner, Monfardini, 2009

Chen, Li, Bruna, 2017

Numerical performance. SBM $k = 2$



Theoretical result: Under simplifications one can show that all local minima have small loss.

Chen, Li, Bruna, 2017

Yao, V., Bandeira, 2019

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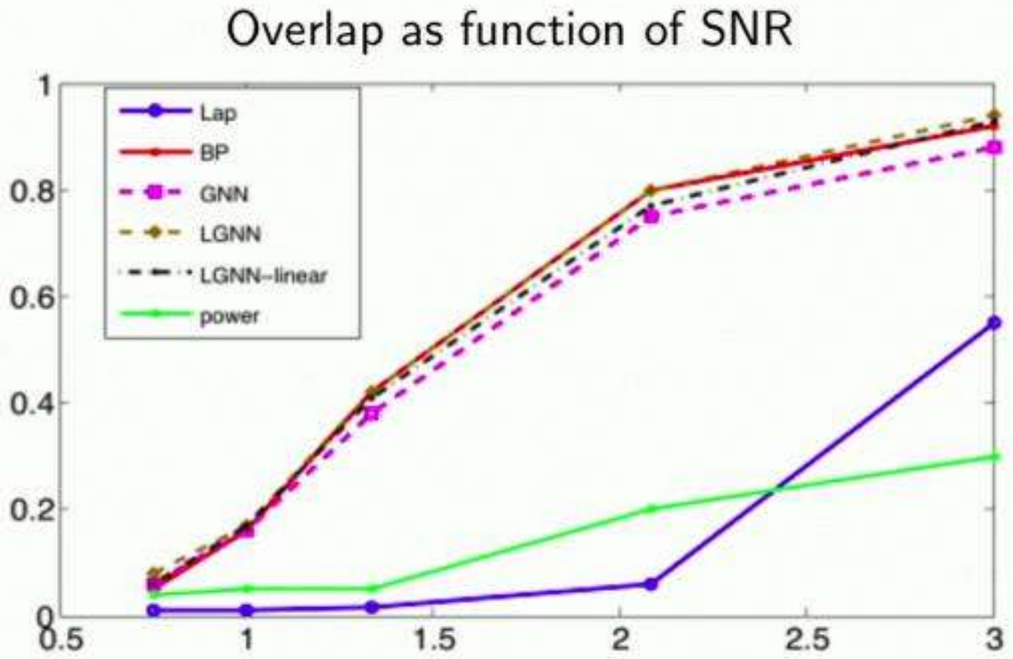

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Extension to unsupervised setting: Max-cut on random regular graphs.

Chen, Li, Bruna, 2017

Yao, V., Bandeira, 2019

Motivating example 2

Quadratic assignment problem

A, B $n \times n$ matrices. Π : set of $n \times n$ permutation matrices.

$$\text{Quadratic assignment} : \max_{X \in \Pi} \text{Trace}(AXBX^\top)$$

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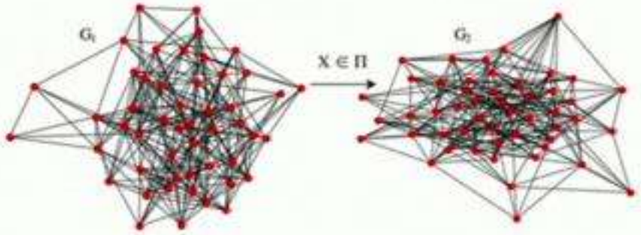

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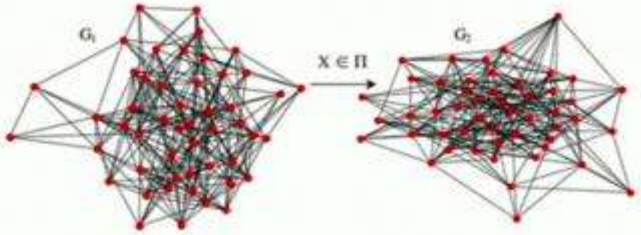

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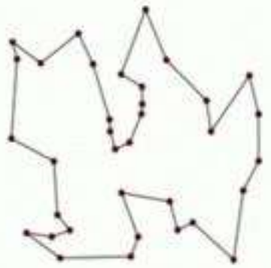

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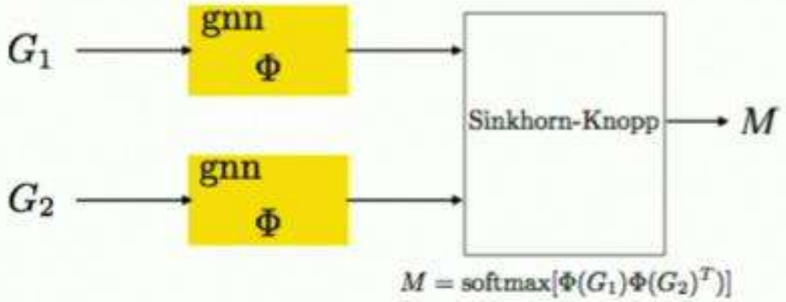
- Graph matching: $\min_{X \in \Pi} \|AX - XB\|_F^2$.
- Graph isomorphism.
- Traveling salesman problem.
- Gromov-Hausdorff distance of finite metric spaces.

It is NP-hard, even to approximate it.

GNN approach to quadratic assignment

Siamese neural network:

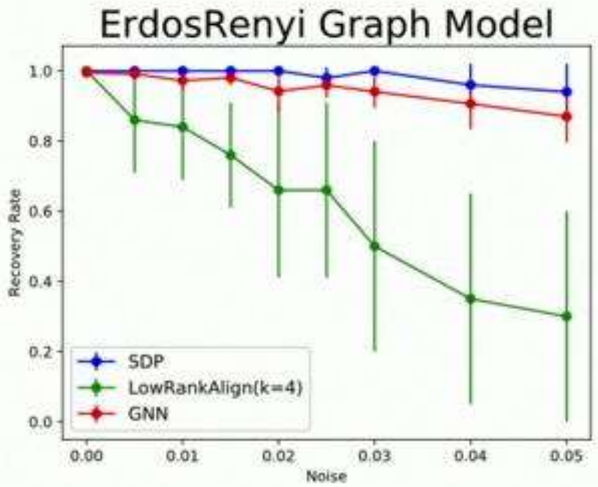


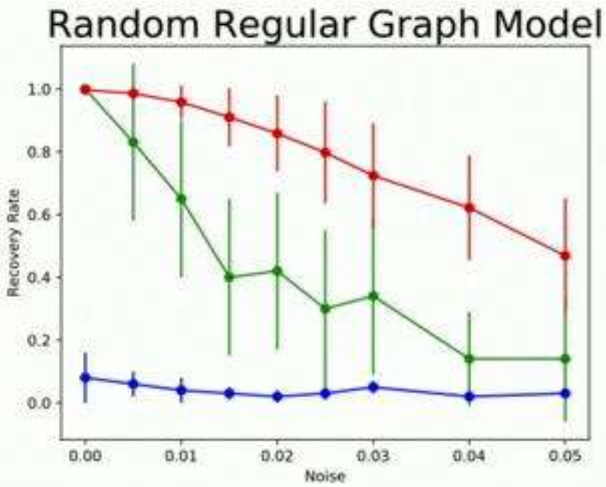
$G_2 = \pi \star G_1 \oplus N \qquad N \sim$ i.i.d. bit flip

$G_1 \sim$ Erdos-Renyi

$G_1 \sim$ Random regular

Numerical experiments





Nowak, V., Bandeira, Bruna, 2017

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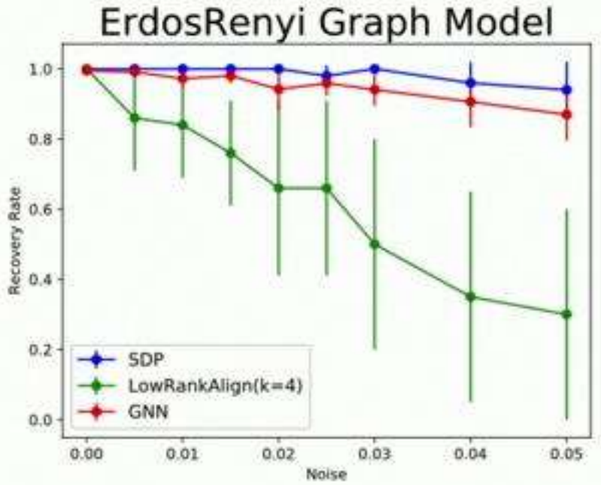

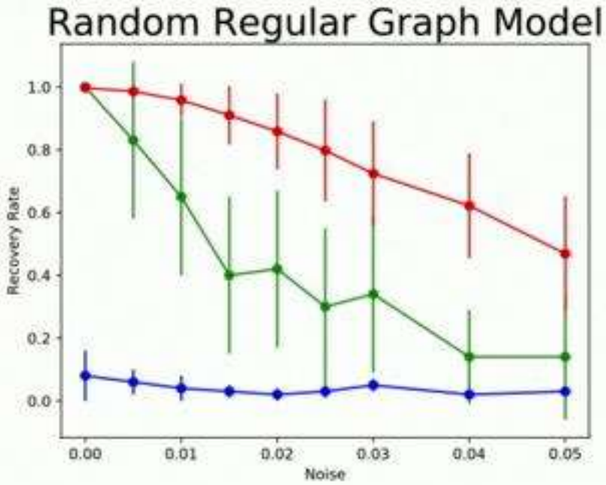

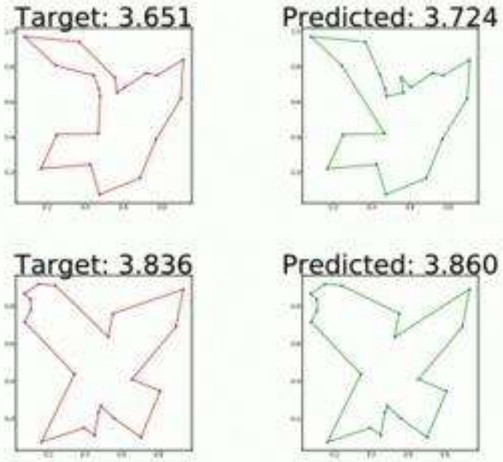

Nowak, V., Bandeira, Bruna, 2017

Other GNN formulation

Message passing neural network

$$a_v^{(k)} = \text{AGGREGATE}^{(k)}\left(\{h_u^{(k-1)} : u \in \mathcal{N}(u)\}\right)$$

$$h_v^{(k)} = \text{COMBINE}^{(k)}\left(h_v^{(k-1)}, a_v^{(k)}\right)$$

Hamilton, Ying, Leskovec, 2017

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- There exist many formulations of GNN
- All satisfy one essential property:
  - invariance or equivariance with respect to permutations
  - node labels are not intrinsic

Hamilton, Ying, Leskovec, 2017

How powerful are graph neural networks?

Q: How good are they at distinguishing non-isomorphic graphs?

Xu, Hu, Leskovec, Jekelga 2019

How powerful are graph neural networks?

Q: How good are they at distinguishing non-isomorphic graphs?

A: MPNN can be as powerful as the Weisfeler-Lehman test (1968).
W-L test is as powerful as the LP relaxation (Ullman et al 1994).

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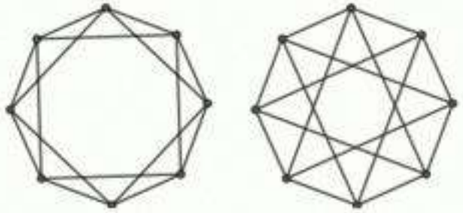
A: MPNN can be as powerful as the Weisfeler-Lehman test (1968).
W-L test is as powerful as the LP relaxation (Ullman et al 1994).

In particular MPNN cannot distinguish between non-isomorphic regular graphs with the same degree.



Xu, Hu, Leskovec, Jekelga 2019

Invariant functions on graphs

- Linear case:
  - If $L : \mathbb{R}^{n^k} \to \mathbb{R}$ invariant, then $vec(L) = \pi^{\otimes k} vec(L)$.
  - If $L : \mathbb{R}^{n^k} \to \mathbb{R}^{n^k}$ equivariant, then $vec(L) = \pi^{\otimes 2k} vec(L)$

  - The space of invariant [equivariant] linear functions on k-tensors has dimension $b(k)$ $[b(2k)]$.
    ($b(k)$ denotes Bell Number: number of partitions of a size k set).

Maron, Ben-Hamu, Shamir, Lipman, 2019

Maron, Fetaya, Segol, Lipman, 2019

Keriven, Peyré, 2019

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- Universal approximation:
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  - Extension to equivariant functions.

Maron, Ben-Hamu, Shamir, Lipman, 2019

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    Arbitrary high order tensors are needed.

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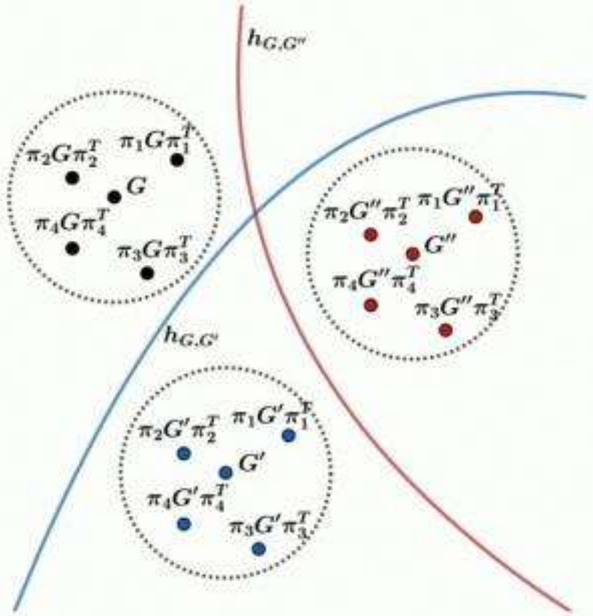
Graph isomorphism equivalence to universal approximation

GIso-discriminating class of functions

A class $\mathcal{C}$ of permutation-invariant functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$ so that for all pairs $G_1 \not\simeq G_2 \in \mathcal{X}^{n\times n}$, there exists $h \in \mathcal{C}$ such that $h(G_1) \neq h(G_2)$.



Chen, V., Chen, Bruna, 2019

Graph isomorphism equivalence to universal approximation

Universally approximating

A class $\mathcal{C}$ of permutation-invariant functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$ so that for all permutation-invariant function f from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$, and for all $\epsilon > 0$, there exists $h_{f,\epsilon} \in \mathcal{C}$ such that
$\|f - h_{f,\epsilon}\|_\infty := \sup_{G\in\mathcal{X}^{n\times n}} |f(G) - h_{f,\epsilon}(G)| < \epsilon$

Remark

Universally approximating classes of functions are also GIso-discriminating.

Chen, V., Chen, Bruna, 2019

Graph isomorphism equivalence to universal approximation

$\mathcal{C}^{+L}$

If $\mathcal{C}$ is a collection of functions from $\mathcal{X}^{n\times n}$ to $\mathbb{R}$, consider the set of functions from graphs G to $\mathcal{NN}([h_1(G), ..., h_d(G)])$ for some finite d and $h_1, ..., h_d \in \mathcal{C}$, where $\mathcal{NN}$ is a feed-forward neural network with ReLU and L layers.

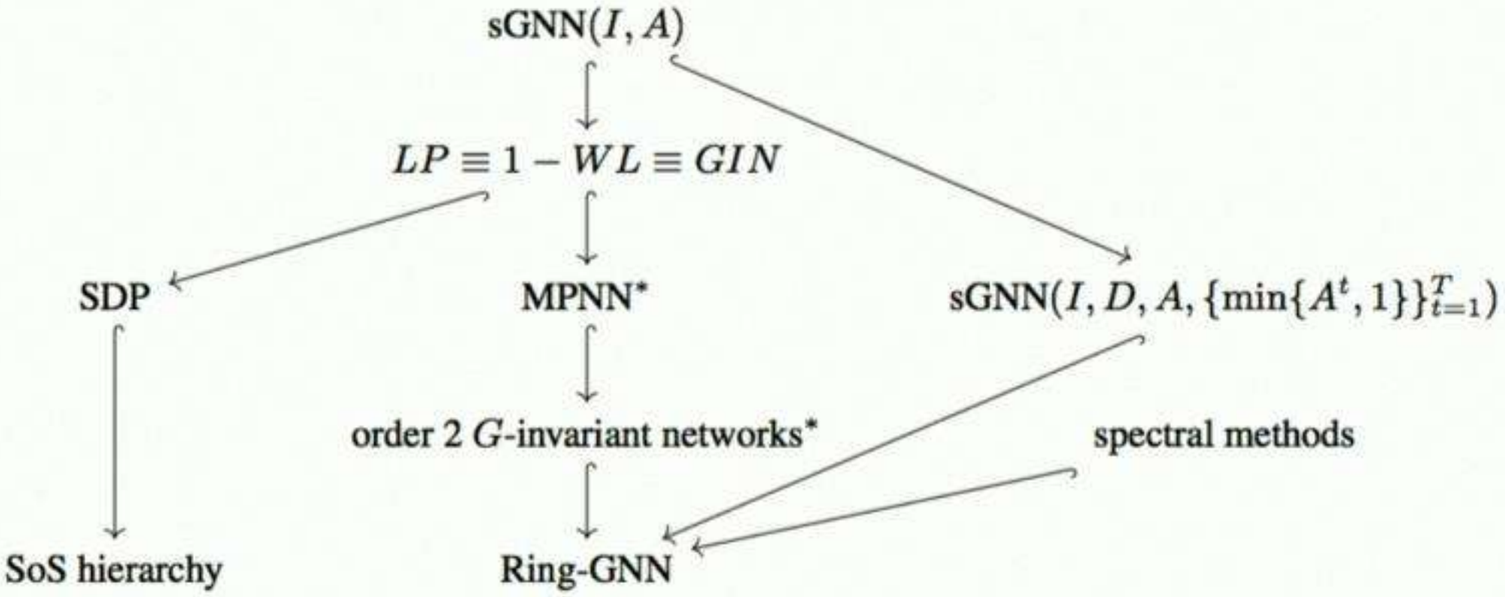
Theorem

If $\mathcal{C}$ is GIso-discriminating $\mathcal{C}^{+2}$ is universally approximating.

Chen, V., Chen, Bruna, 2019

Comparison of classes of functions through GIso

$\mathcal{C} \subseteq \mathcal{C}'$ if for all pairs of non-isomorphic graphs G_1, G_2, if there exists $h \in \mathcal{C}$ so that $h(G_1) \neq h(G_2)$ then there exists $h' \in \mathcal{C}'$ so that $h'(G_1) \neq h'(G_2)$.



Ring GNN

Input: Graph with n nodes and d features: $A \in \mathbb{R}^{n \times n \times d}$.

Equivariant linear layer from $\mathbb{R}^{n \times n \times d}$ to $\mathbb{R}^{n \times n \times d'}$. For $\theta \in \mathbb{R}^{d \times d' \times 17}$:
$L_\theta(A)_{\cdot,\cdot,k'} = \sum_{k=1}^{d} \sum_{i=1}^{15} \theta_{k,k',i} L_i(A_{\cdot,\cdot,i}) + \sum_{i=16}^{17} \theta_{k,k',i} \overline{L}_i$.
Set $A^{(0)} = A$.

$$\begin{aligned} B_1^{(t)} &= \rho(L_{\alpha^{(t)}}(A^{(t)})) \\ B_2^{(t)} &= \rho(L_{\beta^{(t)}}(A^{(t)}) \cdot L_{\gamma^{(t)}}(A^{(t)})) \\ A^{(t+1)} &= k_1^{(t)} B_1^{(t)} + k_2^{(t)} B_2^{(t)} \end{aligned}$$

where $k_1^{(t)}, k_2^{(t)} \in \mathbb{R}$, $\alpha^{(t)}, \beta^{(t)}, \gamma^{(t)} \in \mathbb{R}^{d^{(t)} \times d'^{(t)} \times 17}$ are learnable parameters.

Scalar output: $\theta_S \sum_{i,j} A_{ij}^{(T)} + \theta_D \sum_{i,i} A_{ii}^{(T)} + \sum_i \theta_i \lambda_i(A^{(T)})$, where $\theta_S, \theta_D, \theta_1, \ldots, \theta_n \in \mathbb{R}$ are trainable parameters, and $\lambda_i(A^{(T)})$ is the i-th eigenvalue of $A^{(T)}$.

Extensions - Future work

- Explicit rates:
  Connect GNN depth/architecture with classes of graphs they separate.

- Optimization landscape of GNNs:
  Current analysis of optimization landscape relies in simplified models to show that all local minima are confined in low-energy configurations.

- Connection with SoS:
  For some classes of "detecting hidden structures problems" existence of degree-d SoS refutations implies success of certain (typically non-explicit) spectral methods.
  - Can we express such class of spectral methods with GNNs.
  - Can we learn them?

Hopkins, Kothari, Potechin, Raghavendra, Schramm, Steurer, 2017

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