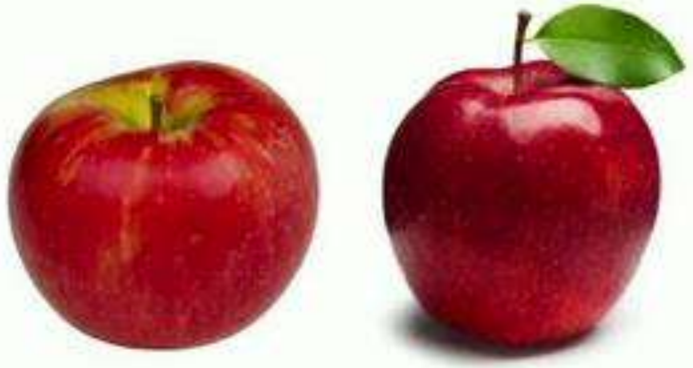
Universality and limitations of deep learning

Emmanuel Abbe (EPFL/Princeton) and Colin Sandon (MIT)

MSR, 08.19

Class 1



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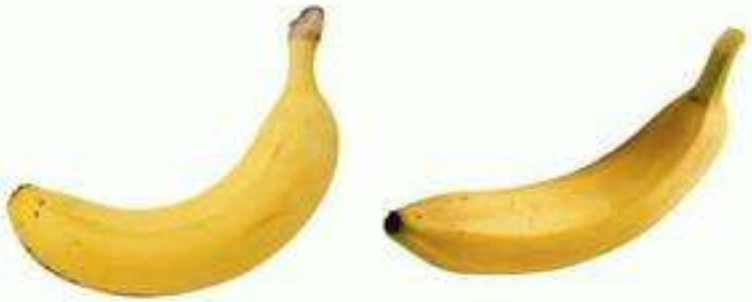

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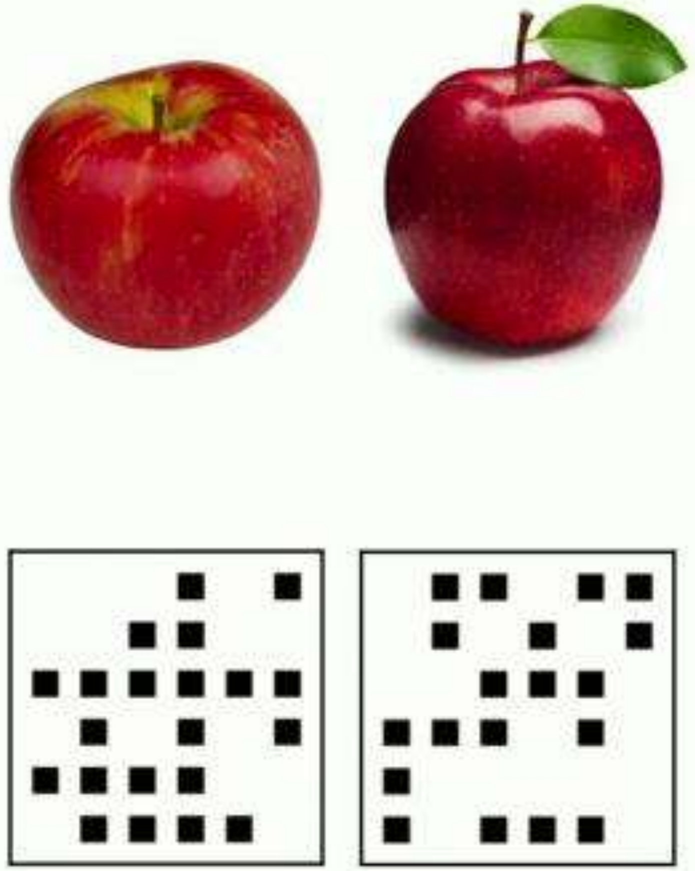

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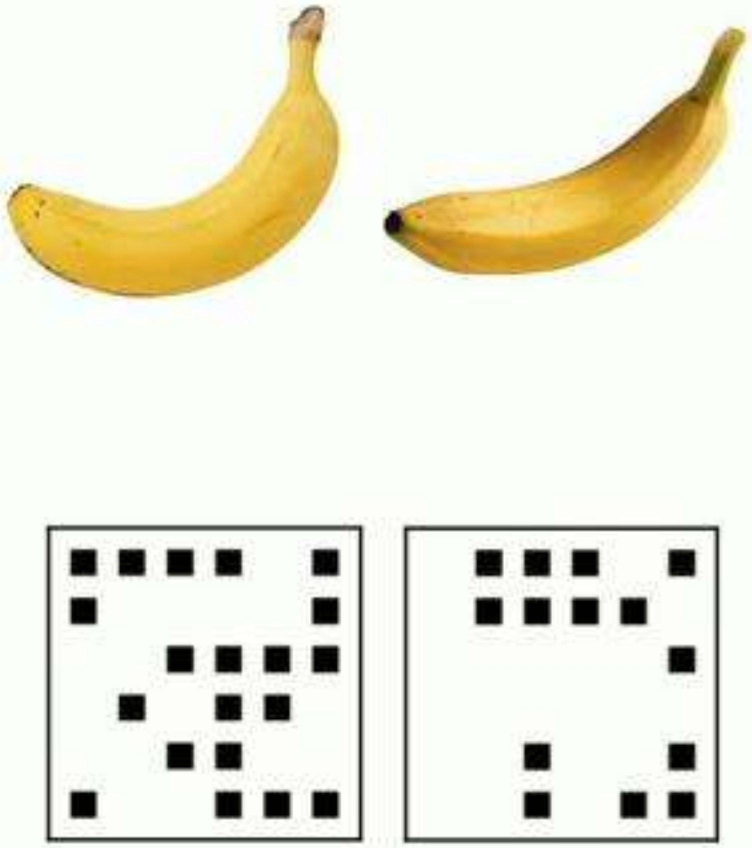

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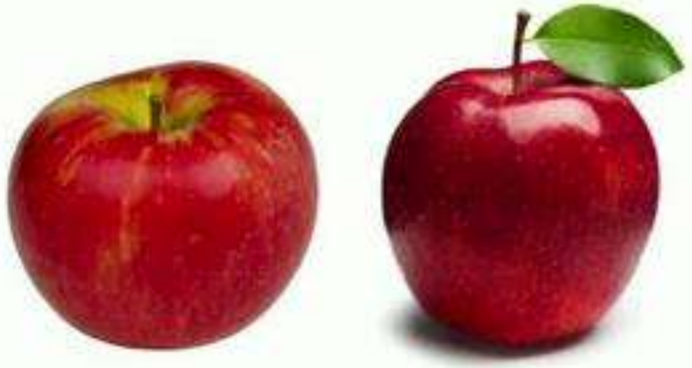

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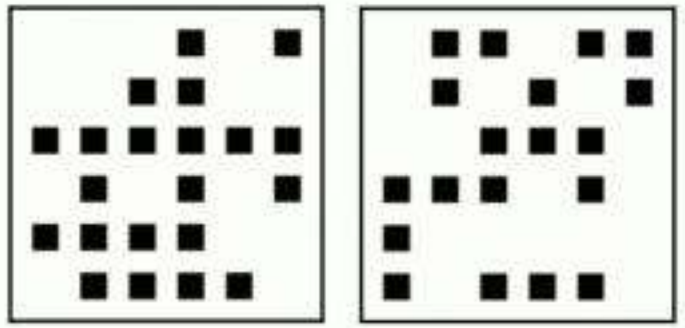

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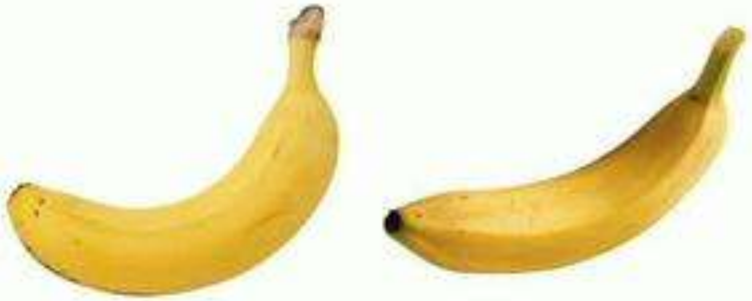

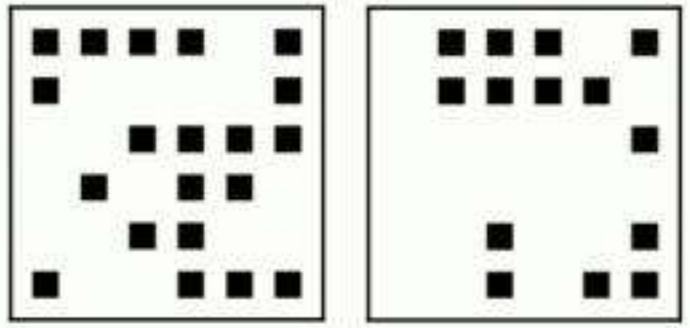

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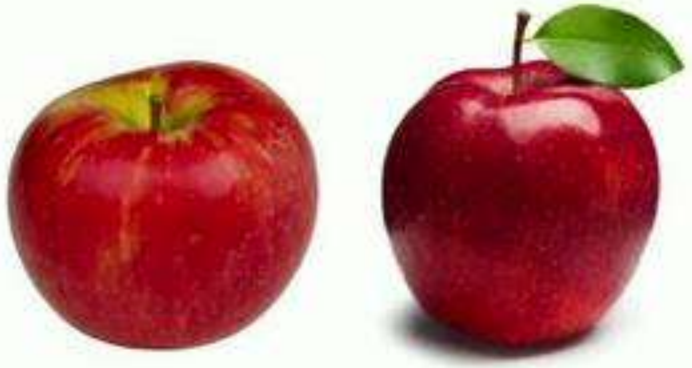

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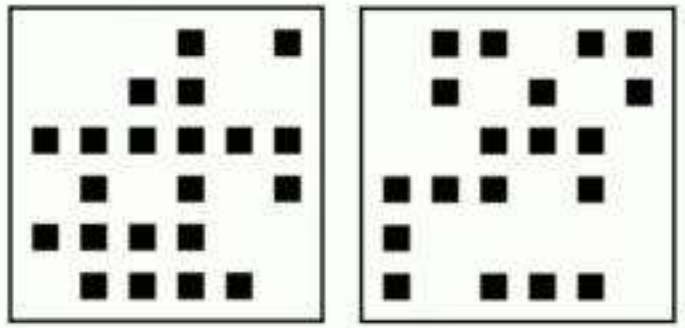

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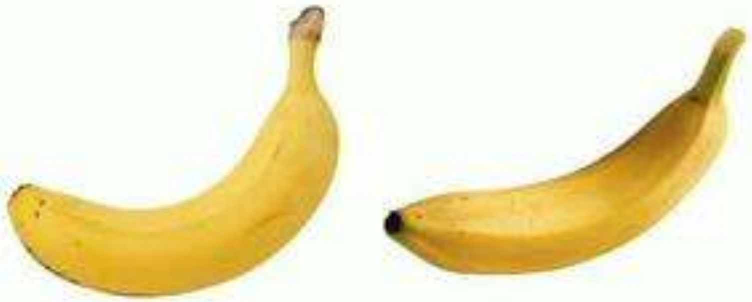

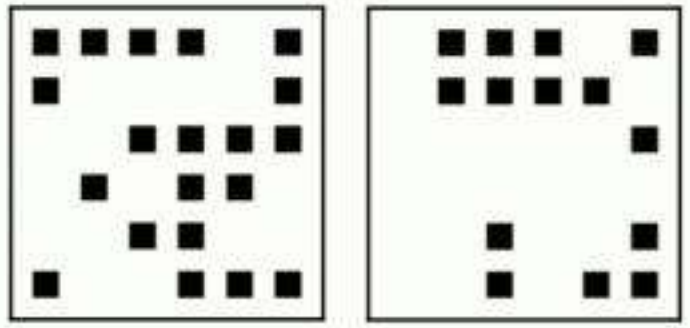

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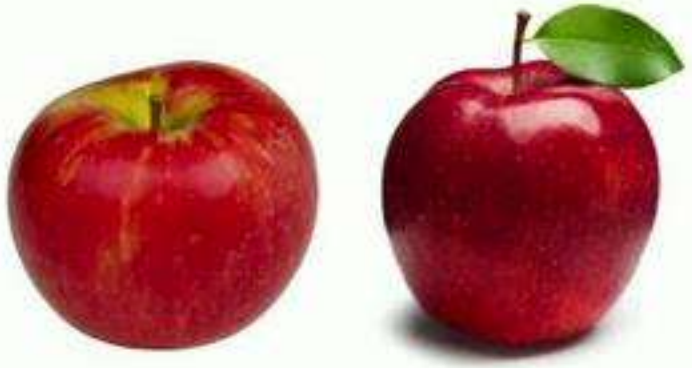

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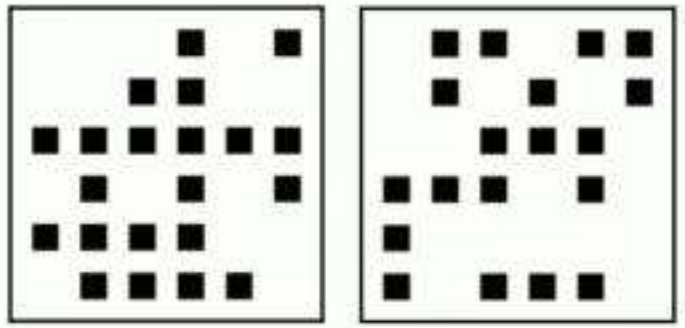

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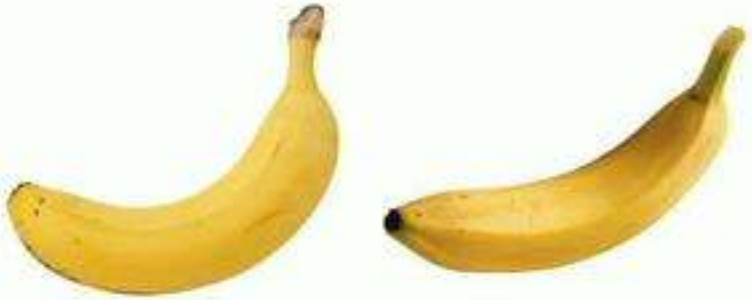

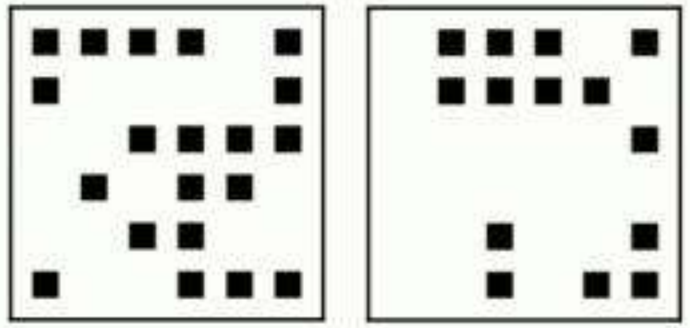

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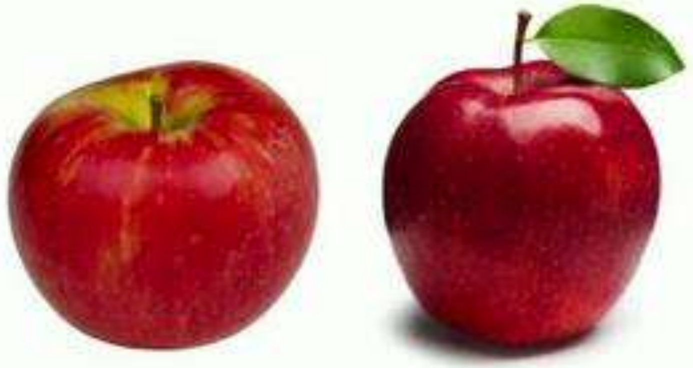

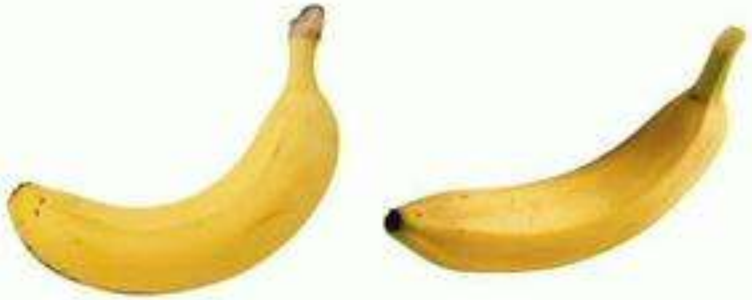

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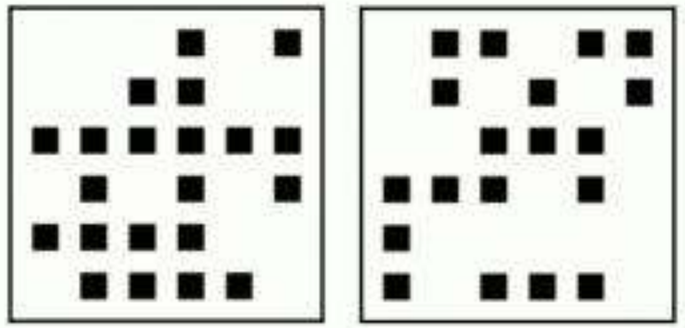

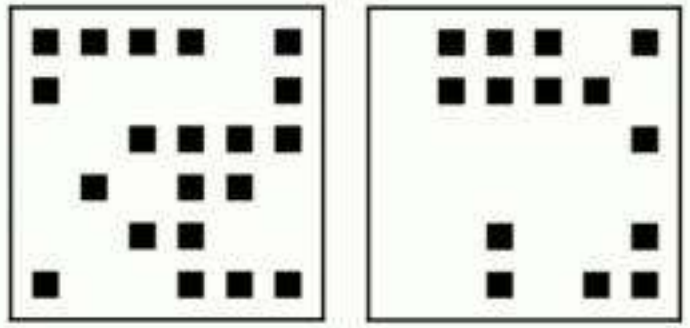

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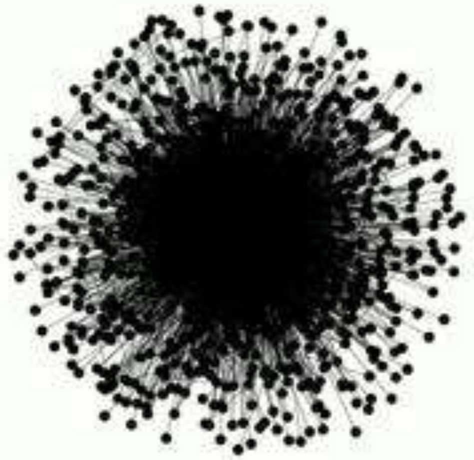

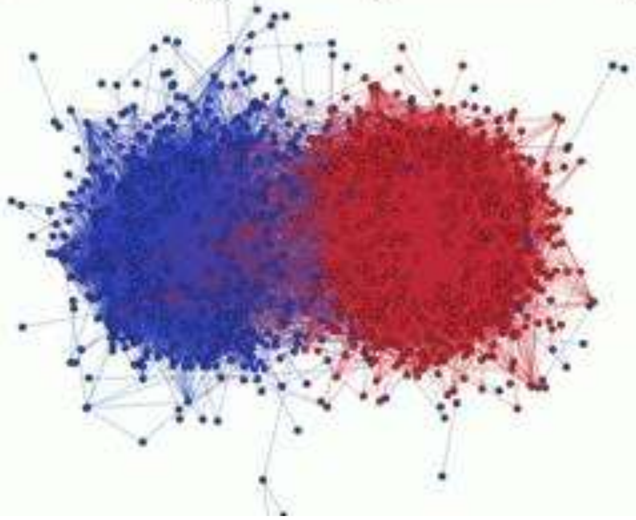

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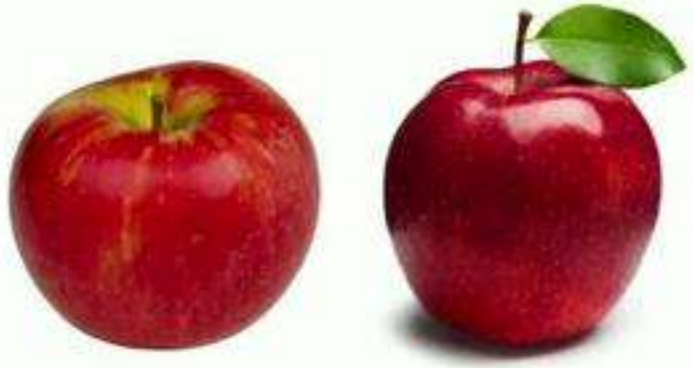

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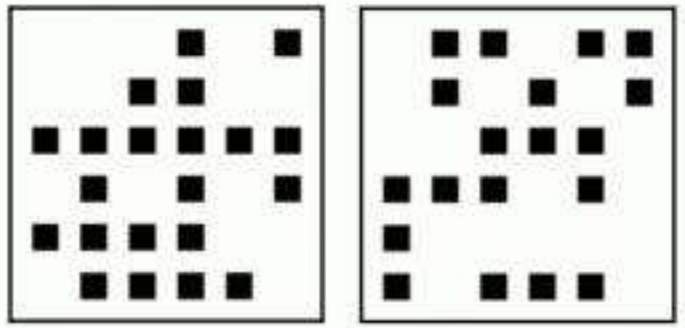

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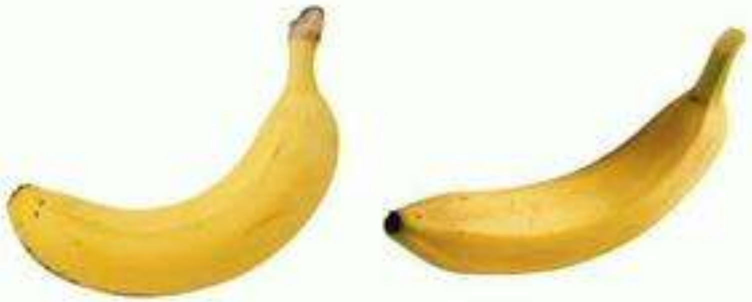

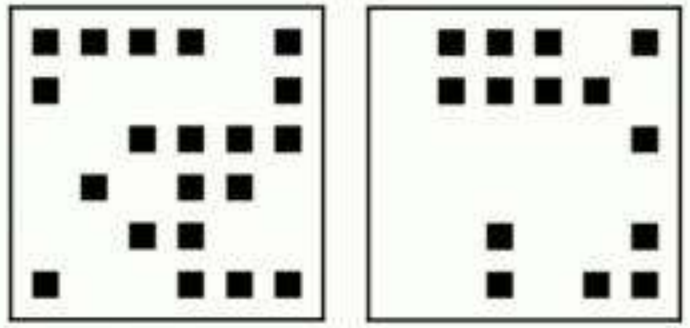

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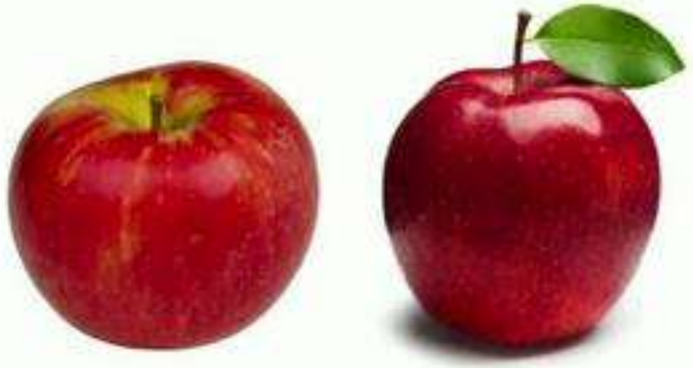

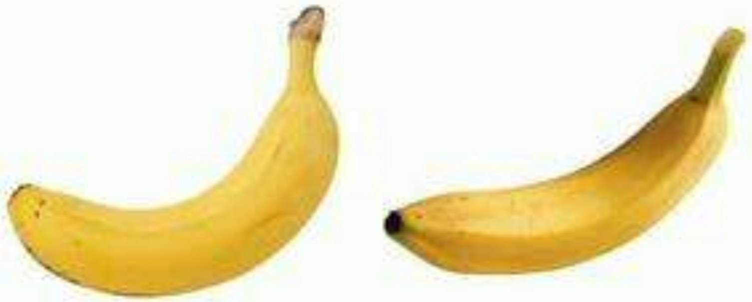

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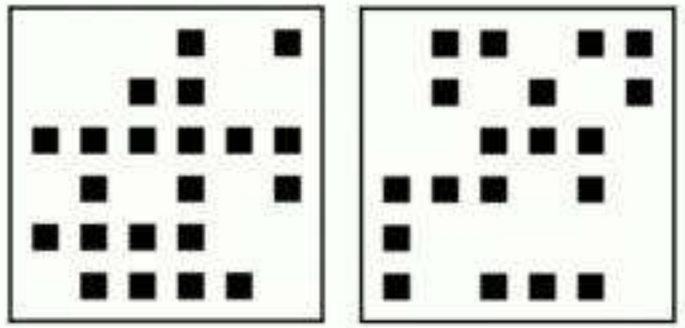

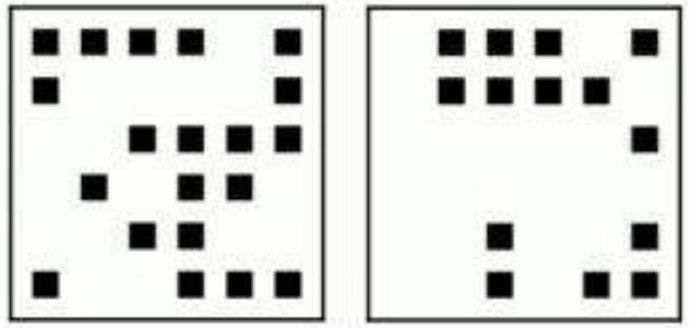

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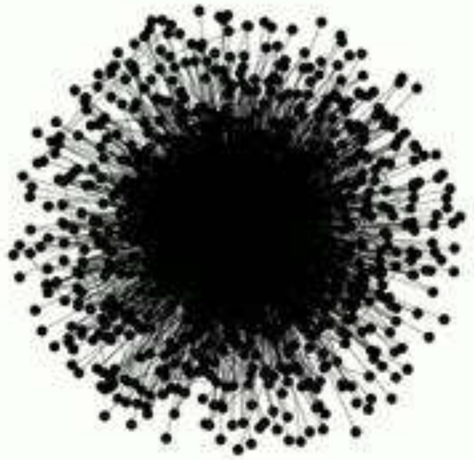
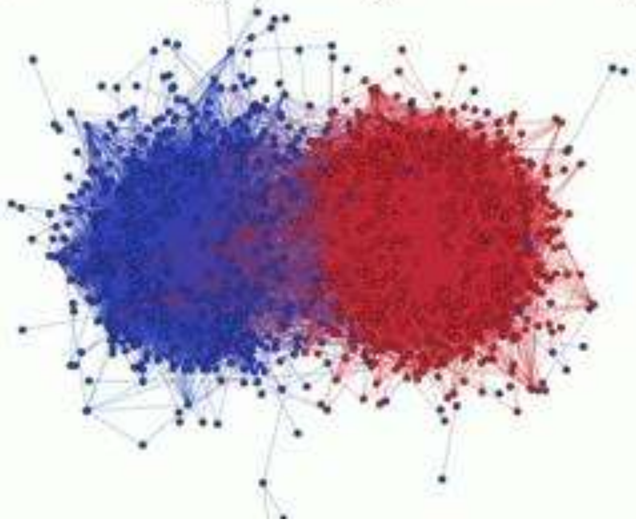
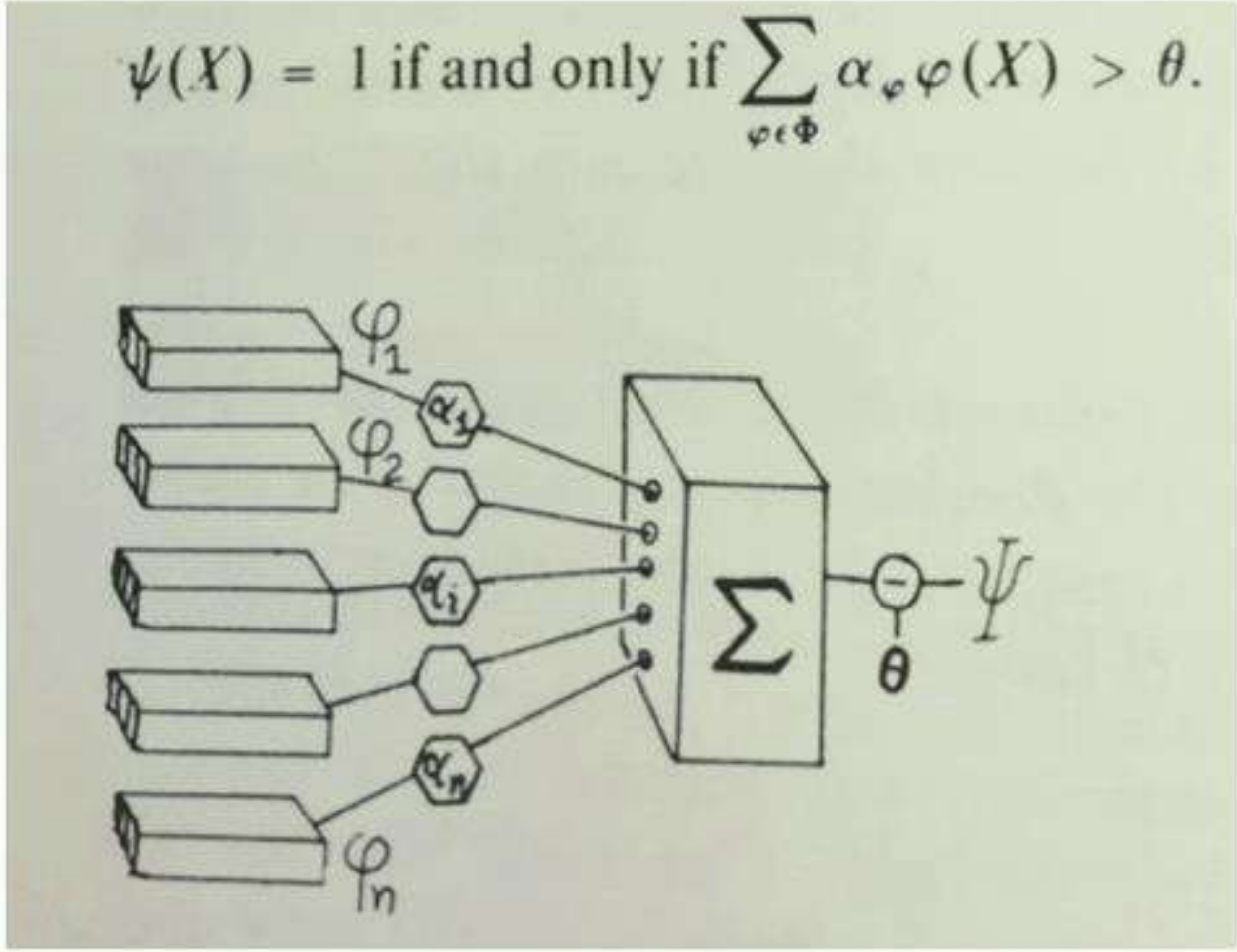
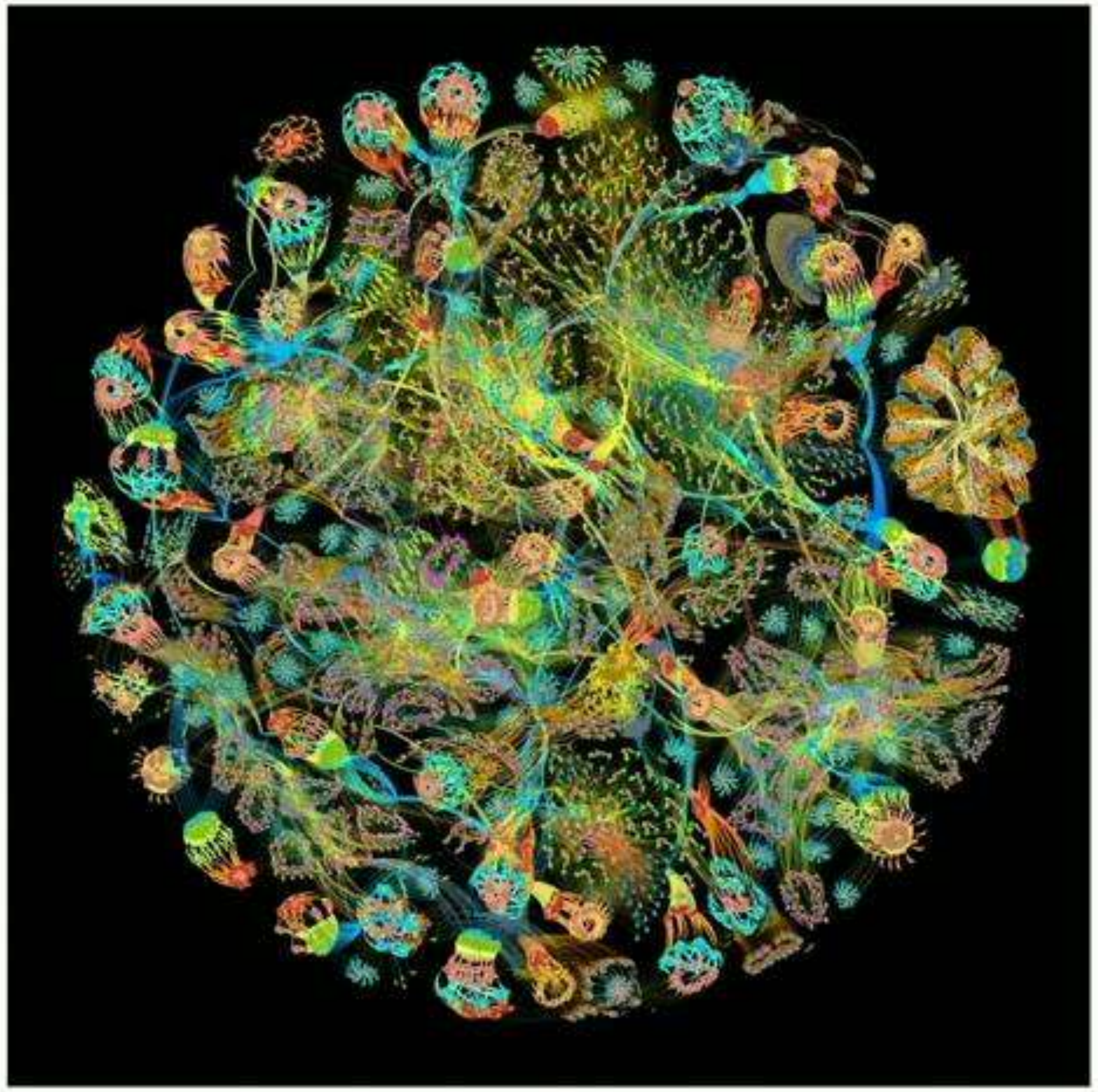




1969


$\psi(X) = 1$ if and only if $\sum_{\varphi \in \Phi} \alpha_\varphi \varphi(X) > \theta$.
φ_1
φ_2
φ_n
α_1
α_i
α_n
Σ
θ
Ψ

2019



u/mattfyles: ResNet-50 neural network from Microsoft Research.
~3 million nodes and ~10 million edges (layout in Gephi)

https://i.redd.it/55tffb8uh6uz.jpg

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What do we mean by ‘deep learning’
and ‘can learn’?

Formalizing the problem

Approximation. Any function on n variables that can be implemented in poly(n)-time can be expressed by a poly(n)-size NN [Parberry 94, Sipser 06]

Estimation. Poly(n)-size NN can be learned with empirical risk minimization (ERM) with poly(n)-samples [VC 71, Anthony-Bartlett 99]

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under symmetry: failure at 2 implies failure at 1 for a typical function

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$\mathcal{X}$: the data domain ($\{+1,-1\}^n$)

$\mathcal{Y}$: the label domain ($\{+1,-1\}$)

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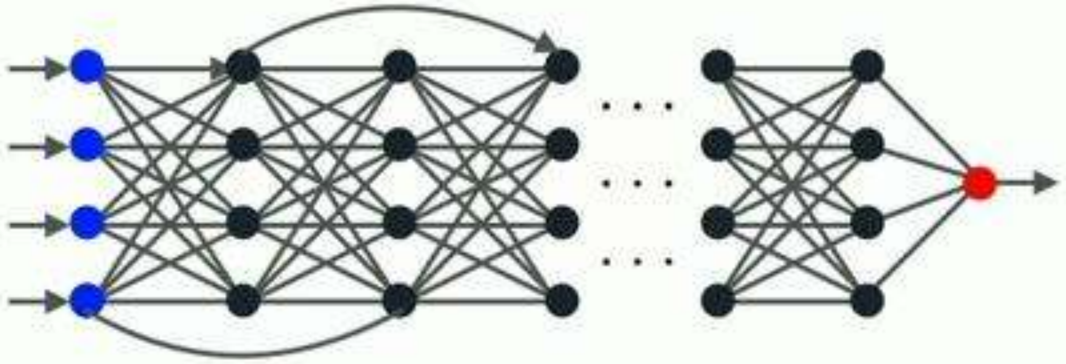

results

Results

Theorem 1. GD cannot learn efficiently function distributions having low CP

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- poly-steps
- poly-rate
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Corollary. GD can learn efficiently monomials of degree k if and only if k is finite

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population gradient

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- **poly-noise /poly-precision**

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- **poly-noise /poly-precision**

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Corollary. SGD can learn efficiently parities while Perceptron, GD or SQ cannot

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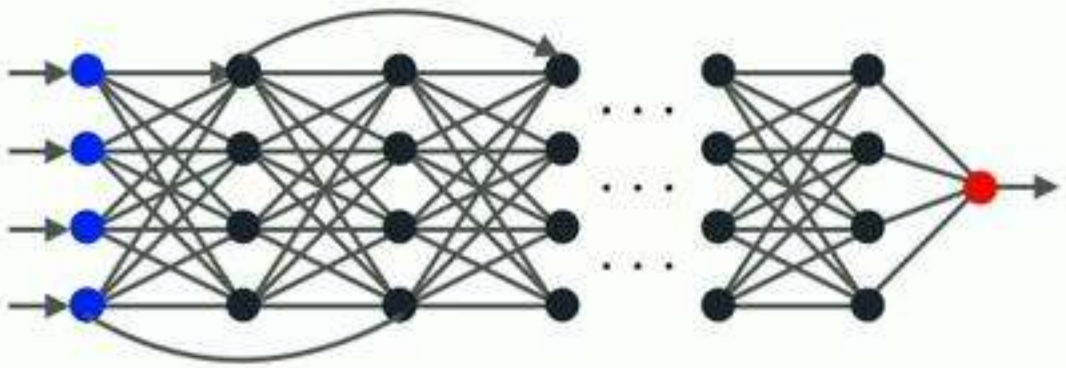

Results

Theorem 1. GD cannot learn efficiently function distributions having low CP

Results

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- poly-size NN
- any initialization
- poly-steps
- poly-rate
- poly-range
- poly-noise

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low = super-poly decay in n

related to statistical dim. [Kearns 98, Blum et al. 01]

"average-case" v.s. "worst-case" SQ (E. Boix)

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Results

Theorem 2. SGD can learn efficiently any efficiently learnable distribution

- poly-size NN
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- **poly-noise /poly-precision**

any $(P_{\mathcal{X}}, P_{\mathcal{F}})$ that can be learned by some algorithm in poly-time with poly-samples

Corollary. SGD can learn efficiently parities while Perceptron, GD or SQ cannot

proof techniques

CP: information-theoretic argument

$$W_H{}^{(t)} = W_H{}^{(t-1)} - \gamma \mathbb{E}_{(X,Y)\sim D_H} \nabla L(W_H{}^{(t-1)}(X), Y) + Z_\sigma^{(t)} \qquad H \in \{F, \star\}$$

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$$\le (\mathbb{E}_{D_\star} \nabla_e^2)(\mathbb{E}_{F,F'} \mathbb{E}_{D_\star} (1 - D_F / D_\star)^{\otimes 2} (1 - D_{F'} / D_\star)^{\otimes 2})^{1/2}$$

(CS+replica)

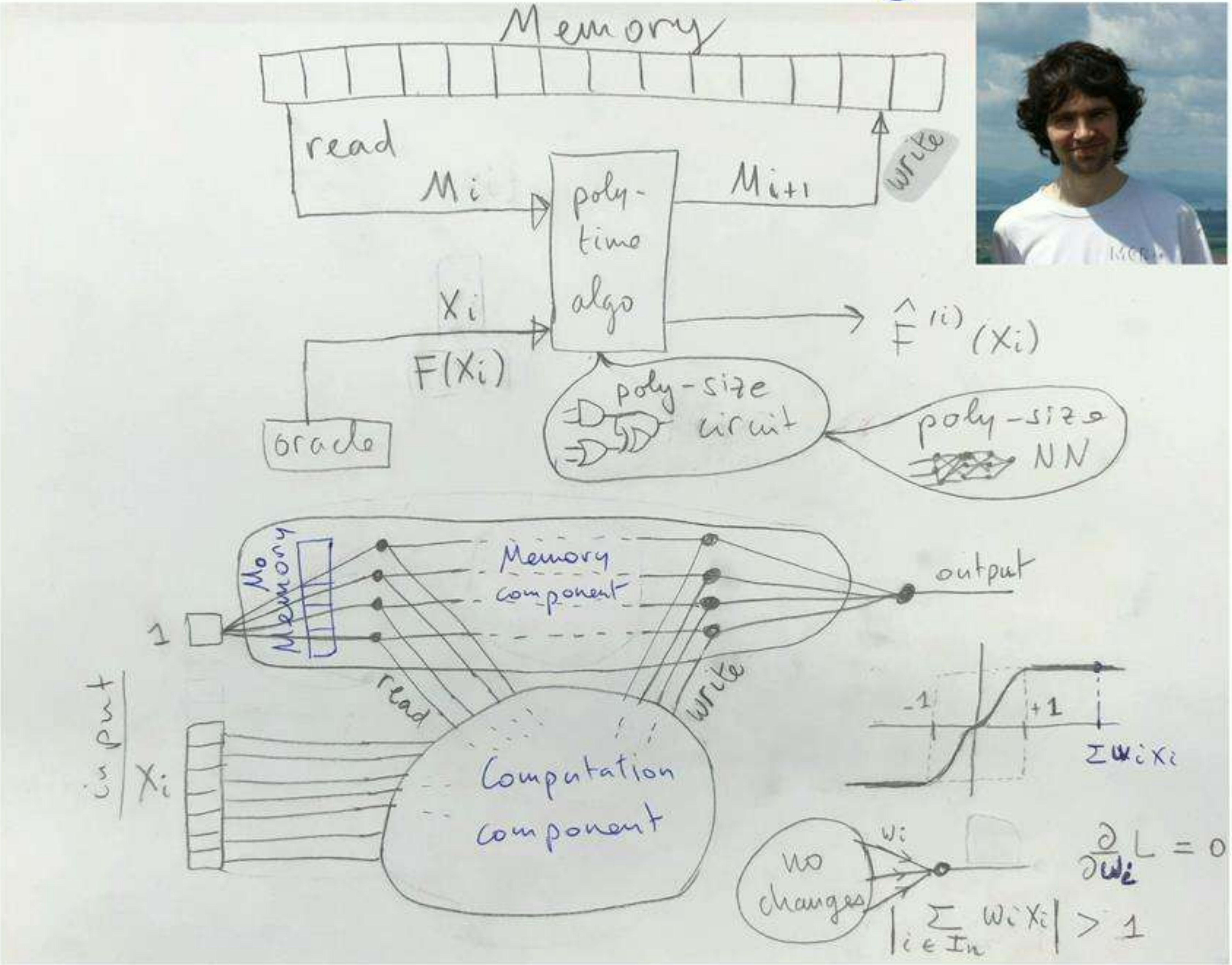
Junk-flow and cross-predictability

Theorem. $\mathbb{P}\{{W_F}^{(T)}(X) = F(X)\} \leq 1/2 + \frac{1}{\sigma} \cdot \mathrm{JF} \cdot \mathrm{CP}^{1/4}$

$$\mathrm{JF} := \sum_{t=1}^{T} \gamma_t \|\mathbb{E}_{D_\star} \nabla^{(t)}\|_2$$

$$\mathrm{CP} := \mathbb{E}_{F,F'} (\mathbb{E}_X F(X) F(X'))^2$$

The universal emulation argument



thank you

Towards demystifying Generalization and Early Stopping in Neural Networks

Mahdi Soltanolkotabi
Department of Electrical and Computer Engineering
USC University of Southern California

August 26, 2019
AI Institute “Geometry of Deep Learning”
Microsoft Research, Redmond, WA

Collaborators:

Samet Oymak, Zalan Fabian, Mingchen Li

Motivation: overparameterization without overfitting

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Mystery

$$\# \text{ of parameters} \quad >> \quad \# \text{ training data}$$

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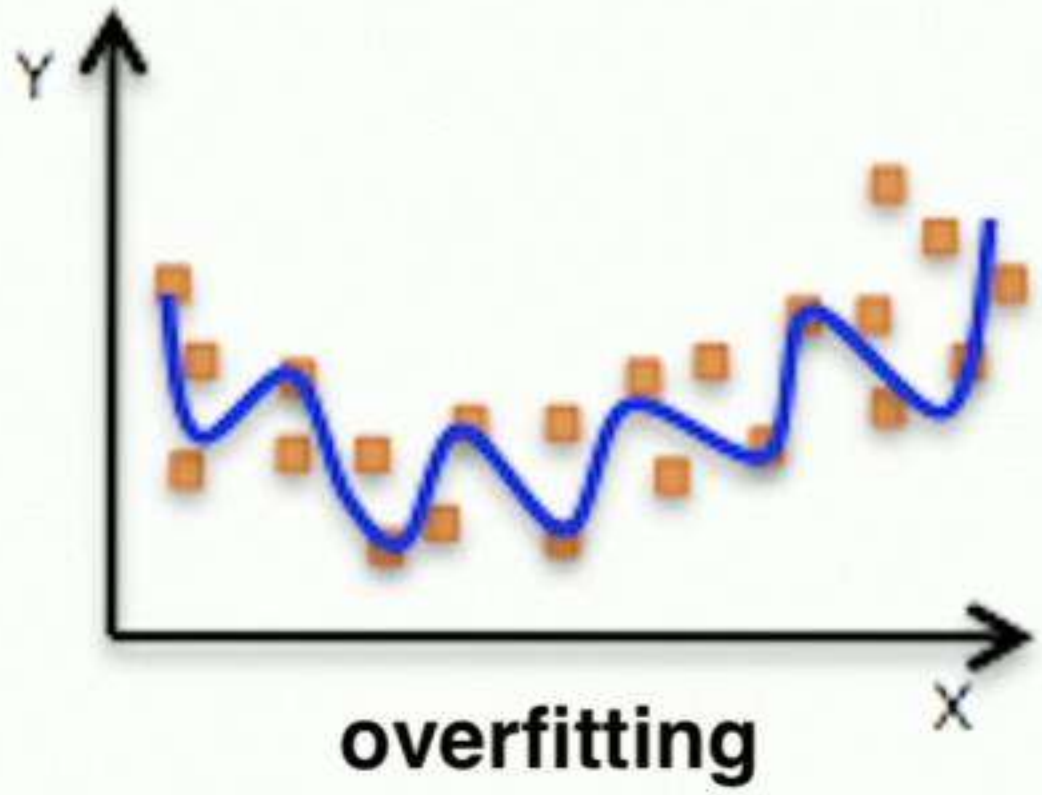

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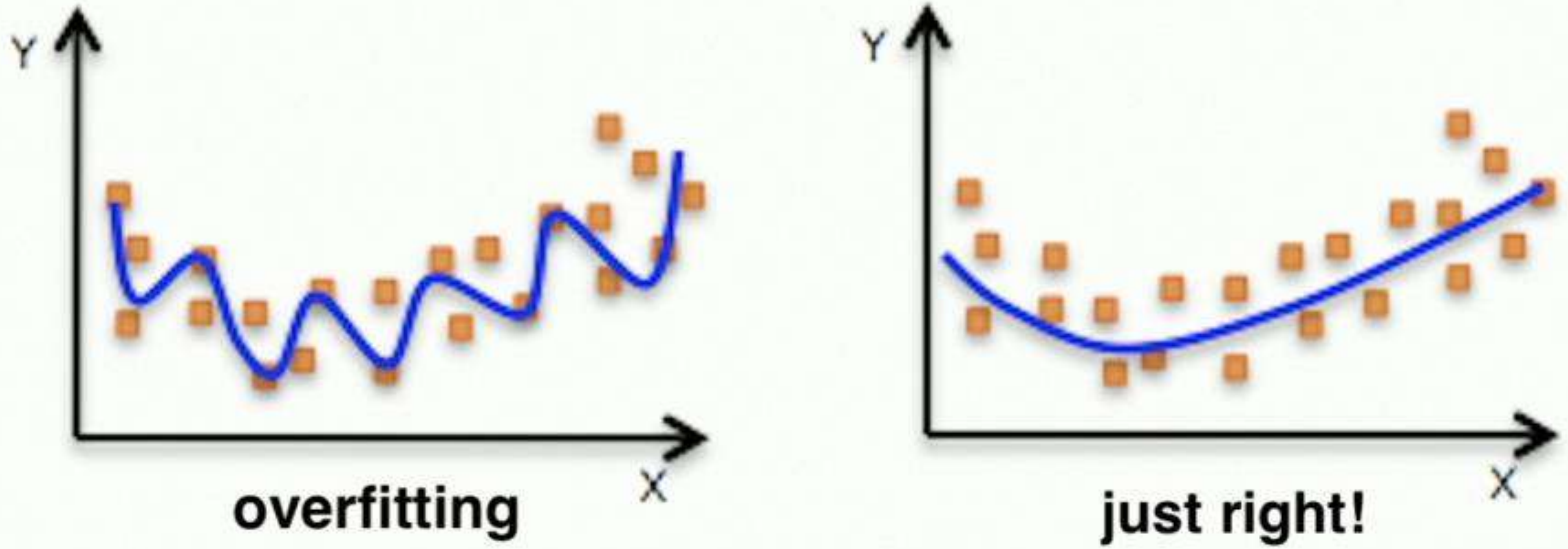

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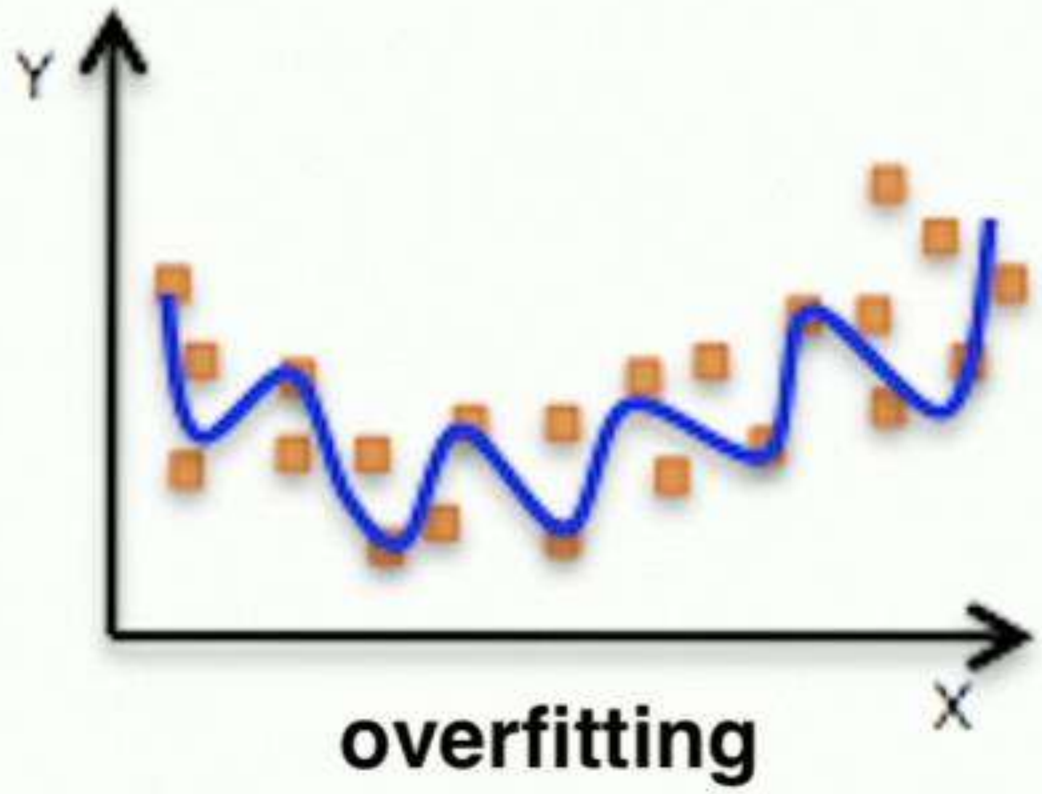

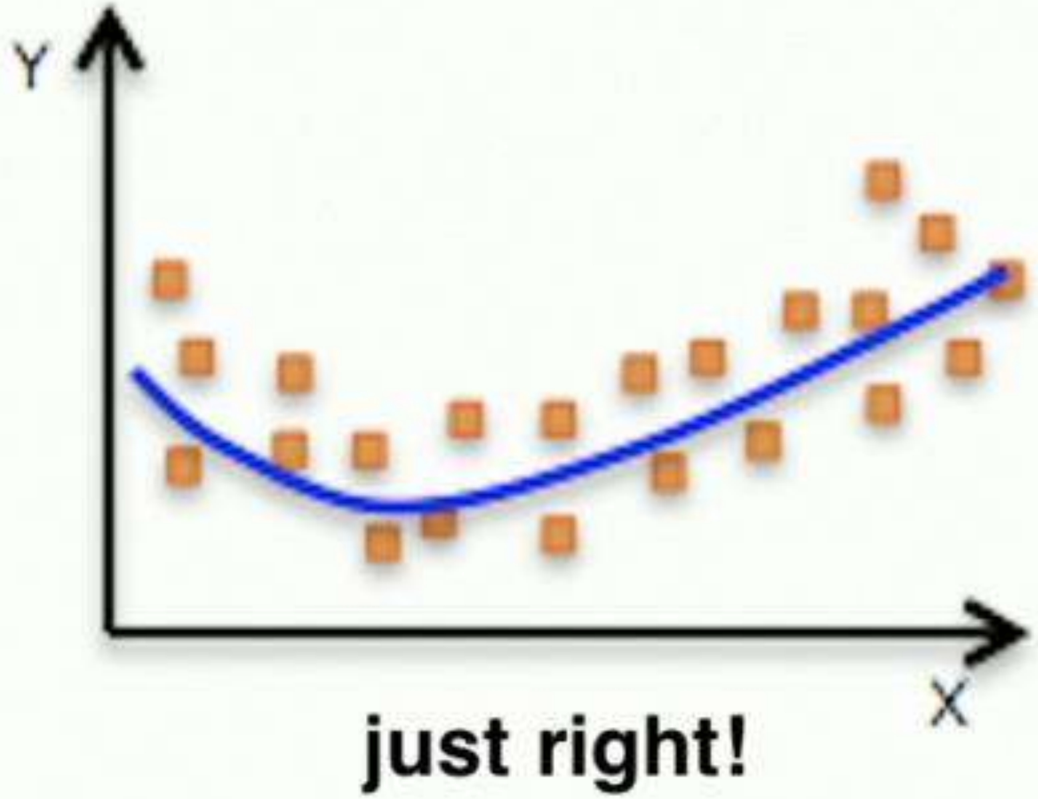

Challenges:

- *Optimization: Why can neural nets fit to the training data?*
- *Generalization: Why can neural nets predict?*

Experiment I: Overfitting to corruption

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Add corruption

- Corrupt a fraction of training labels by replacing with another random label
- No corruption on test labels

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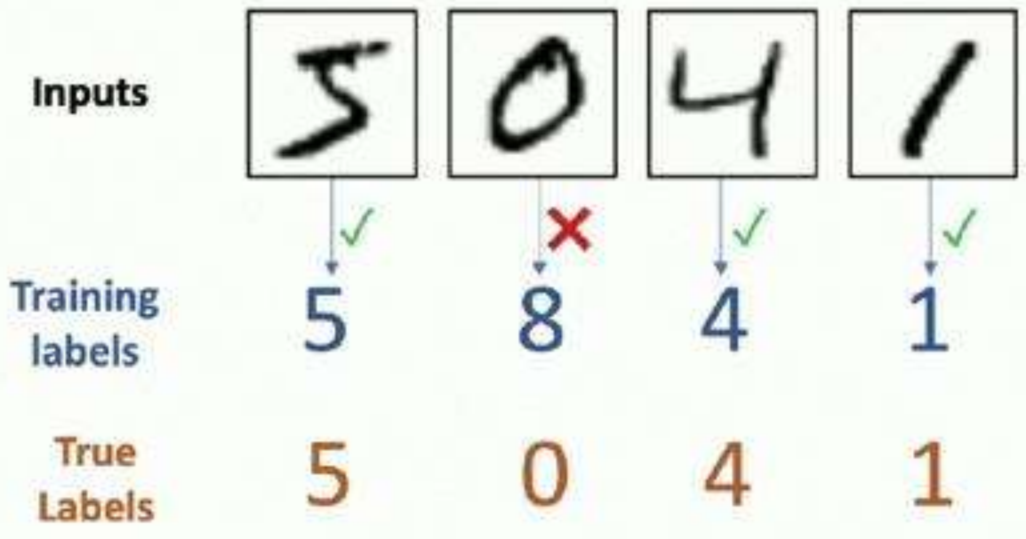

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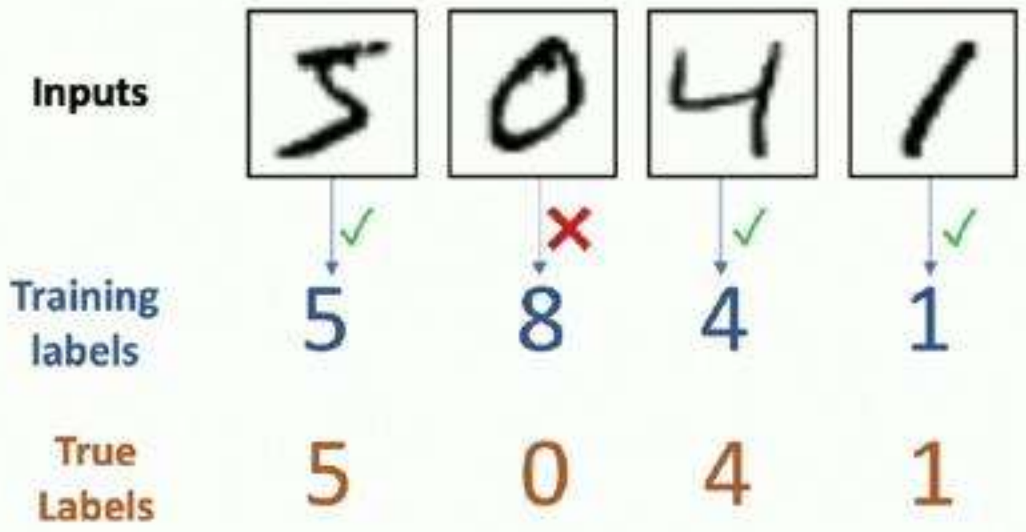

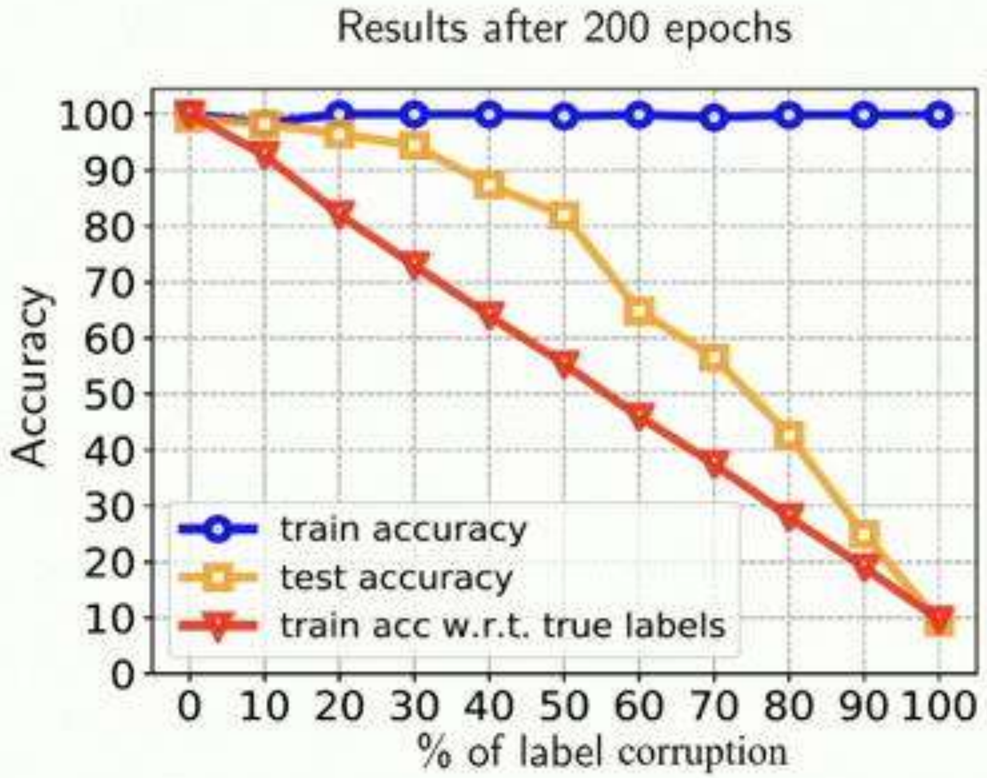

Experiment II-Early stopping and robustness

Repeat the same experiment but stop early

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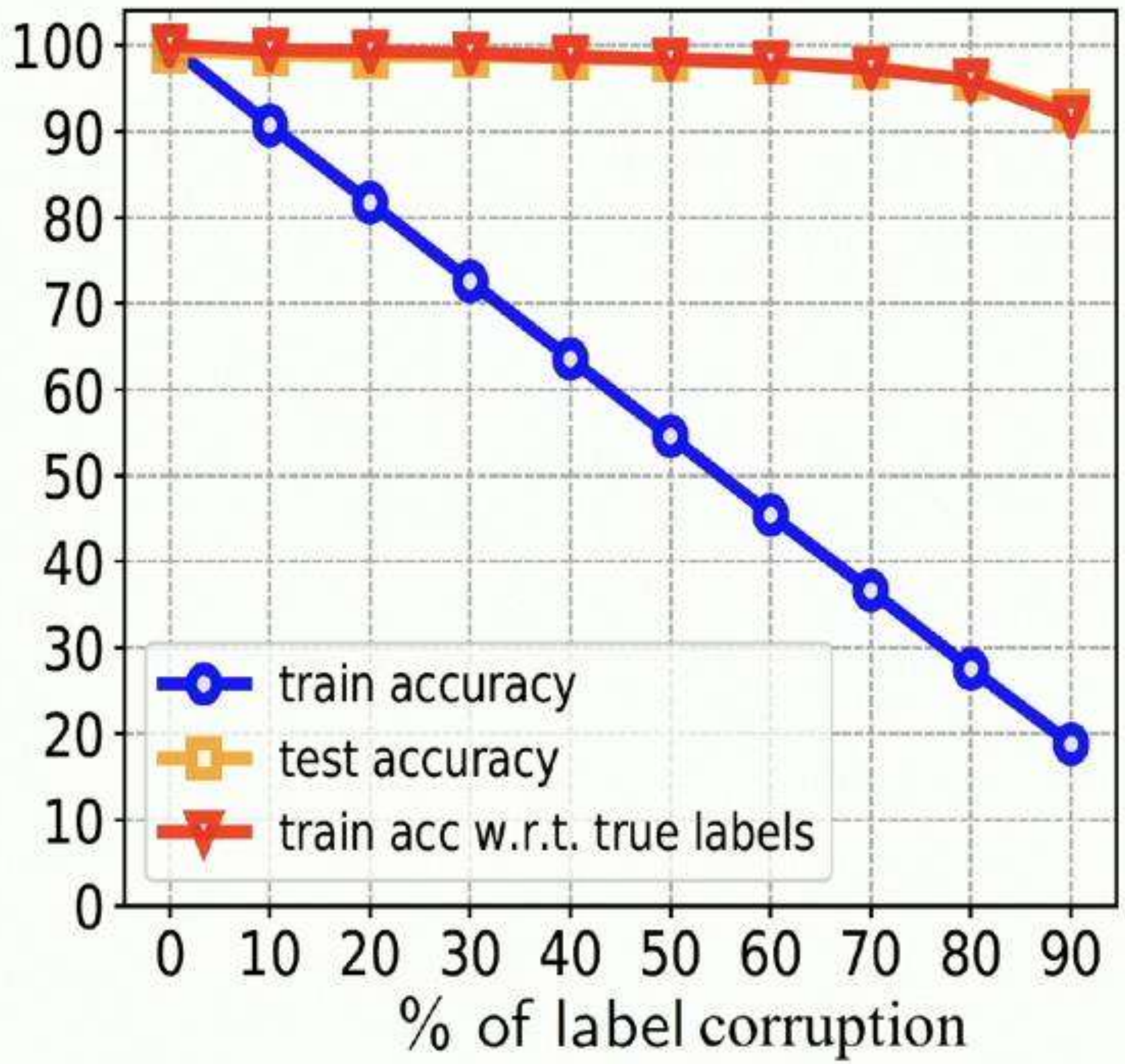

Focus: optimization/generalization dynamics

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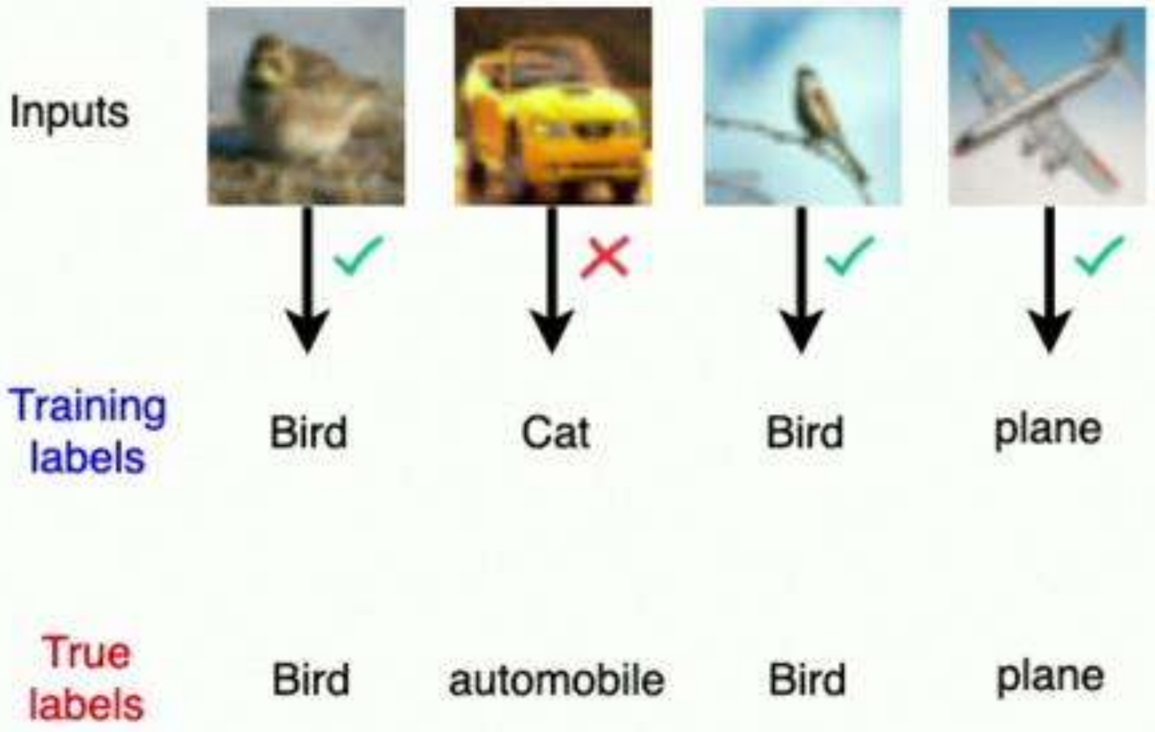
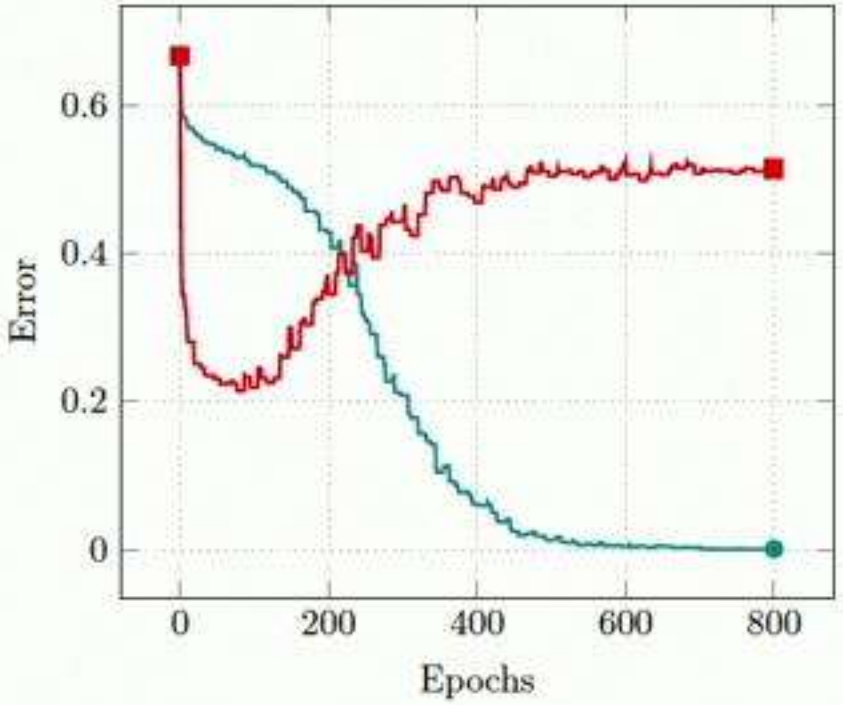
Add corruption

- Corrupt 50% of training labels by replacing with another random label
- No corruption on test labels





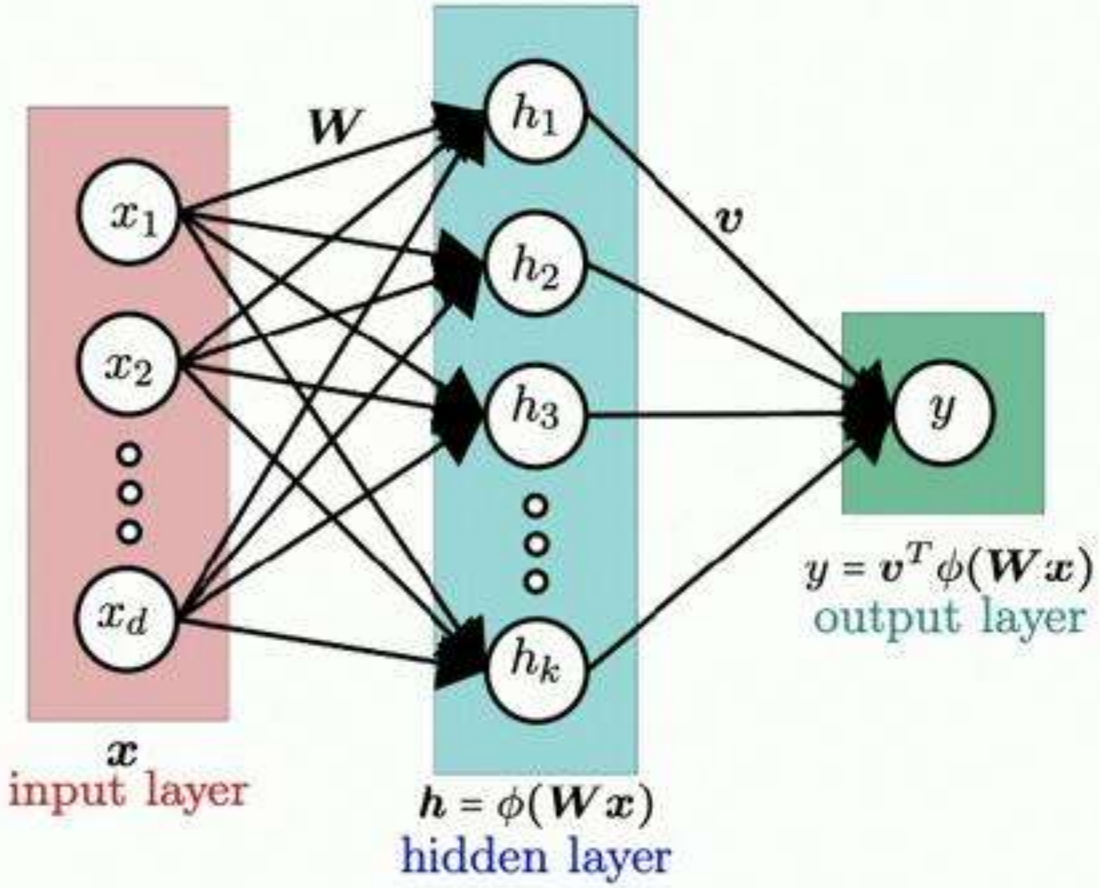
train error (green)
test error (red)

Theory for overparameterization without overfitting

- *Optimization*
- *Generalization*
- *Early stopping*

Optimization

One-hidden layer



$$\boldsymbol{y}_i = \boldsymbol{v}^T\phi(\boldsymbol{W}\boldsymbol{x}_i)$$

Theory for smooth activations

- Data set $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n \in \mathbb{R}^d \times \mathbb{R}$
- Loss

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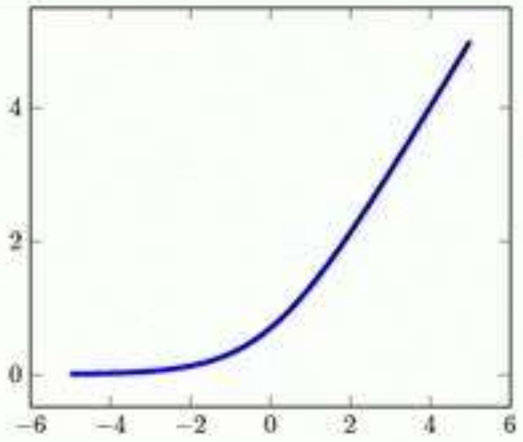

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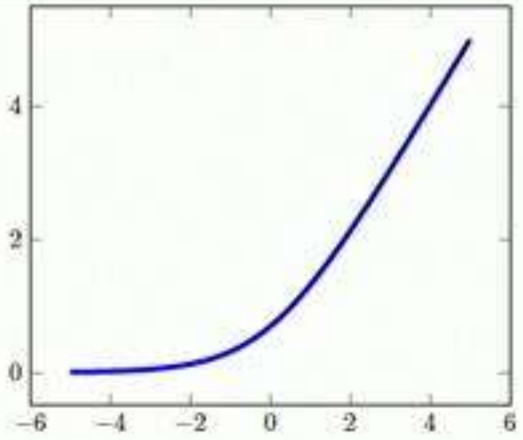

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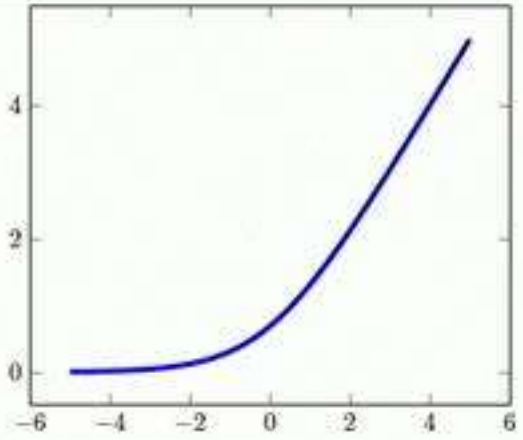

Theorem

Assume

- *Distinct data points* ($\boldsymbol{x}_i \neq \boldsymbol{x}_j$)
- *Smooth activations e.g.* $\phi(z) = \log(1 + e^z)$
- *Overparameterization: # training data* $\leq 2 \times$ *# width* ($k \geq \frac{n}{2}$)
- *Initialization* $\boldsymbol{v}_0$ *at random i.i.d.* $\mathcal{N}(0, \nu^2)$ *and* $\boldsymbol{W}_0$ *i.i.d.* $\mathcal{N}(0,1)$ *with* $\nu >> 1$

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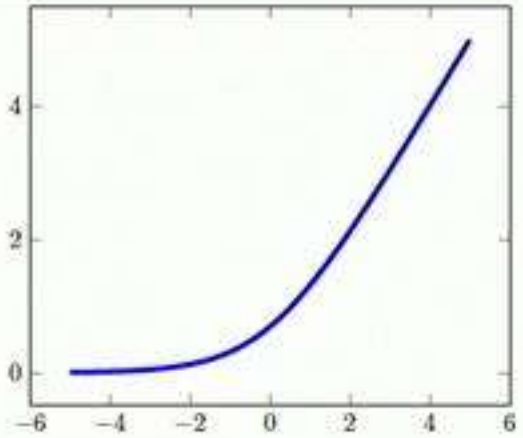

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Then, with high probability

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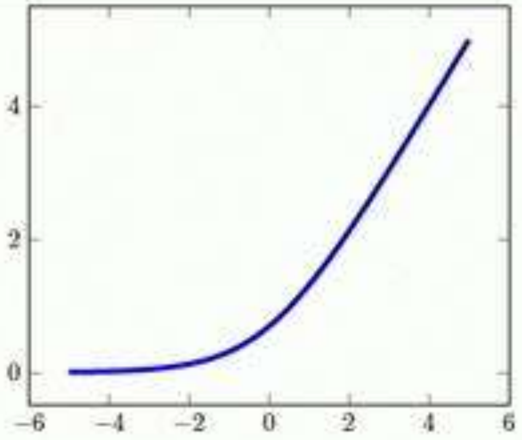

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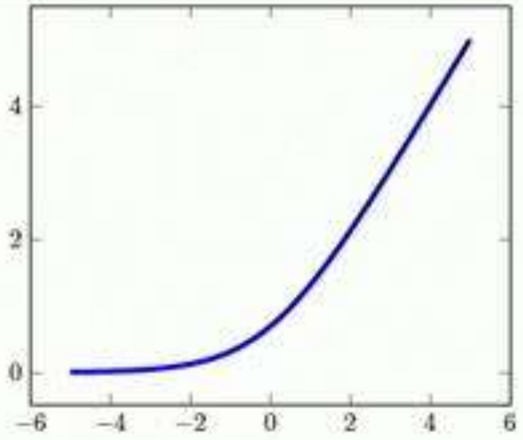
Possible extension: If rank$(\boldsymbol{X}) = d$, # training data $\leq 2 \times$ # parameters*

Theory for smooth activations



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Then, with high probability

- *Zero training error:* $\mathcal{L}(\boldsymbol{v}_\tau, \boldsymbol{W}_\tau) \leq (1-\rho)^\tau \mathcal{L}(\boldsymbol{v}_0, \boldsymbol{W}_0)$

Possible extension: If rank$(\boldsymbol{X}) = d$, # training data $\leq 2 \times$ # parameters*
Prior work [Du et. al., Allen-Zhu et. al., Oymak et. al. ...]
require very wide networks $k \gtrsim \frac{n^4}{\lambda^4}$

Generalization

Model and training

- Data: $(\boldsymbol{x}_1, \boldsymbol{y}_1), \ldots, (\boldsymbol{x}_n, \boldsymbol{y}_n) \in \mathbb{R}^d \times \mathbb{R}^K$
- Training Loss:
  $\mathcal{L}(\boldsymbol{W}) := \frac{1}{2}\sum_{i=1}^{n} \|\boldsymbol{V}\phi(\boldsymbol{W}\boldsymbol{x}_i) - \boldsymbol{y}_i\|_{\ell_2}^2$

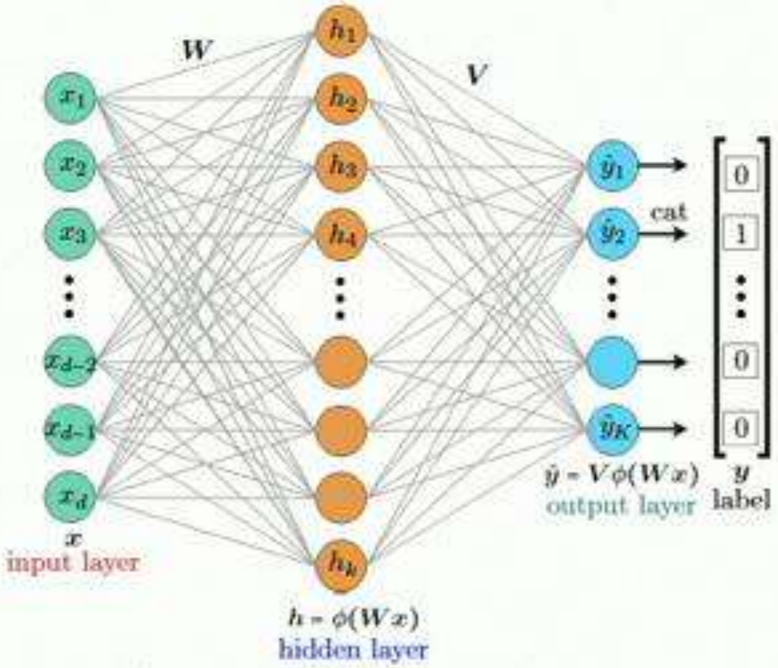
  Concatenate label and prediction vectors

$$\boldsymbol{y} = \begin{bmatrix} \boldsymbol{y}_1 \\ \vdots \\ \boldsymbol{y}_n \end{bmatrix}, f(\boldsymbol{W}) = \begin{bmatrix} \boldsymbol{V}f(\boldsymbol{x}_1; \boldsymbol{W}) \\ \vdots \\ \boldsymbol{V}f(\boldsymbol{x}_n; \boldsymbol{W}) \end{bmatrix} \in \mathbb{R}^{nK}.$$

$$\min_{\boldsymbol{W} \in \mathbb{R}^{k \times d}} \mathcal{L}(\boldsymbol{W}) := \frac{1}{2}\|f(\boldsymbol{W}) - \boldsymbol{y}\|_{\ell_2}^2 .$$

- Algorithm: gradient descent from random initialization

$$\boldsymbol{W}_{\tau+1} = \boldsymbol{W}_{\tau} - \eta \nabla \mathcal{L}(\boldsymbol{W}_{\tau})$$



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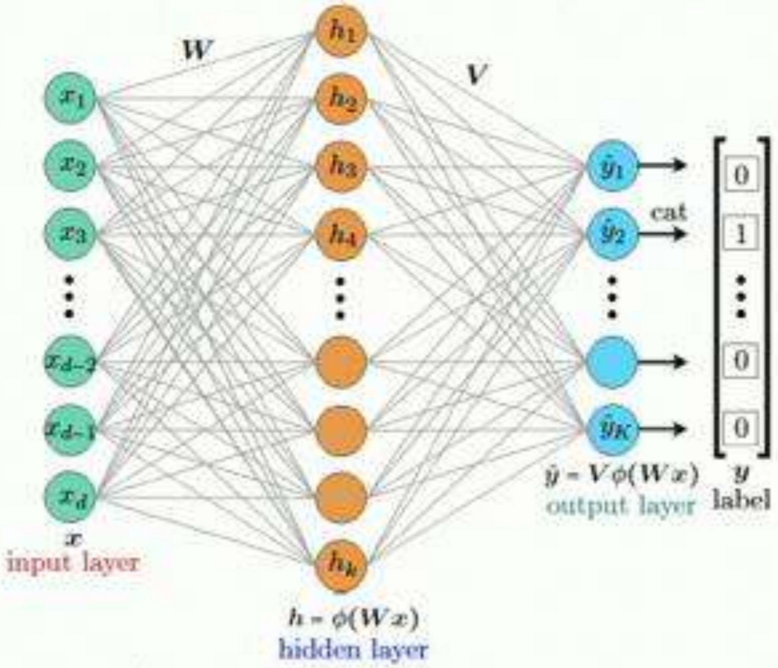

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$$\nabla\mathcal{L}(\boldsymbol{W}) = \mathcal{J}^T(\boldsymbol{W})\left(f(\boldsymbol{W}) - \boldsymbol{y}\right) \quad \text{with} \quad \mathcal{J}(\boldsymbol{W}) = \frac{\partial f(\boldsymbol{W})}{\partial \text{vect}(\boldsymbol{W})}.$$

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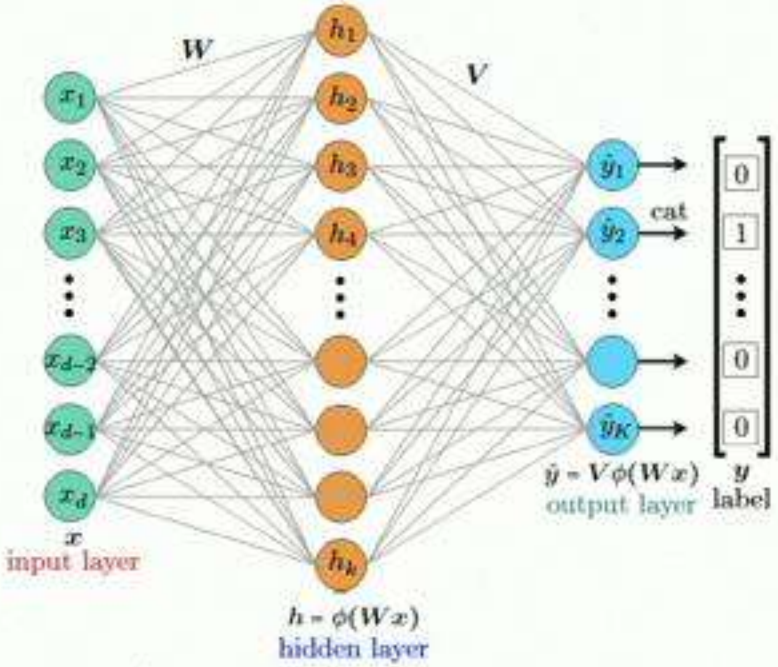

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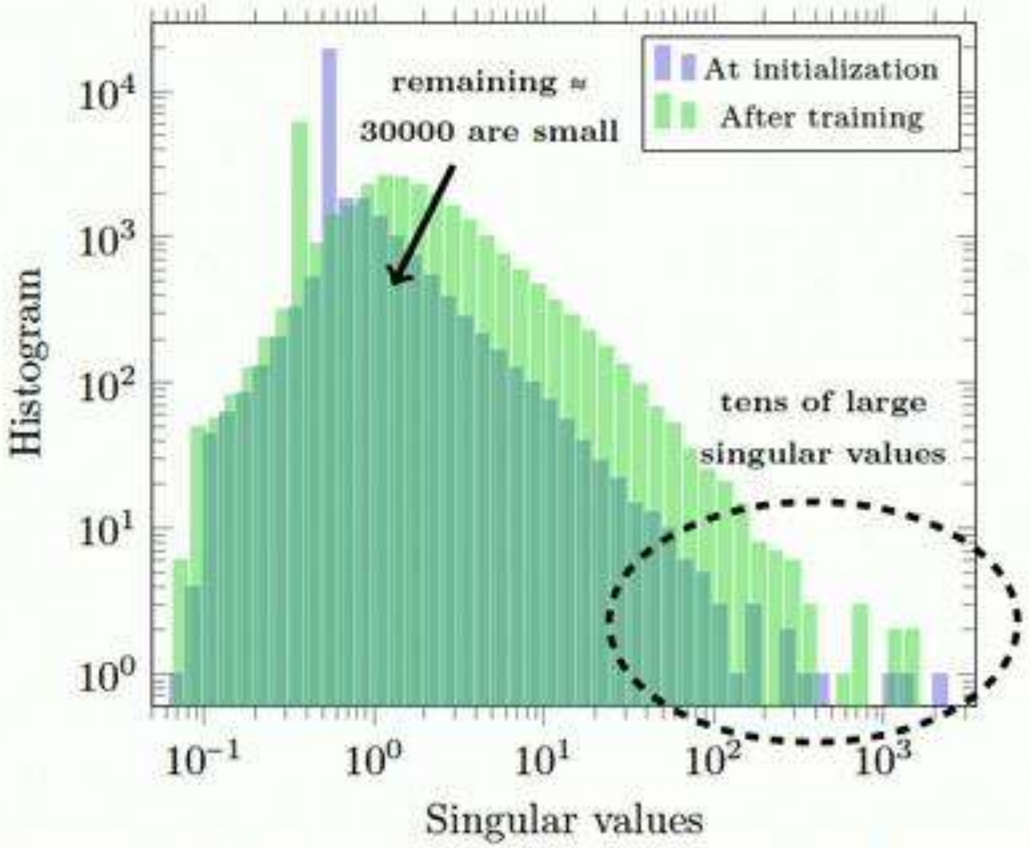
- Prediction: pass through softmax and pick maximum

Key observation

- Dataset: CIFAR10
- Model: ResNET20
- Task: Three-way classification (automobile, airplane, bird)
- $n = 10,000$ and $p = 270,000$



Histogram of the singular values of the initial final Jacobian of neural net during training.

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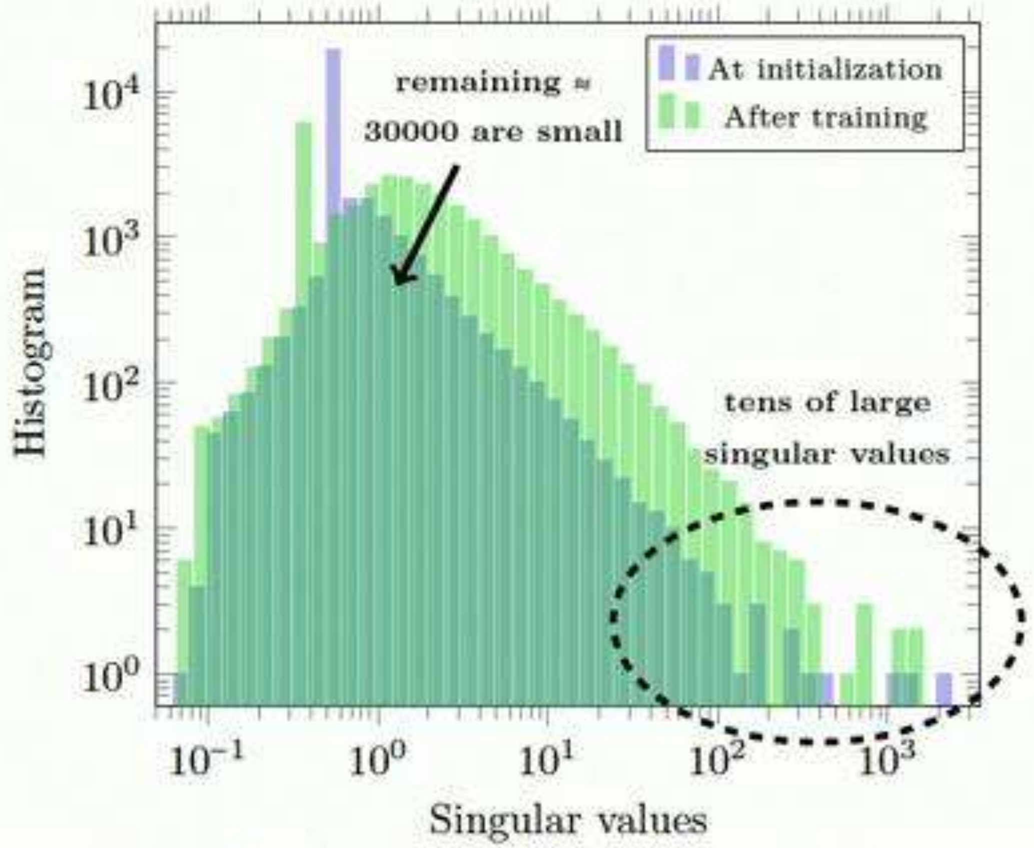

Histogram of the singular values of the initial final Jacobian of neural net during training.

Jacobian has low-rank structure

Information and nuisance spaces

$$\nabla \mathcal{L}(\boldsymbol{W}) = \mathcal{J}^T(\boldsymbol{W})\,(f(\boldsymbol{W}) - \boldsymbol{y}) \quad \text{with} \quad \mathcal{J}(\boldsymbol{W}) = \frac{\partial f(\boldsymbol{W})}{\partial \mathsf{vect}(\boldsymbol{W})}.$$

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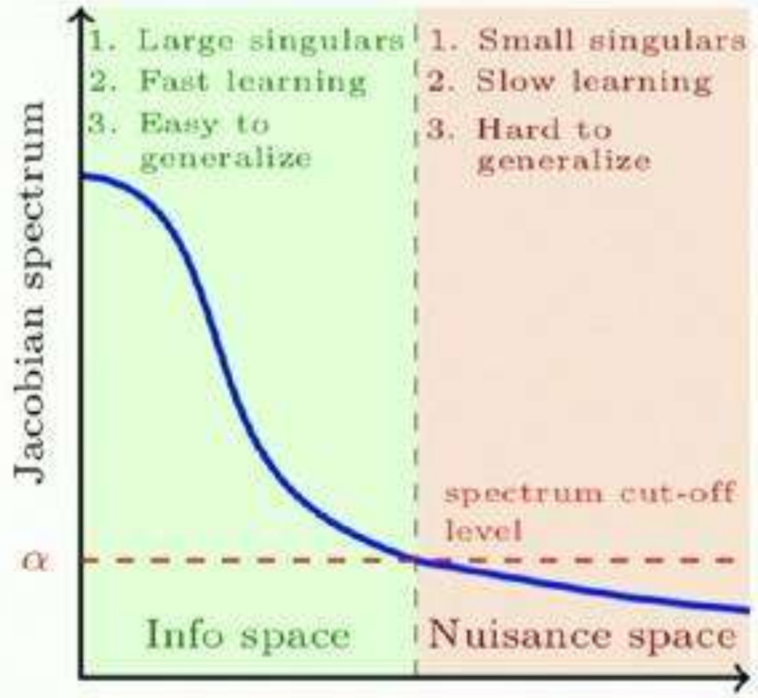
Information and nuisance space of the Jacobian

Jacobian $\boldsymbol{J} \in \mathbb{R}^{nK \times p}$

$$\boldsymbol{J} = \sum_{s=1}^{nK} \lambda_s \boldsymbol{u}_s \boldsymbol{v}_s^T = \boldsymbol{U}\, diag\,(\lambda_1, \lambda_2, \ldots, \lambda_{nK})\, \boldsymbol{V}^T$$

- *Information space:* $\mathcal{I} =$*span*$(\{\boldsymbol{u}_s\}_{s=1}^r)$
- *nuisance space:* $\mathcal{N} =$*span*$(\{\boldsymbol{u}_s\}_{s=r+1}^n)$



Theory (random initialization)

Fix output layer to i.i.d. $\frac{1}{\sqrt{kK\log(K)}}$ and initialize $\boldsymbol{W}_0$ i.i.d. $\mathcal{N}(0,1)$

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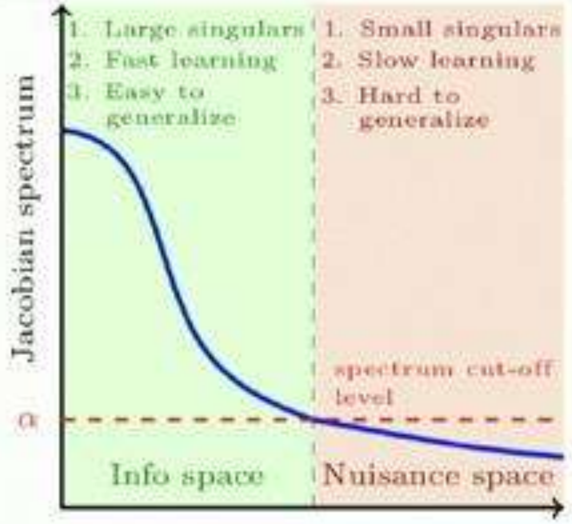

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- Structured datasets generalize easier and require smaller networks.
- with constant $\bar{\alpha}$, constant iterations and width is sufficient for learning.
- Picking cut-off small ($\mathcal{I} = \mathbb{R}^n$) and $K = 1$ improves upon [Arora et. al.]

$$\text{missclass error} \lesssim \sqrt{\frac{\boldsymbol{y}^T\left(\boldsymbol{J}\boldsymbol{J}^T\right)^{-1}\boldsymbol{y}}{n}} \quad \text{with} \quad k \gtrsim \frac{n^4 \log n}{\lambda_{\min}^4\left(\boldsymbol{J}\boldsymbol{J}^T\right)}$$

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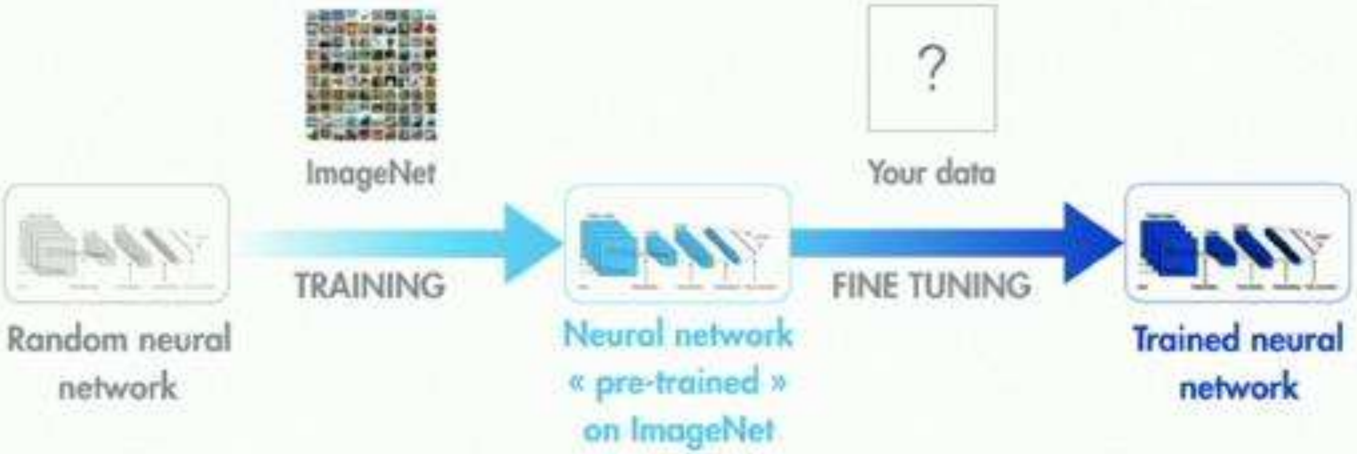
- Applies to pre-trained models e.g. meta/transfer learning



Question: What can we say about pretrained networks vs random?

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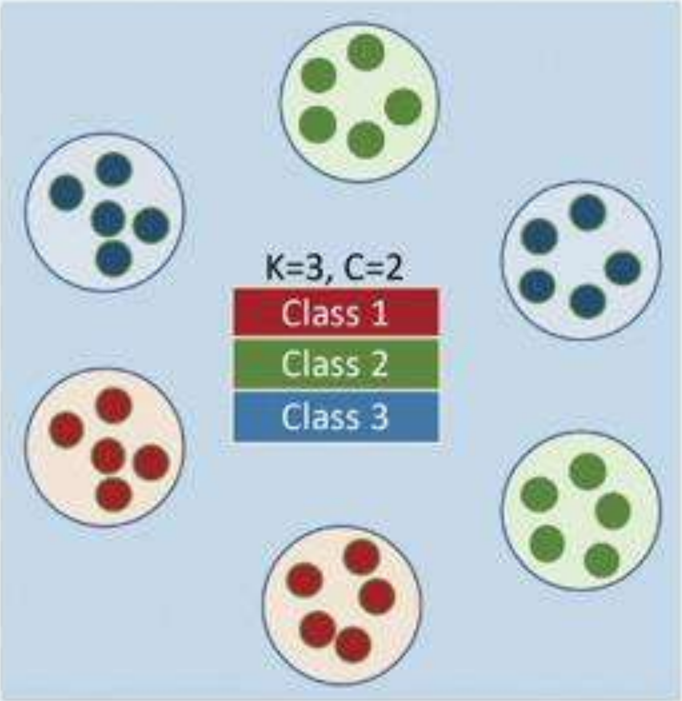
- Applies to any iteration $\boldsymbol{J} = \boldsymbol{J}(\boldsymbol{W}_\tau)$
- A step towards kernel adaptation $\mathcal{K}_\tau = \boldsymbol{J}(\boldsymbol{W}_\tau)\boldsymbol{J}^T(\boldsymbol{W}_\tau)$

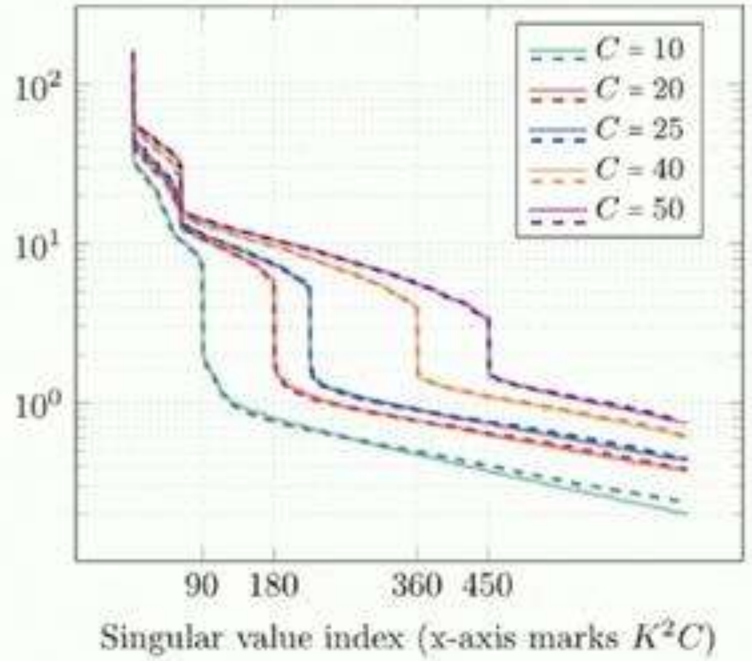
$$\mathcal{K}_0 \rightarrow \mathcal{K}_1 \rightarrow \mathcal{K}_2 \rightarrow \ldots \rightarrow$$

see [Bach and Chizat 2018], [Mei and Montanari], [Yang], [Soudry et. al.] and many others

Concrete example: Gaussian Mixture Model (GMM)

Data set a GMM with K classes each containing C components per class with small σ^2





Theorem

With high probability

- *Jacobian has* K^2C *large singular values that grow* $\propto \sqrt{n}$
- *If* $k \gtrsim \Gamma^4 K^8 C^4$ *after* $T \propto \Gamma K^2 C$ *iterations,*

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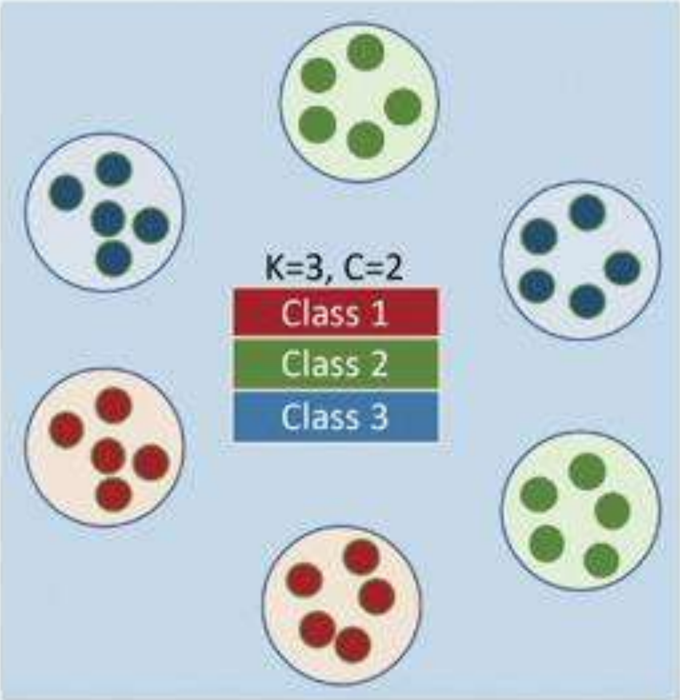

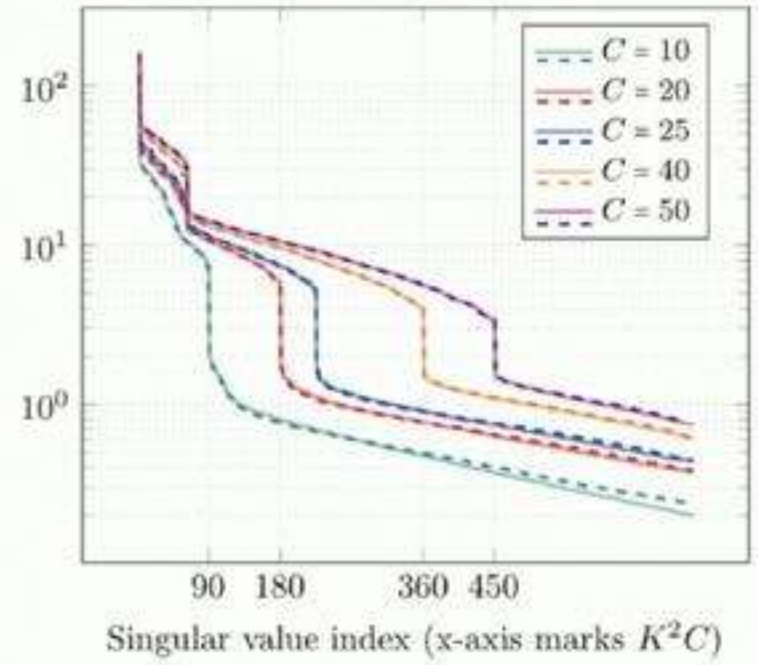

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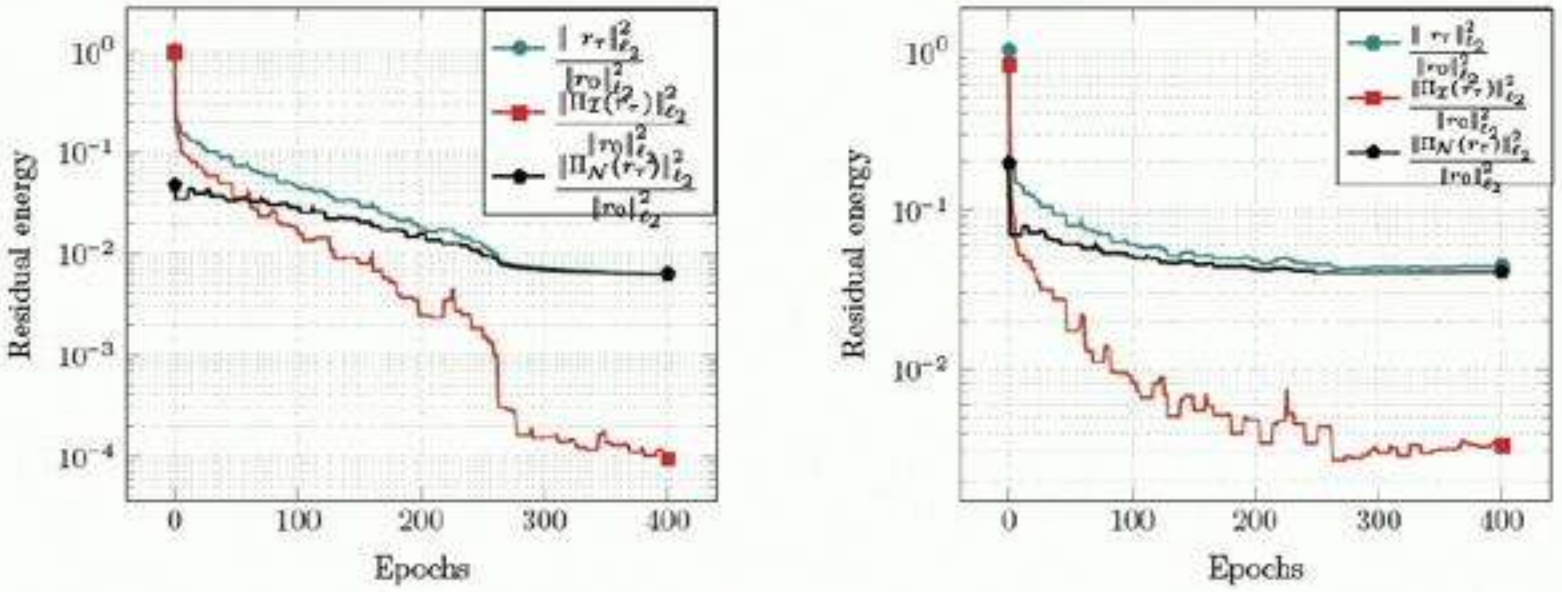
[Arora et. al. 2019] $k \to \infty$ as $\sigma \to 0$

Numerical experiments

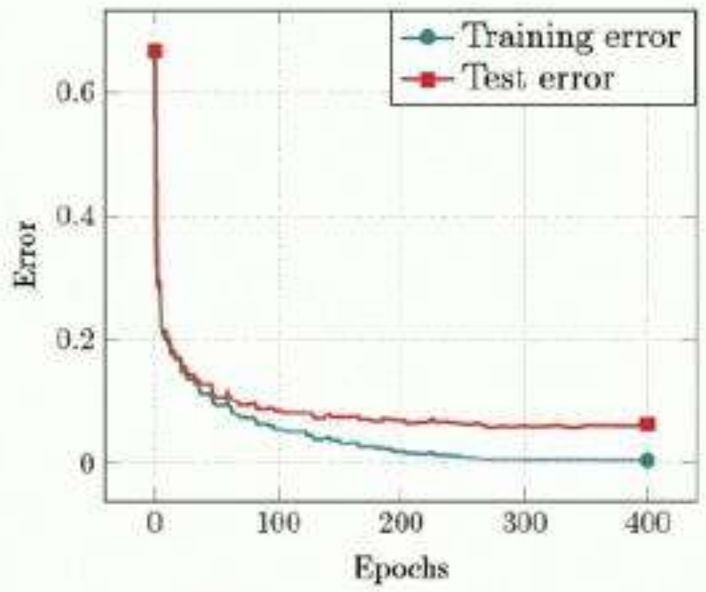
No label corruption

$$K = 3 \text{ classes}, \quad \dim(\mathcal{I}) = 50, \quad n = 10,000$$

Consider evolution of residual $\boldsymbol{r}_\tau = f(\boldsymbol{W}_\tau) - \boldsymbol{y}$



Residual along the information/nuisance spaces of the final Jacobian using (a) train data and (b) test data



Train and test error

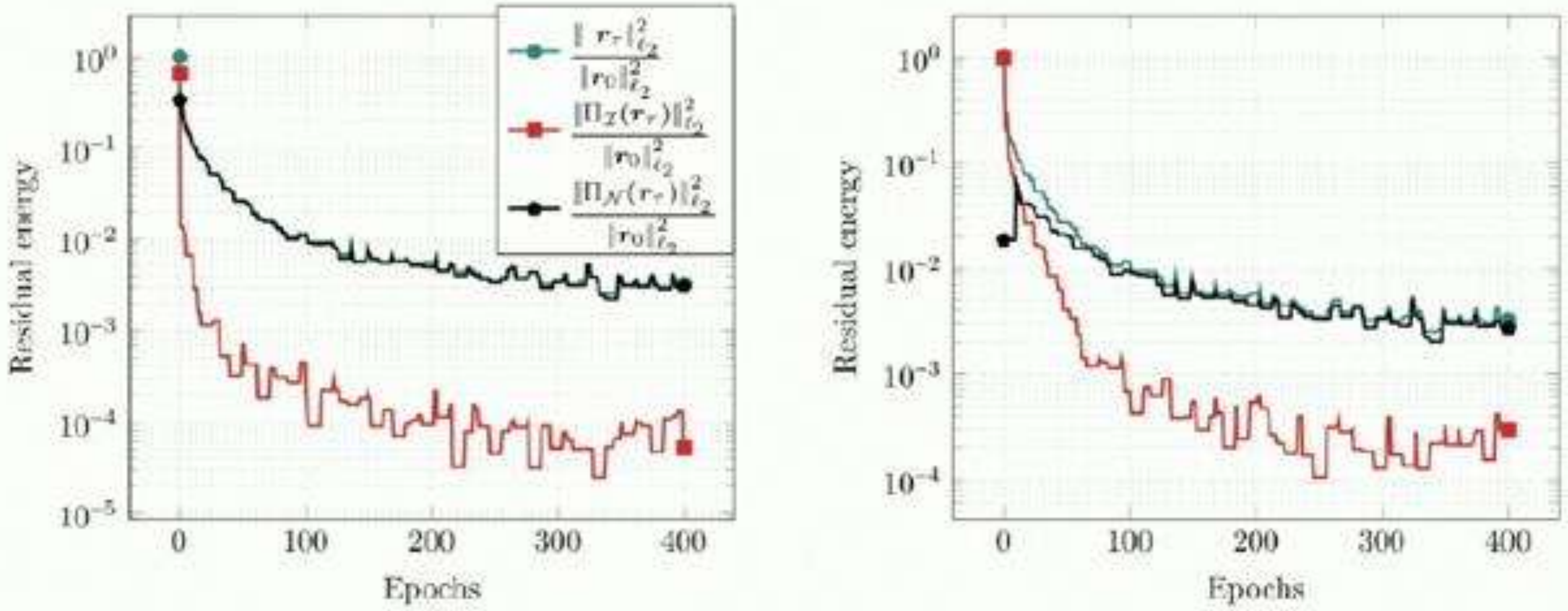
	$\frac{\lVert\Pi_{\mathcal{I}}(\boldsymbol{y})\rVert_{\ell_2}}{\lVert\boldsymbol{y}\rVert_{\ell_2}}$	$\frac{\lVert\Pi_{\mathcal{N}}(\boldsymbol{y})\rVert_{\ell_2}}{\lVert\boldsymbol{y}\rVert_{\ell_2}}$	$\frac{\lVert\boldsymbol{J}_{\mathcal{I}}^{\dagger}\boldsymbol{y}\rVert_{\ell_2}}{\lVert\boldsymbol{y}\rVert_{\ell_2}}$	$\frac{\lVert\Pi_{\mathcal{I}}(\boldsymbol{r}_0)\rVert_{\ell_2}}{\lVert\boldsymbol{r}_0\rVert_{\ell_2}}$	$\frac{\lVert\Pi_{\mathcal{N}}(\boldsymbol{r}_0)\rVert_{\ell_2}}{\lVert\boldsymbol{r}_0\rVert_{\ell_2}}$	$\frac{\lVert\boldsymbol{J}_{\mathcal{I}}^{\dagger}\boldsymbol{r}_0\rVert_{\ell_2}}{\lVert\boldsymbol{r}_0\rVert_{\ell_2}}$
$\boldsymbol{J}_{init}$	0.724	0.690	$5.44 \cdot 10^{-3}$	0.886	0.465	$4.10 \cdot 10^{-3}$
$\boldsymbol{J}_{final}$	0.987	0.158	$3.16 \cdot 10^{-3}$	0.976	0.217	$3.43 \cdot 10^{-3}$

Table 1: Depiction of the alignment of the initial label/residual with the information/nuisance space using uncorrupted data and a Multi-class ResNet20 model trained with SGD.

No label corruption with ADAM

$$K = 3 \text{ classes}, \quad \dim(\mathcal{I}) = 50, \quad n = 10,000$$

Consider evolution of residual $\boldsymbol{r}_\tau = f(\boldsymbol{W}_\tau) - \boldsymbol{y}$
green (total), red (on $\mathcal{I}$), black (on $\mathcal{N}$)



Residual along the information/nuisance spaces of the
(a) initial and (b) final Jacobian using ADAM

	$\frac{\lVert\Pi_{\mathcal{I}}(\boldsymbol{y})\rVert_{\ell_2}}{\lVert\boldsymbol{y}\rVert_{\ell_2}}$	$\frac{\lVert\Pi_{\mathcal{N}}(\boldsymbol{y})\rVert_{\ell_2}}{\lVert\boldsymbol{y}\rVert_{\ell_2}}$	$\frac{\lVert\boldsymbol{J}_{\mathcal{I}}^{\dagger}\boldsymbol{y}\rVert_{\ell_2}}{\lVert\boldsymbol{y}\rVert_{\ell_2}}$	$\frac{\lVert\Pi_{\mathcal{I}}(\boldsymbol{r}_0)\rVert_{\ell_2}}{\lVert\boldsymbol{r}_0\rVert_{\ell_2}}$	$\frac{\lVert\Pi_{\mathcal{N}}(\boldsymbol{r}_0)\rVert_{\ell_2}}{\lVert\boldsymbol{r}_0\rVert_{\ell_2}}$	$\frac{\lVert\boldsymbol{J}_{\mathcal{I}}^{\dagger}\boldsymbol{r}_0\rVert_{\ell_2}}{\lVert\boldsymbol{r}_0\rVert_{\ell_2}}$
$\boldsymbol{J}_{init}$	0.702	0.712	$5.36 \cdot 10^{-3}$	0.814	0.582	$4.43 \cdot 10^{-3}$
$\boldsymbol{J}_{final}$	0.997	0.078	$3.10 \cdot 10^{-3}$	0.991	0.136	$3.06 \cdot 10^{-3}$

Table 2: Depiction of the alignment of the initial label/residual with the information/nuisance space using uncorrupted data and a Multi-class ResNet20 model trained with Adam.

50% label corruption

$$K = 3 \text{ classes}, \quad \dim(\mathcal{I}) = 50, \quad n = 10,000$$

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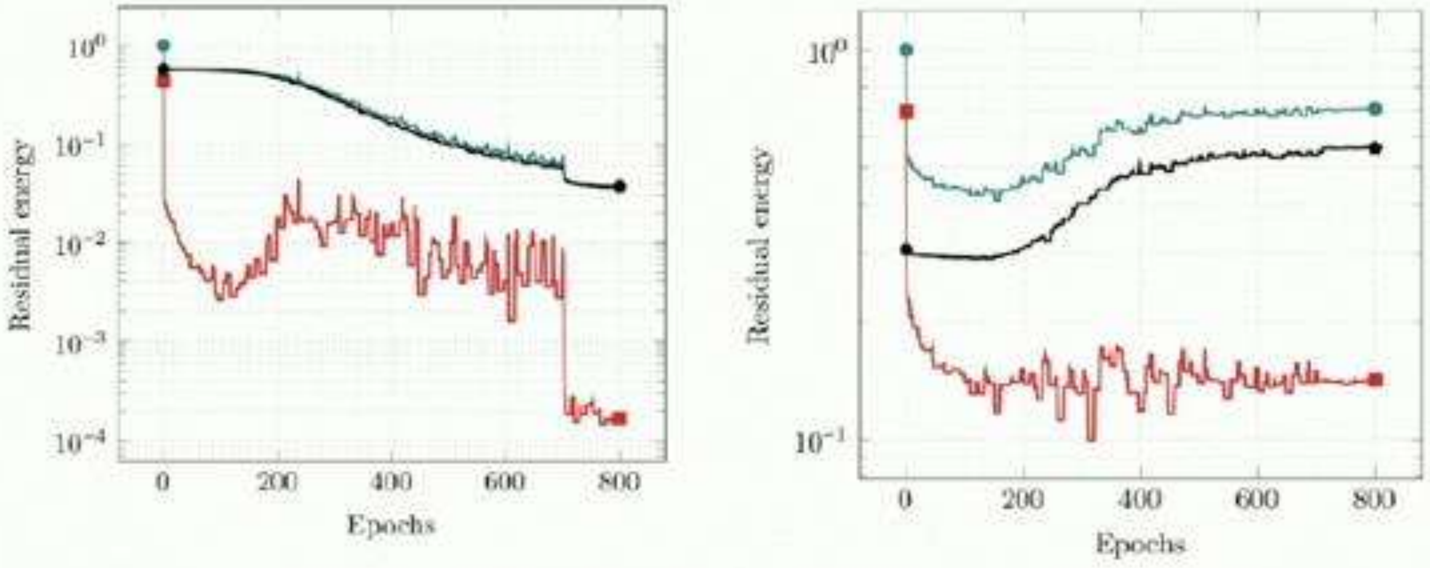
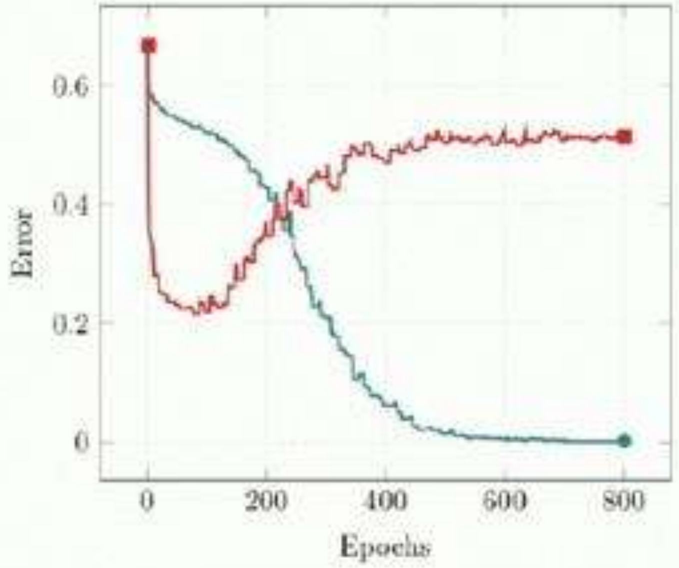


Residual along the information/nuisance spaces of the final Jacobian using (a) train data and (b) test data

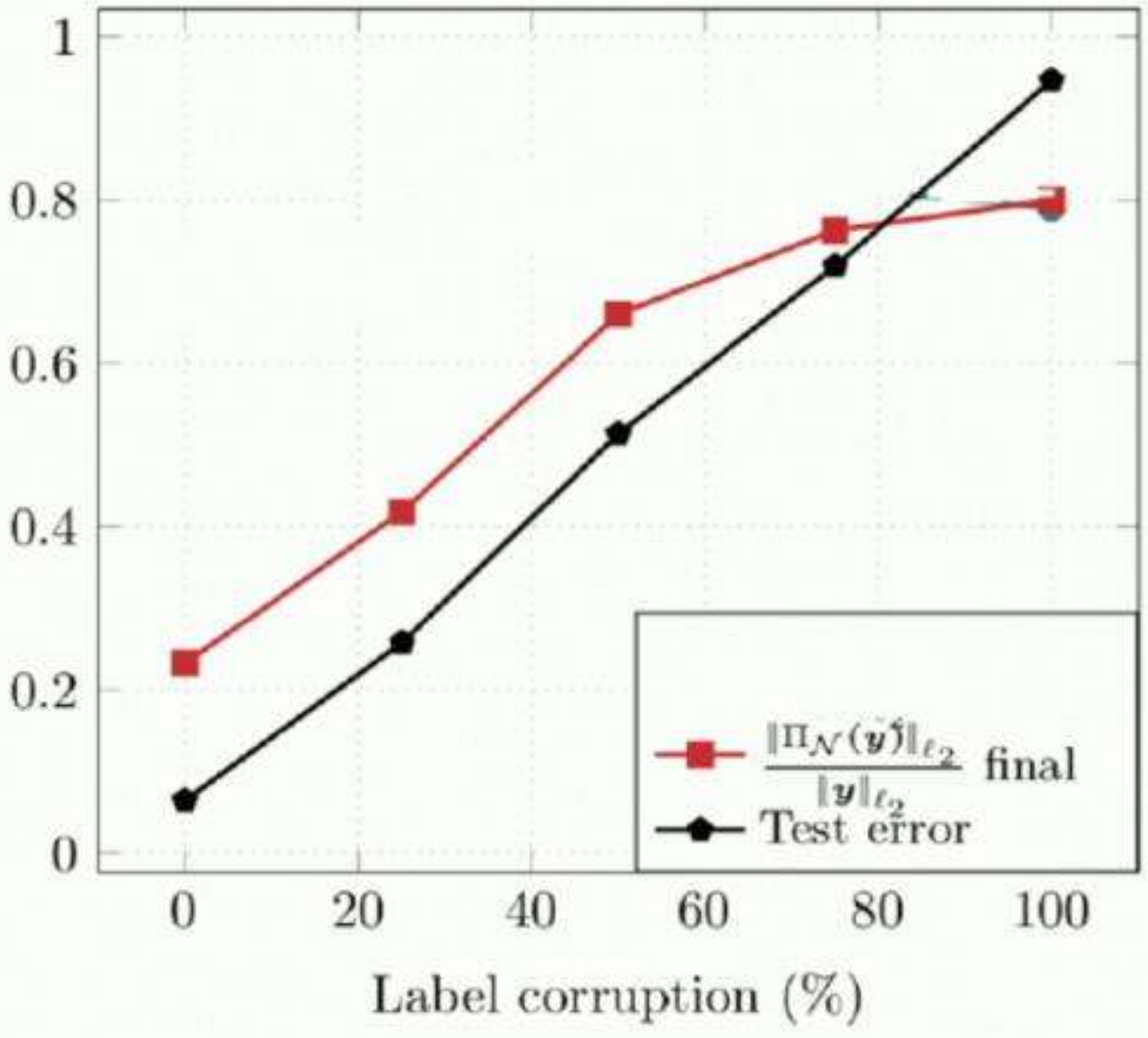


Train and test error

	$\frac{\Vert\Pi_{\mathcal{I}}(\boldsymbol{y})\Vert_{\ell_2}}{\Vert\boldsymbol{y}\Vert_{\ell_2}}$	$\frac{\Vert\Pi_{\mathcal{N}}(\boldsymbol{y})\Vert_{\ell_2}}{\Vert\boldsymbol{y}\Vert_{\ell_2}}$	$\frac{\Vert\boldsymbol{J}_{\mathcal{I}}^{\dagger}\boldsymbol{y}\Vert_{\ell_2}}{\Vert\boldsymbol{y}\Vert_{\ell_2}}$	$\frac{\Vert\Pi_{\mathcal{I}}(\boldsymbol{r}_0)\Vert_{\ell_2}}{\Vert\boldsymbol{r}_0\Vert_{\ell_2}}$	$\frac{\Vert\Pi_{\mathcal{N}}(\boldsymbol{r}_0)\Vert_{\ell_2}}{\Vert\boldsymbol{r}_0\Vert_{\ell_2}}$	$\frac{\Vert\boldsymbol{J}_{\mathcal{I}}^{\dagger}\boldsymbol{r}_0\Vert_{\ell_2}}{\Vert\boldsymbol{r}_0\Vert_{\ell_2}}$
$\boldsymbol{J}_{init}$	0.587	0.810	$1.72 \cdot 10^{-3}$	0.643	0.766	$1.98 \cdot 10^{-3}$
$\boldsymbol{J}_{final}$	0.751	0.660	$1.87 \cdot 10^{-3}$	0.763	0.646	$1.20 \cdot 10^{-3}$

Table 3: Depiction of the alignment of the initial label/residual with the information/nuisance space using 50% label corrupted data and a Multi-class ResNet20 model trained with SGD.

Test error grows in tandem with energy on nuisance space

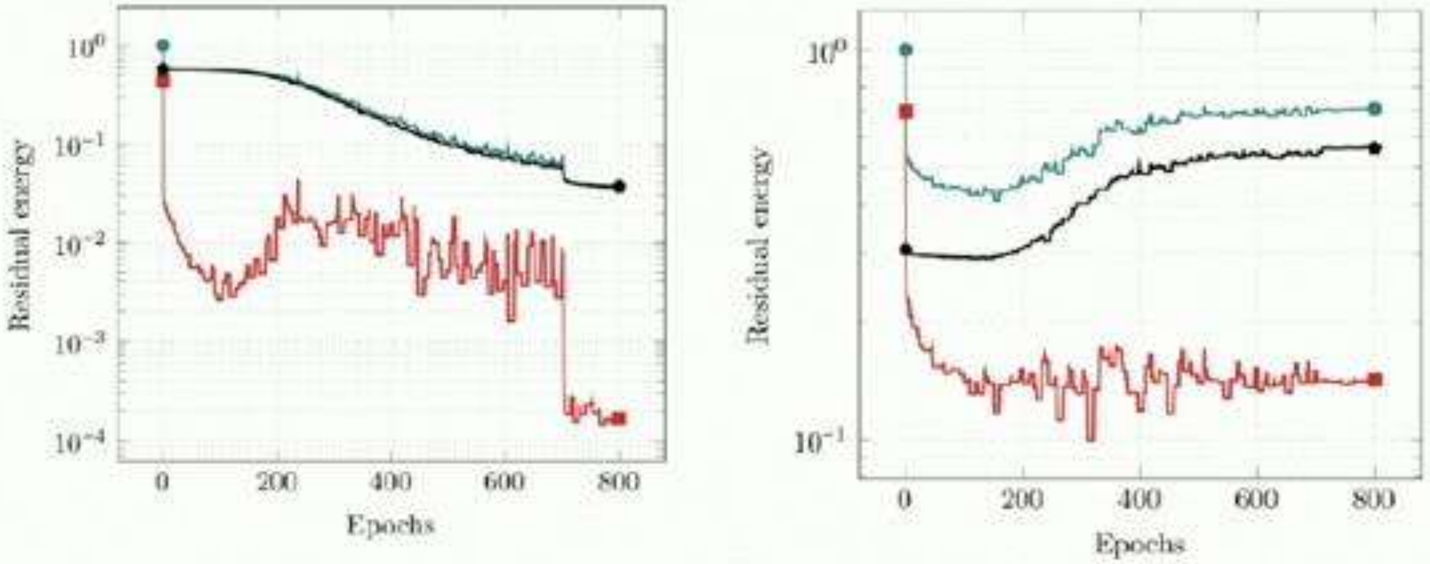


Fraction of the energy of the label vector
as a function of the amount of label corruption.

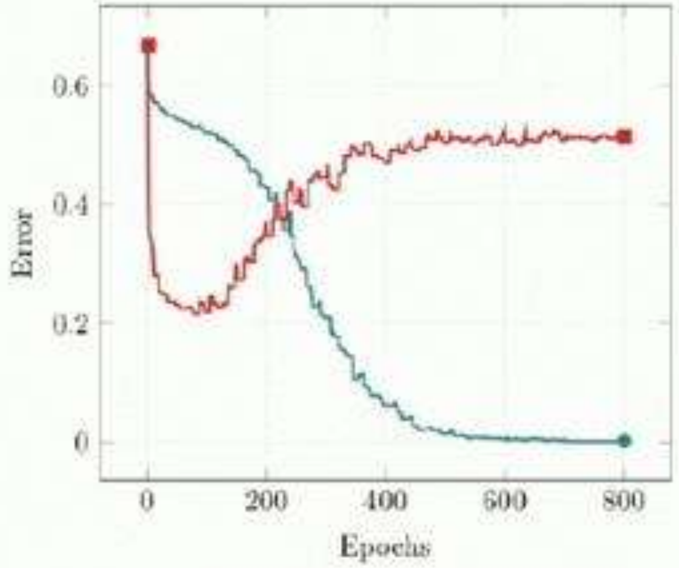
50% label corruption

$$K = 3 \text{ classes}, \quad \dim(\mathcal{I}) = 50, \quad n = 10,000$$

Consider evolution of residual $\boldsymbol{r}_\tau = f(\boldsymbol{W}_\tau) - \boldsymbol{y}$



Residual along the information/nuisance spaces of the final Jacobian using (a) train data and (b) test data



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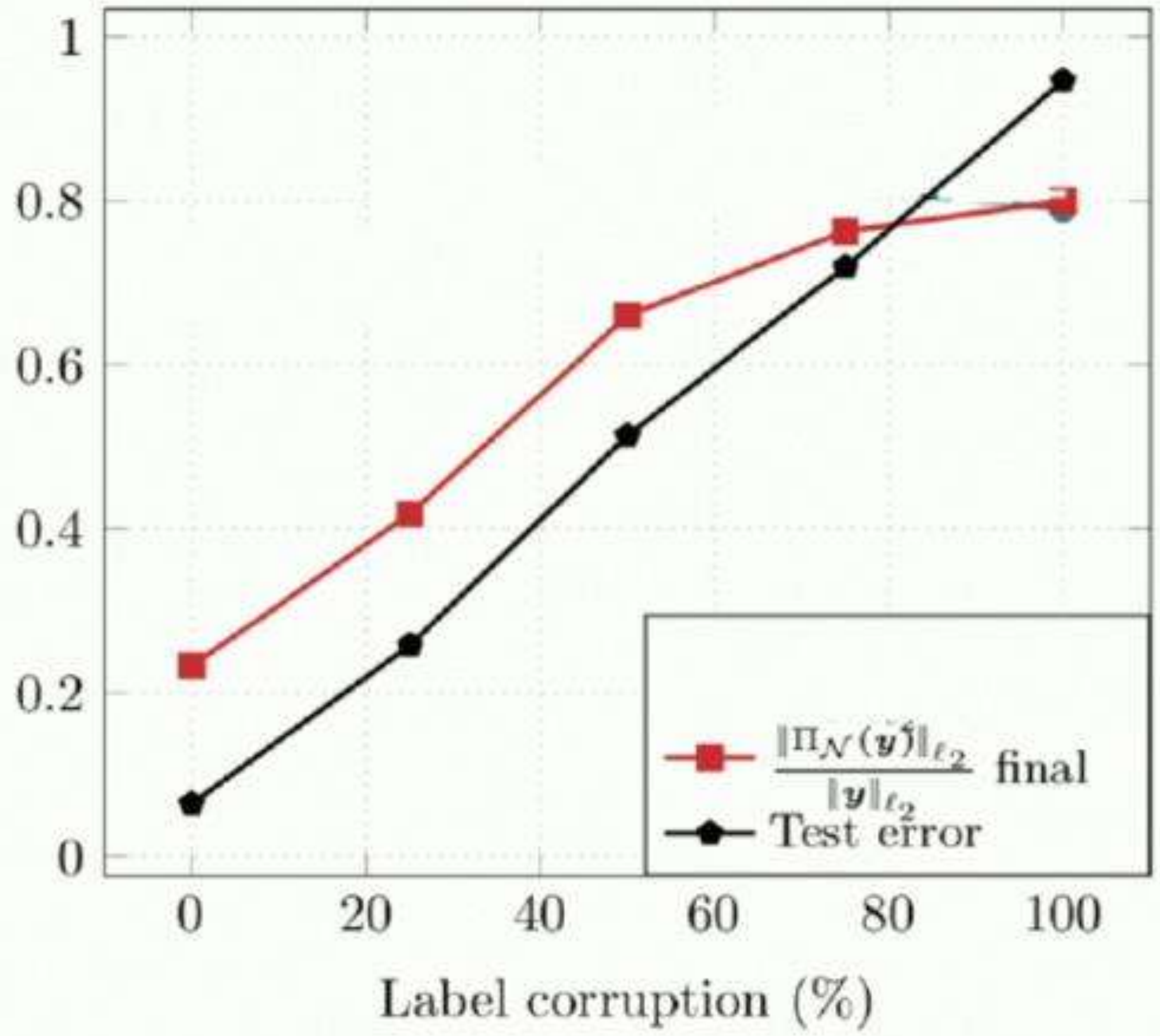

Fraction of the energy of the label vector
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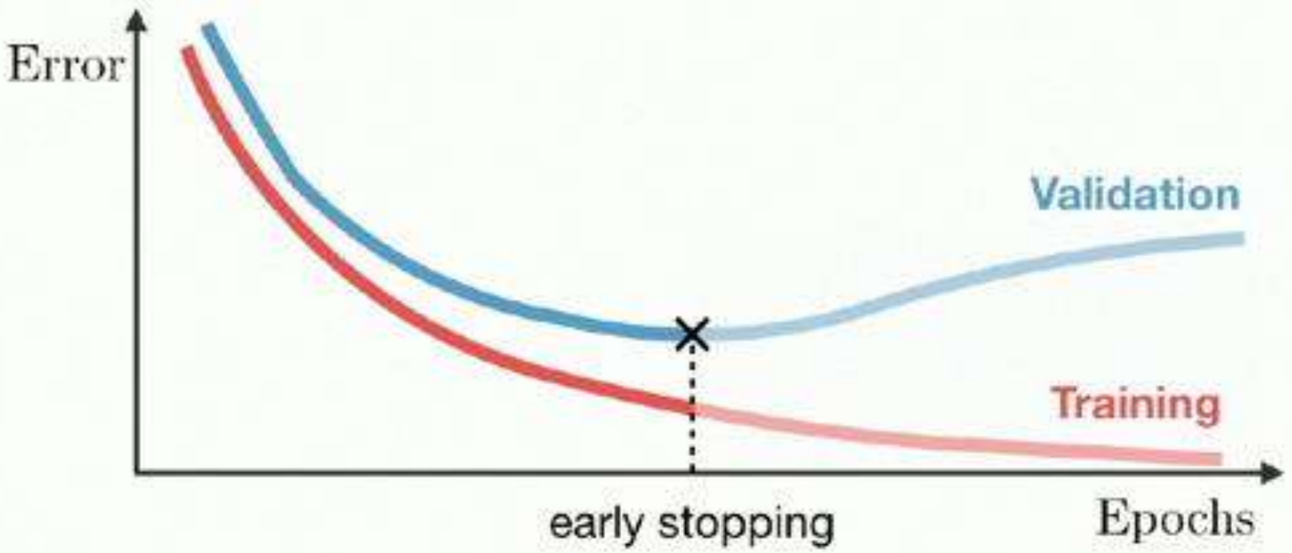
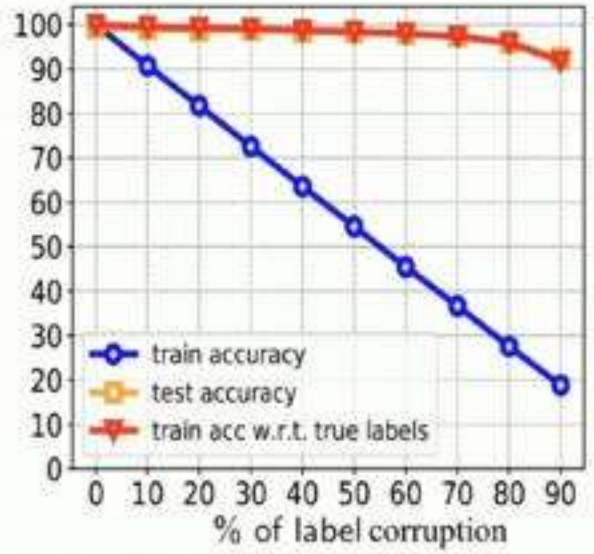
Early stopping and robustness to label corruption





Experiment II-Early stopping and robustness

Repeat the same experiment but stop early

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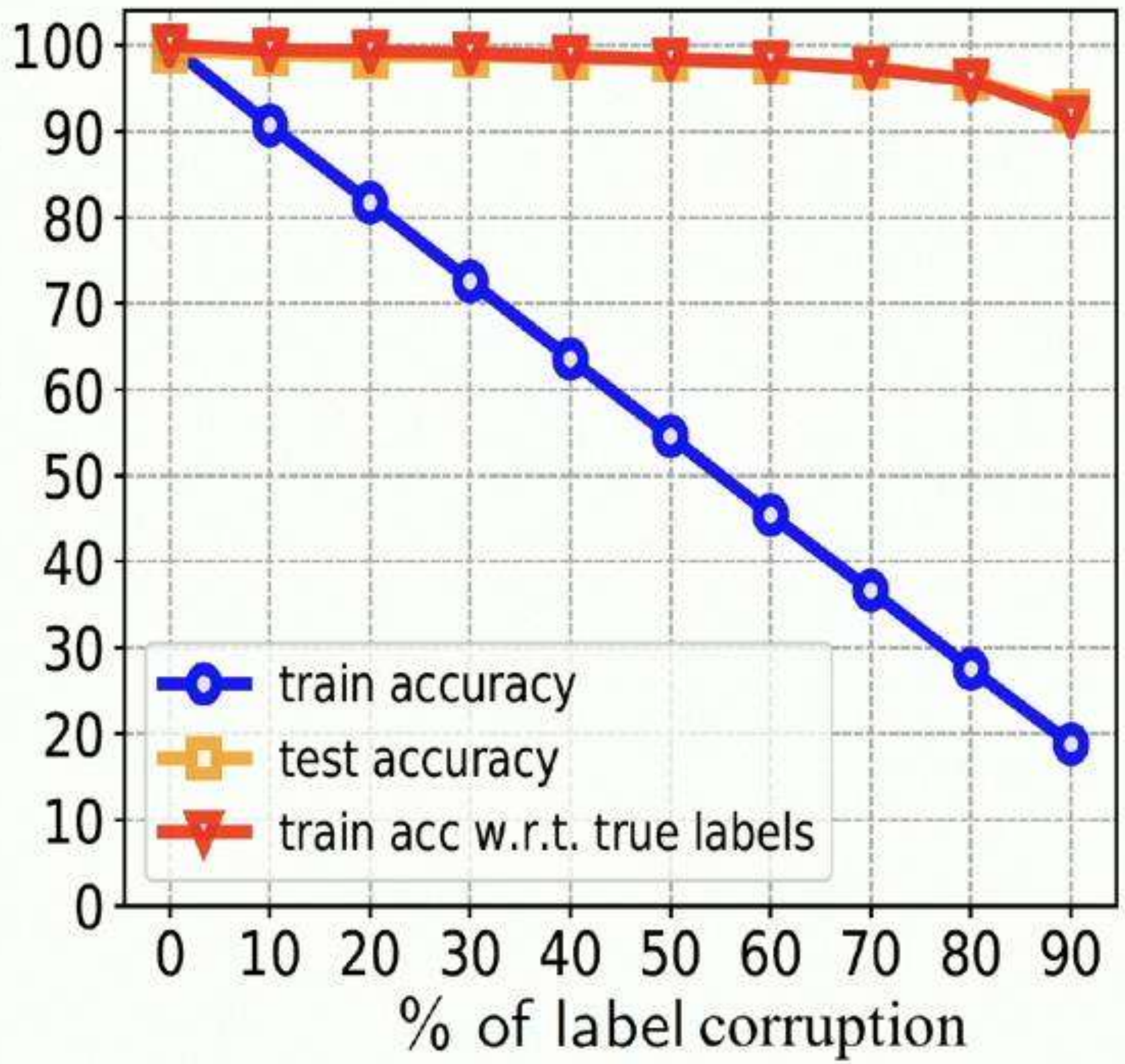
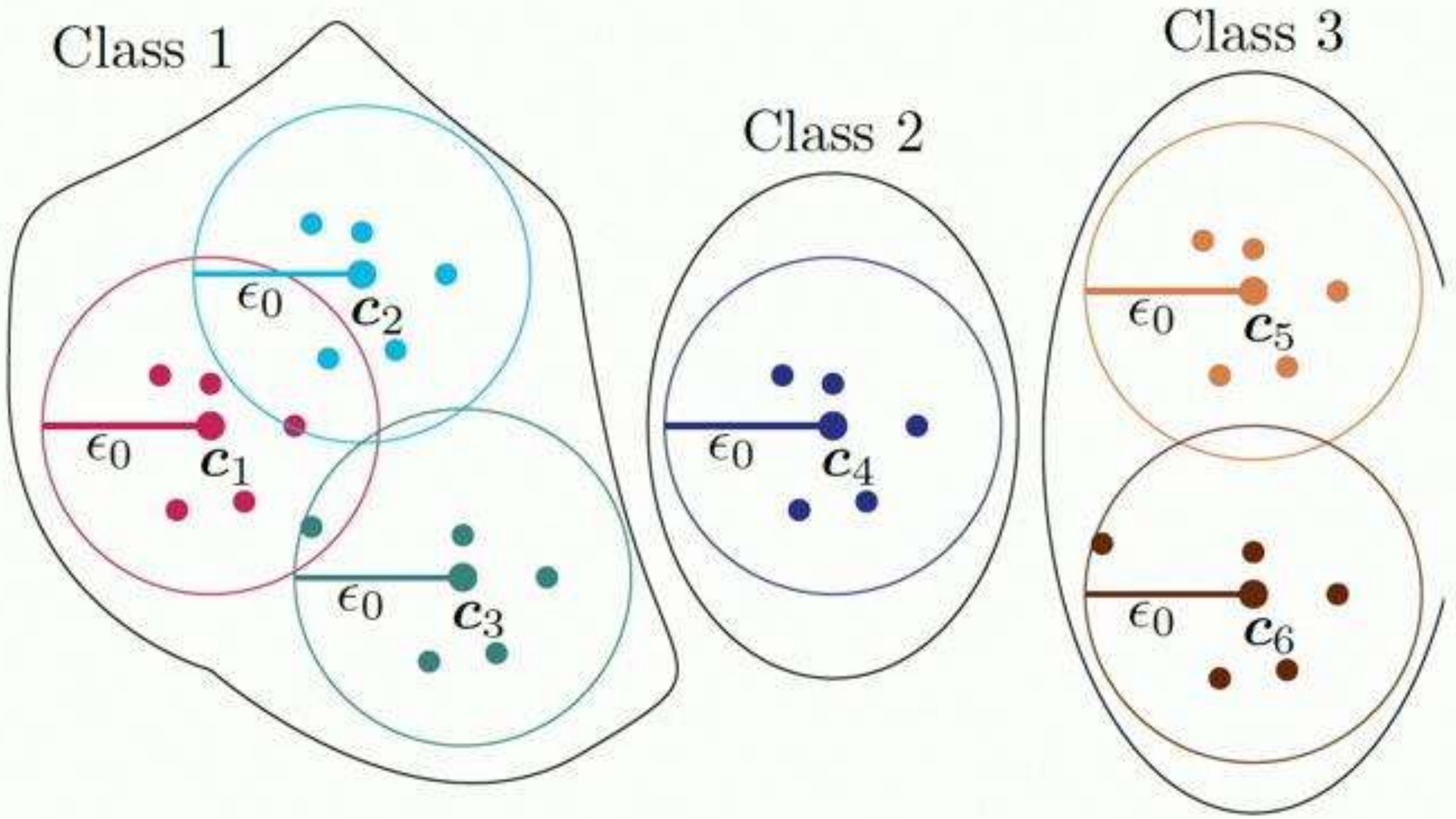


Model (without corruption)

clean data: clusterable data

input/label pairs $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n} \in \mathbb{R}^d \times \mathbb{R}^K$

L clusters and K classes



Robustness to corruption

Clean data points $\{(\boldsymbol{x}_i, \bar{y}_i)\}_{i=1}^n$, corrupt $s := \rho n$ to get corrupted data $\{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$.

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Fit

$$\mathcal{L}(\boldsymbol{W}) := \frac{1}{2}\sum_{i=1}^{n} \|f(\boldsymbol{W}, \boldsymbol{x}_i) - \boldsymbol{y}_i\|_{\ell_2}^2$$

via gradient descent

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Theorem (Oymak and Soltanolkotabi 2019)

Assume

- *Corruption level* $\rho < \frac{1}{16}$
- *Overparameterization:* $\#parameters \gtrsim L^4$

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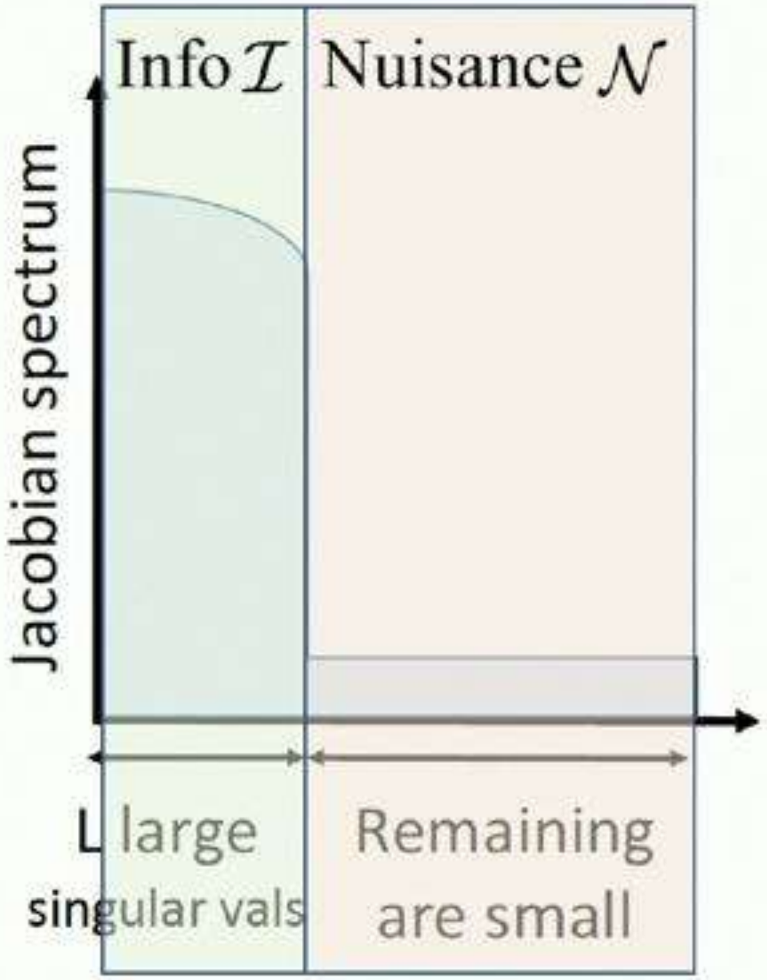
Starting from random initialization, after $\tau \sim L\log(1/\rho)$ *iterations, gradient descent finds a model with perfect accuracy, i.e.*

$$\textit{closest label to } f(\boldsymbol{W}_\tau, \boldsymbol{x}_i) = \textit{true label } \bar{y}_i$$

Key Intuition

Key Intuition

Jacobian is low-rank



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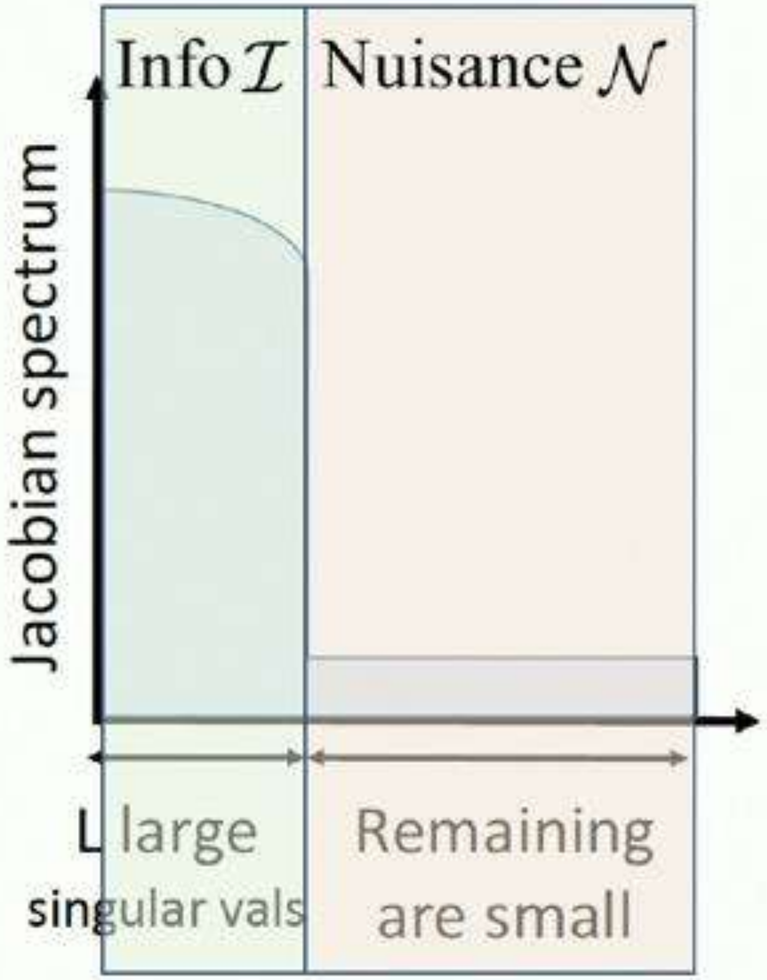
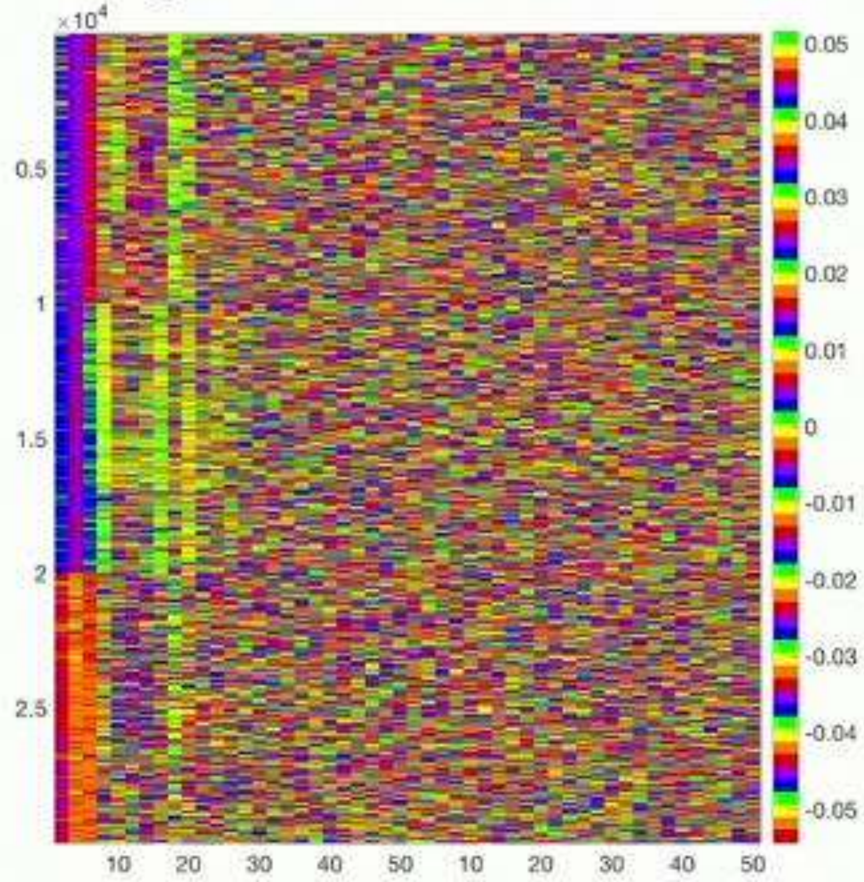


Prominent eigenvects of Jacobian are diffused



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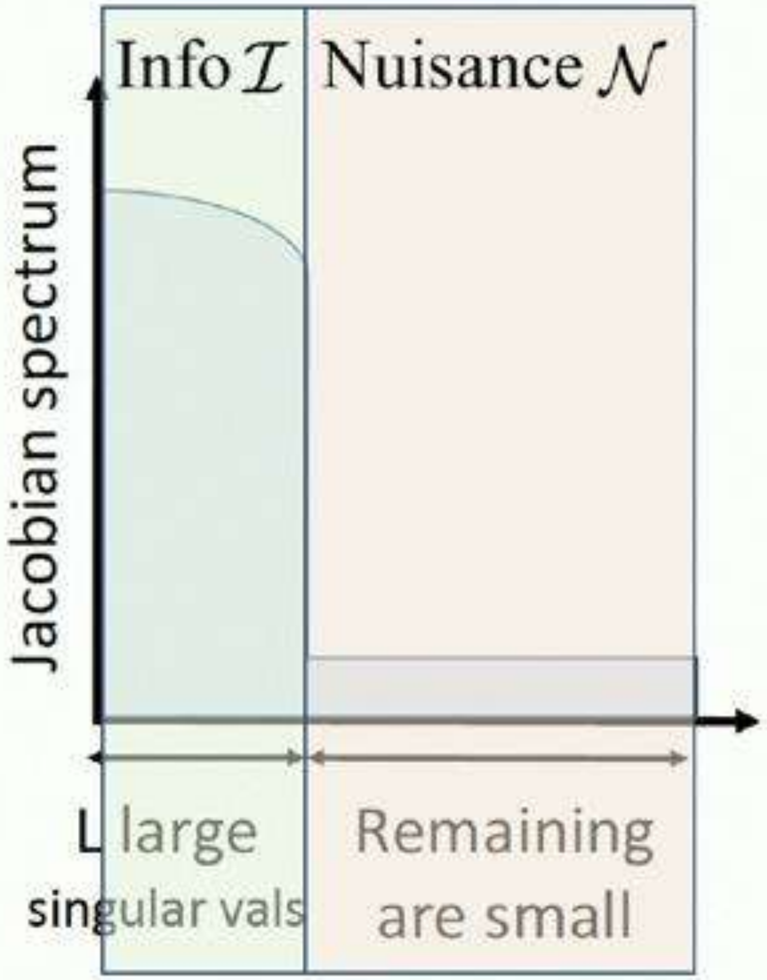

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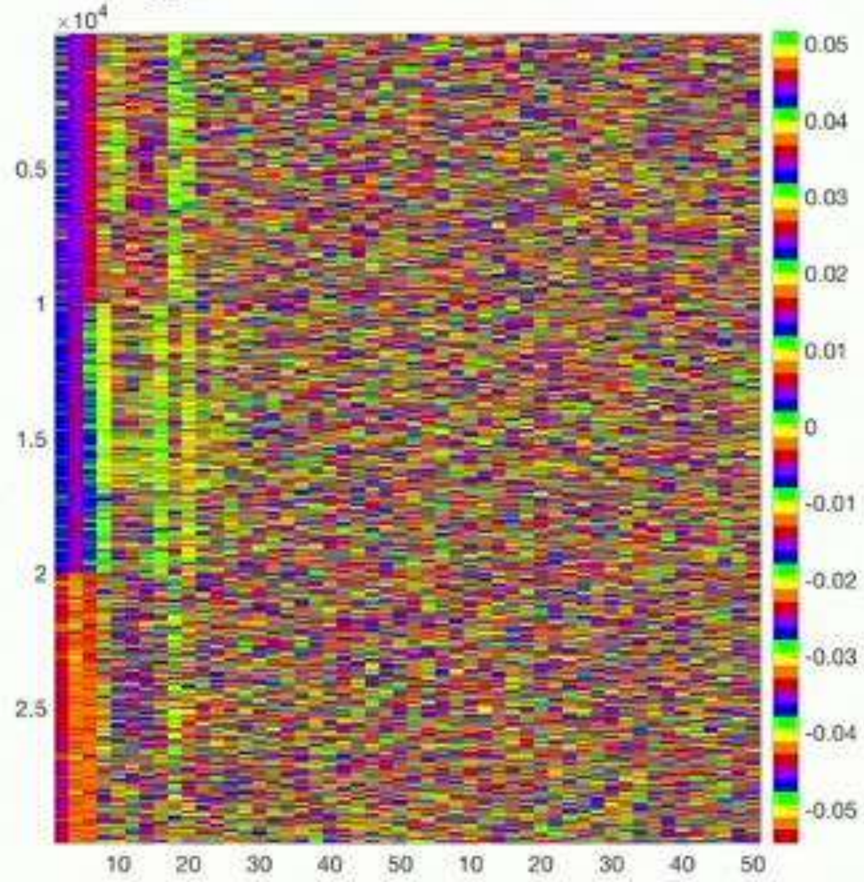

Interaction of Jacobian and residual $\nabla\mathcal{L}(\boldsymbol{\theta}) = \mathcal{J}^T(\boldsymbol{\theta})\,(f(\boldsymbol{\theta}, \boldsymbol{X}) - \boldsymbol{y})$

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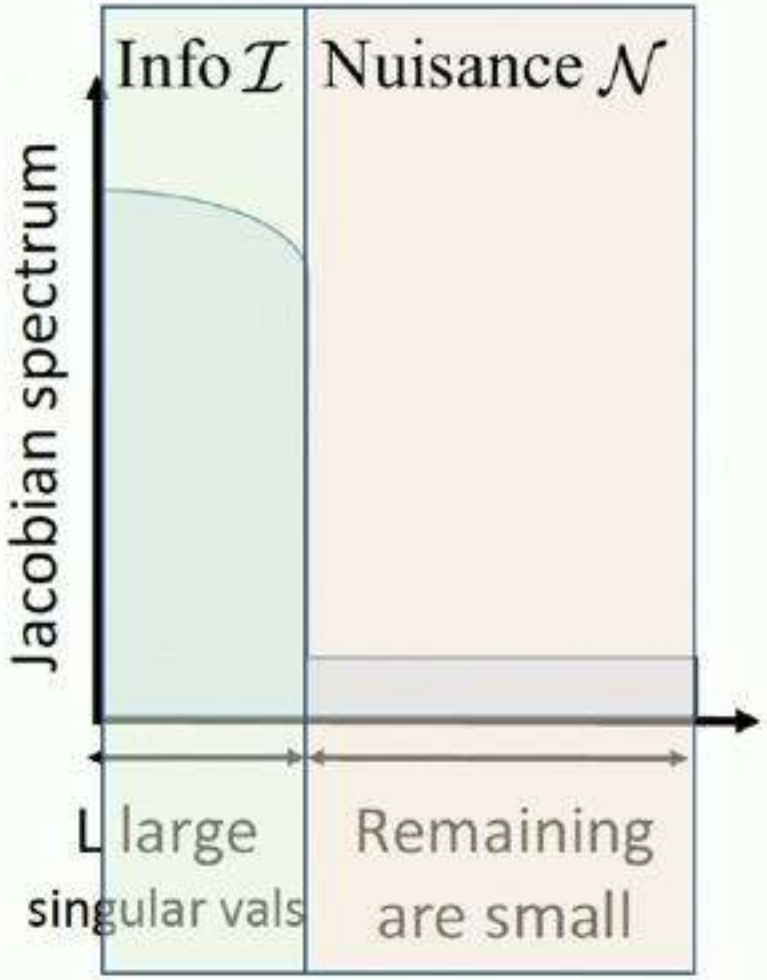

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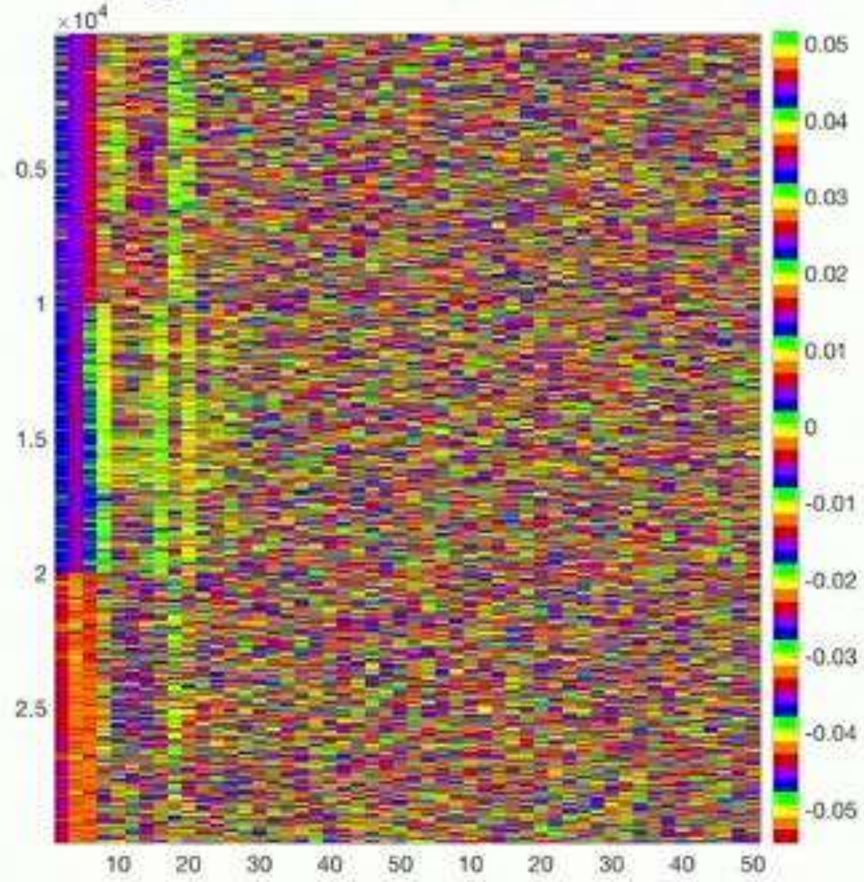

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Residual can be decomposed into two terms

$$r(\boldsymbol{\theta}) := f(\boldsymbol{\theta},\boldsymbol{X}) - \boldsymbol{y} = \underbrace{f(\boldsymbol{\theta},\boldsymbol{X}) - \bar{\boldsymbol{y}}}_{\text{Residual w.r.t. true labels}} + \underbrace{\bar{\boldsymbol{y}} - \boldsymbol{y}}_{corruption}$$

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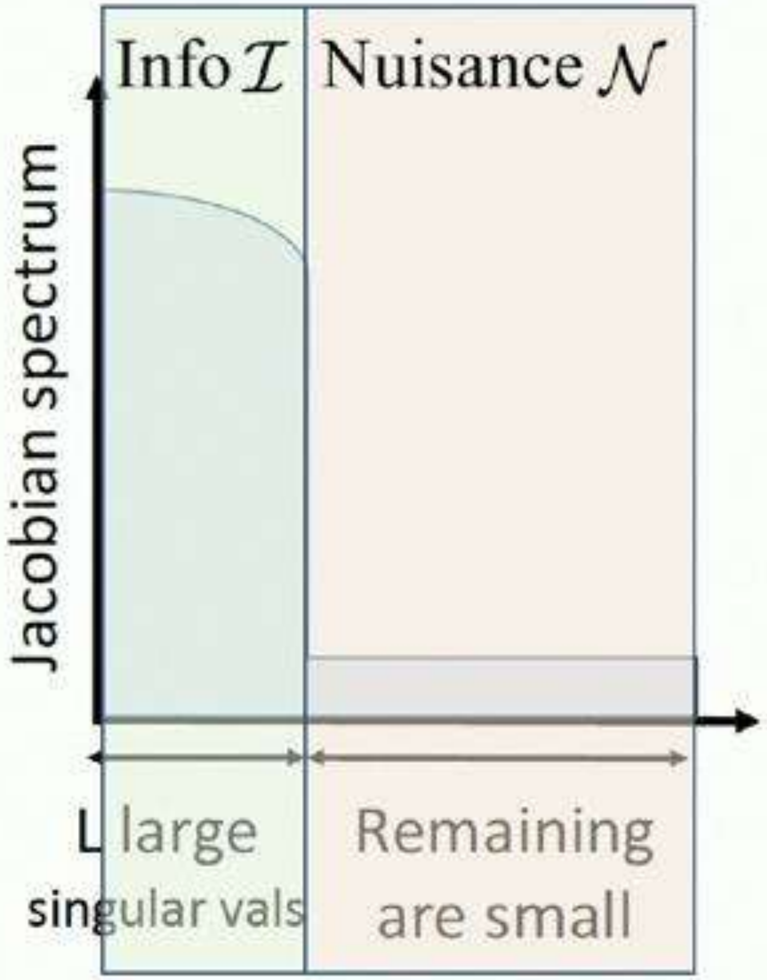

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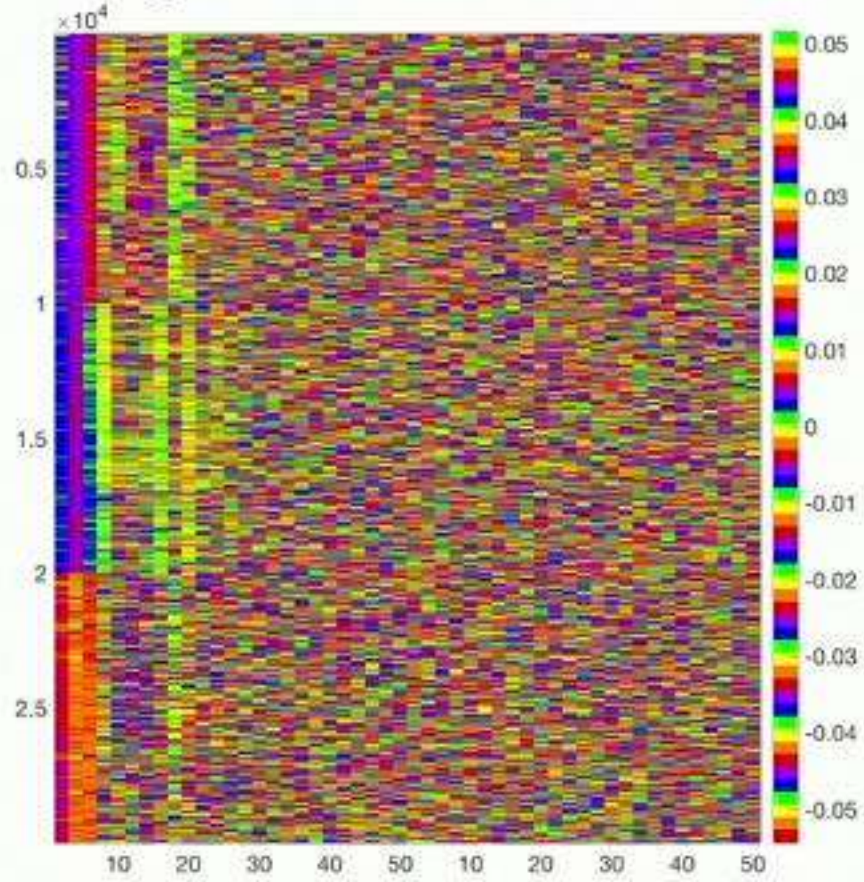

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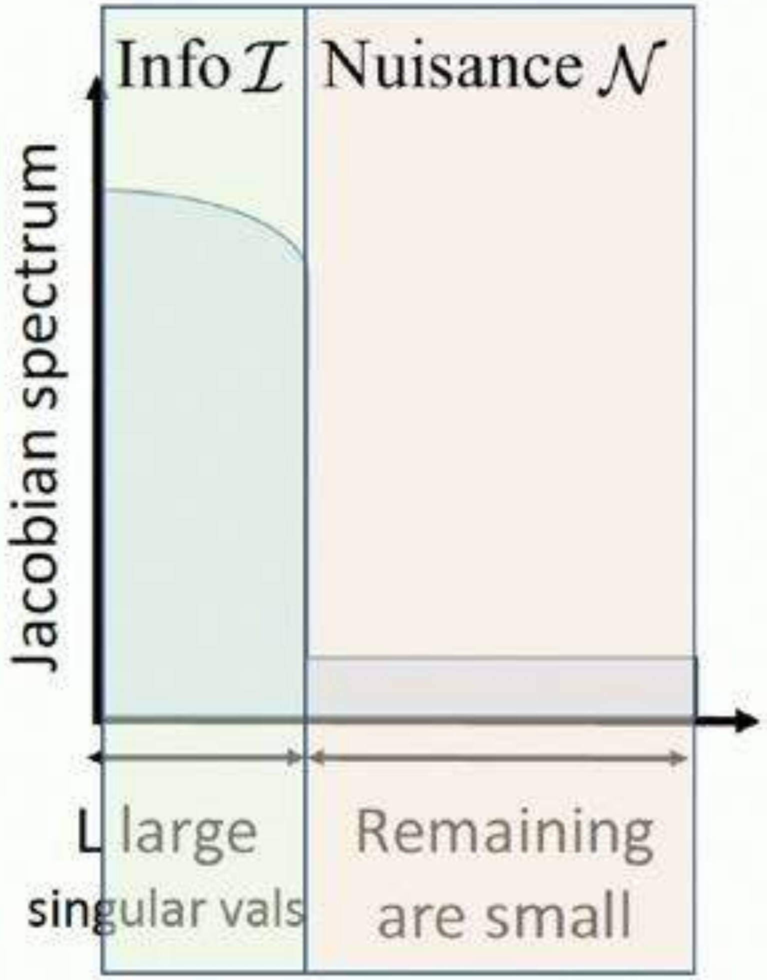

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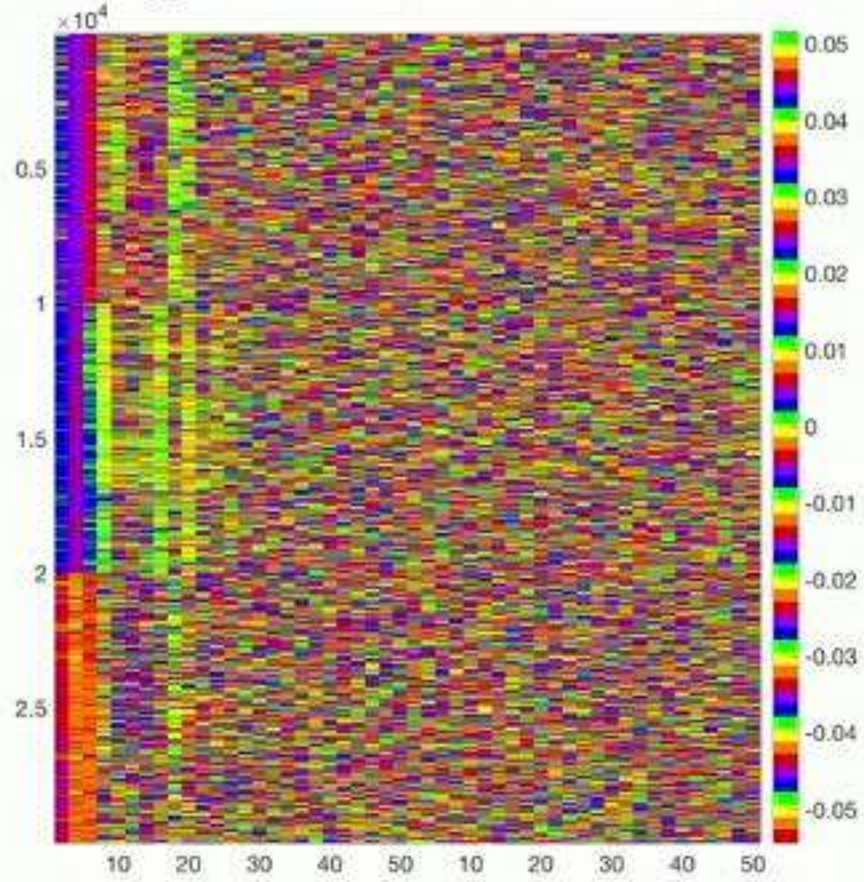

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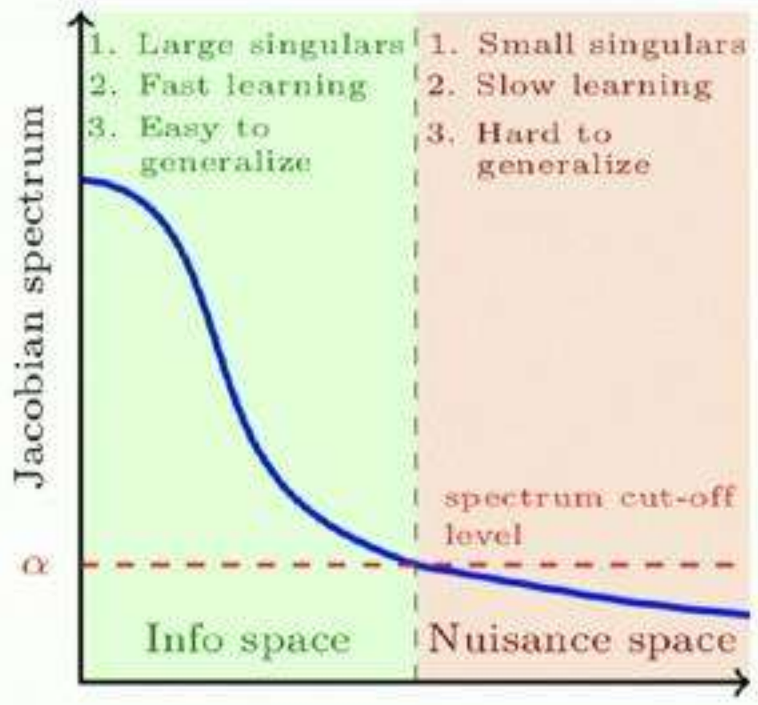
- Residual w.r.t. true labels falls mostly onto $\mathcal{I}$ and quickly goes to zero
- Diffuseness $\Rightarrow$ corruption $\boldsymbol{y} - \bar{\boldsymbol{y}}$ falls mostly onto $\mathcal{N}$ and slowly goes to zero

Conclusion

- Global optimization: With modest overparameterization neural networks can fit any data
- Generalization: Neural networks can predict well on test data when the prominent eigenvectors of the Jacobian are aligned with the labels
- Early stopping and robustness to label corruption: Neural networks are robust to sparse label corruption when the Jacobian is low-rank and prominent eigenvectors are diffused



Thanks!

Funding acknowledgment

the David & Lucile Packard FOUNDATION

ALFRED P. SLOAN FOUNDATION 1934

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UNITED STATES AIR FORCE

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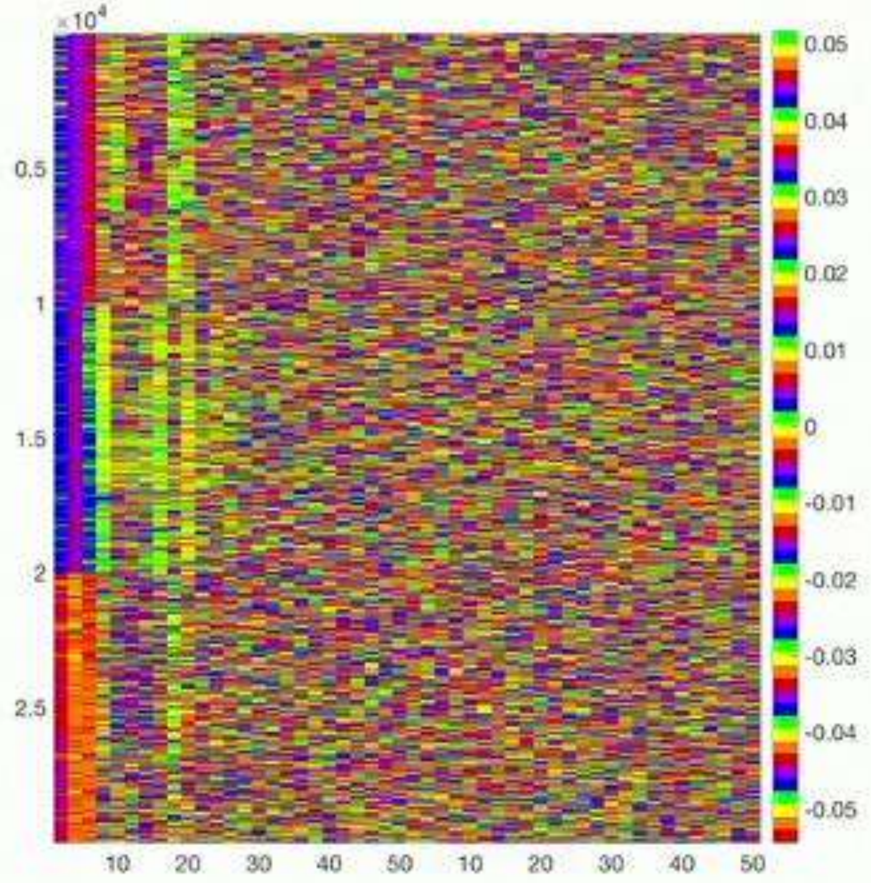
Google

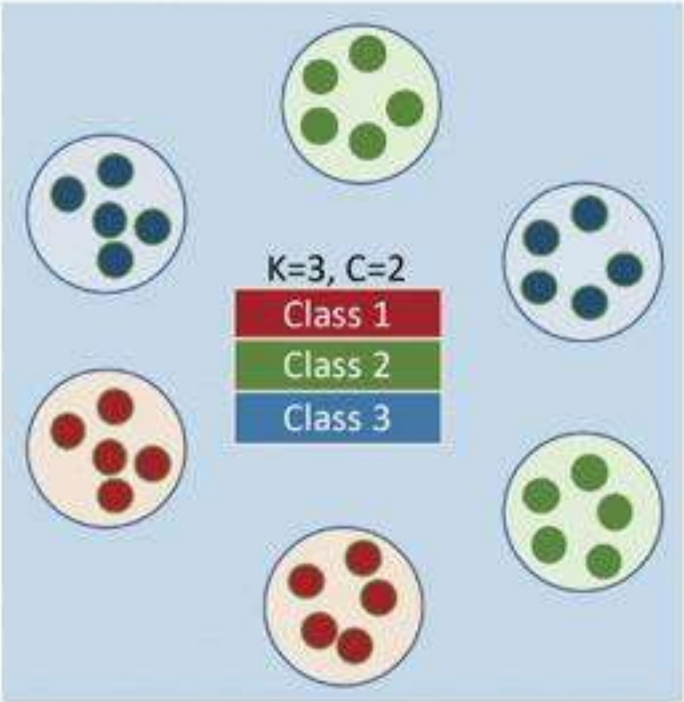
Key Idea II

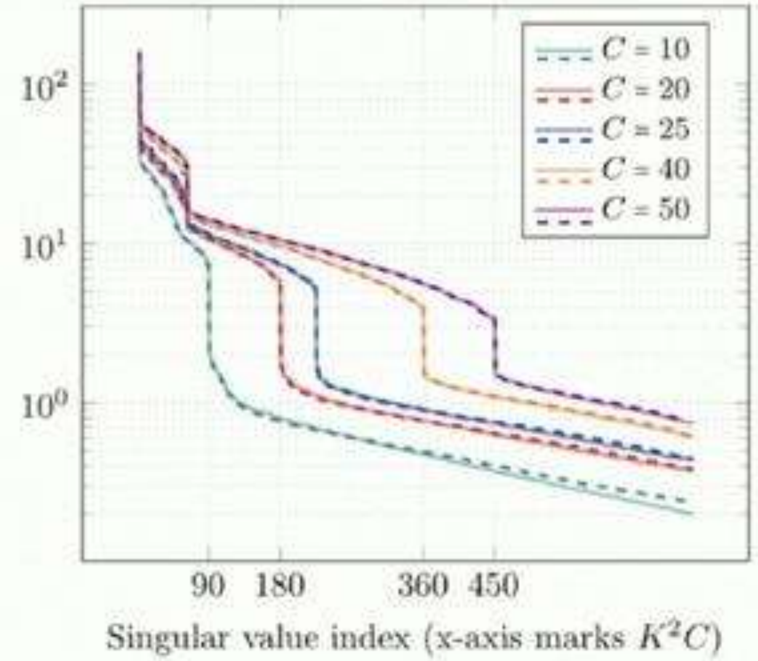
Prominent eigenvects of Jacobian are diffused



Concrete example: Gaussian Mixture Model (GMM)

Data set a GMM with K classes each containing C components per class with small σ^2





Theorem

With high probability

- *Jacobian has* K^2C *large singular values that grow* $\propto \sqrt{n}$
- *If* $k \gtrsim \Gamma^4 K^8 C^4$ *after* $T \propto \Gamma K^2 C$ *iterations,*

$$misclass\,(f(\boldsymbol{W}_T)) \lesssim \Gamma\sqrt{\frac{K^2C}{n}} + e^{-\Gamma}$$

Geometry of Optimization and Learning: Rich vs Kernel Inductive Bias

Nati Srebro (TTIC)

Based on work with **Suriya Gunasekar** (TTIC→MSR), Behnam Neyshabur (TTIC→Google),
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Last Time On...

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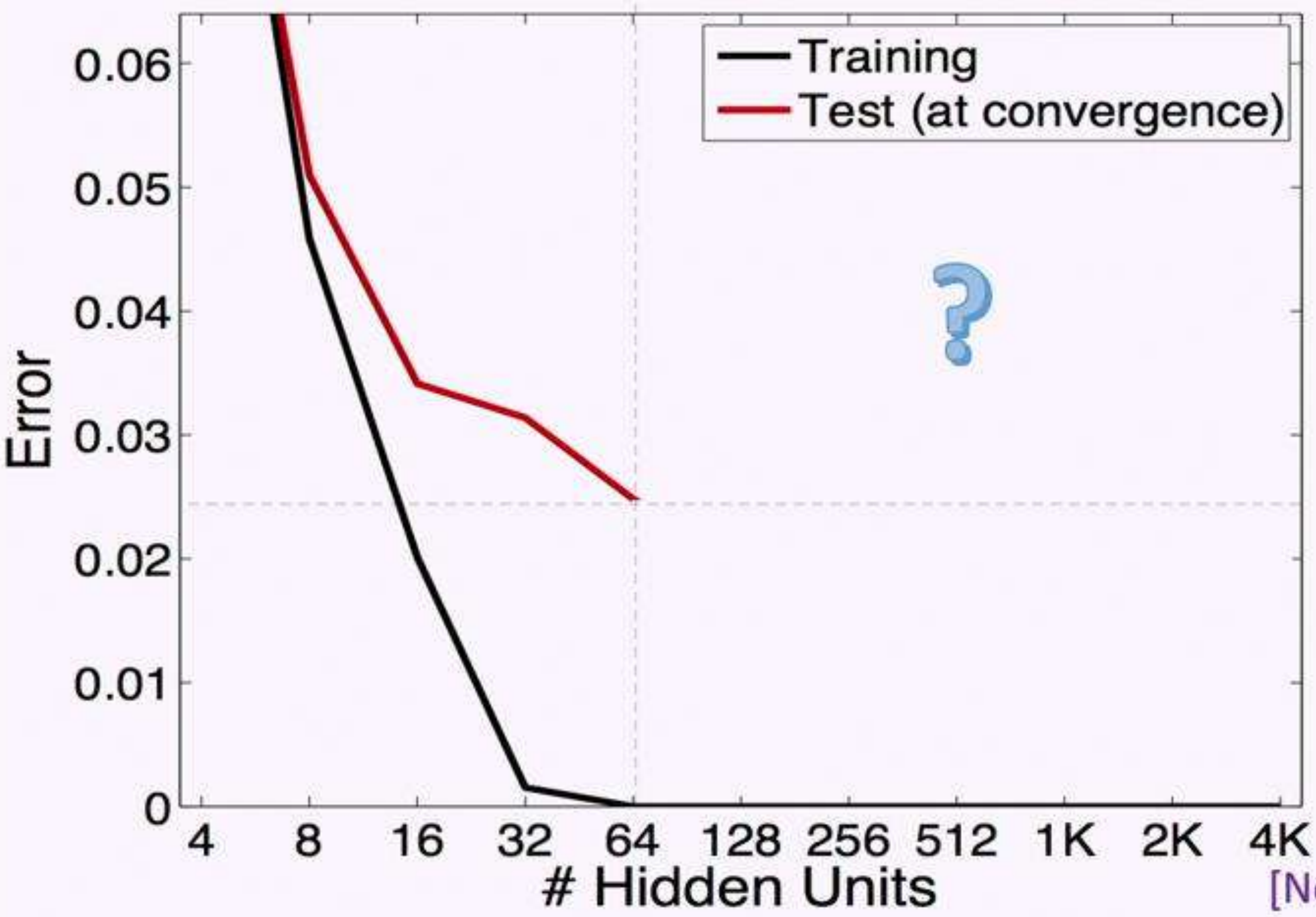
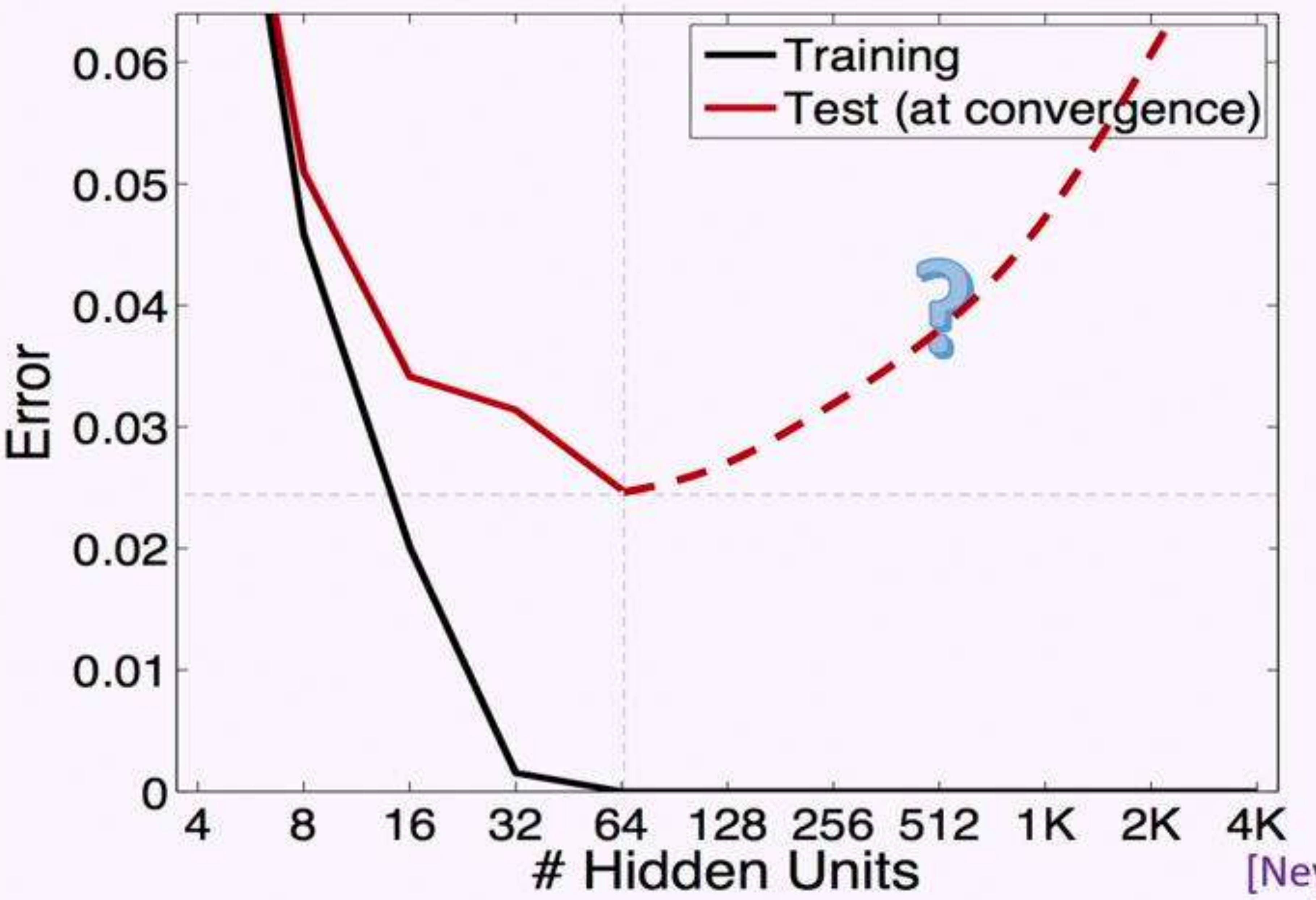


[Neyshabur Tomioka S ICLR'15]



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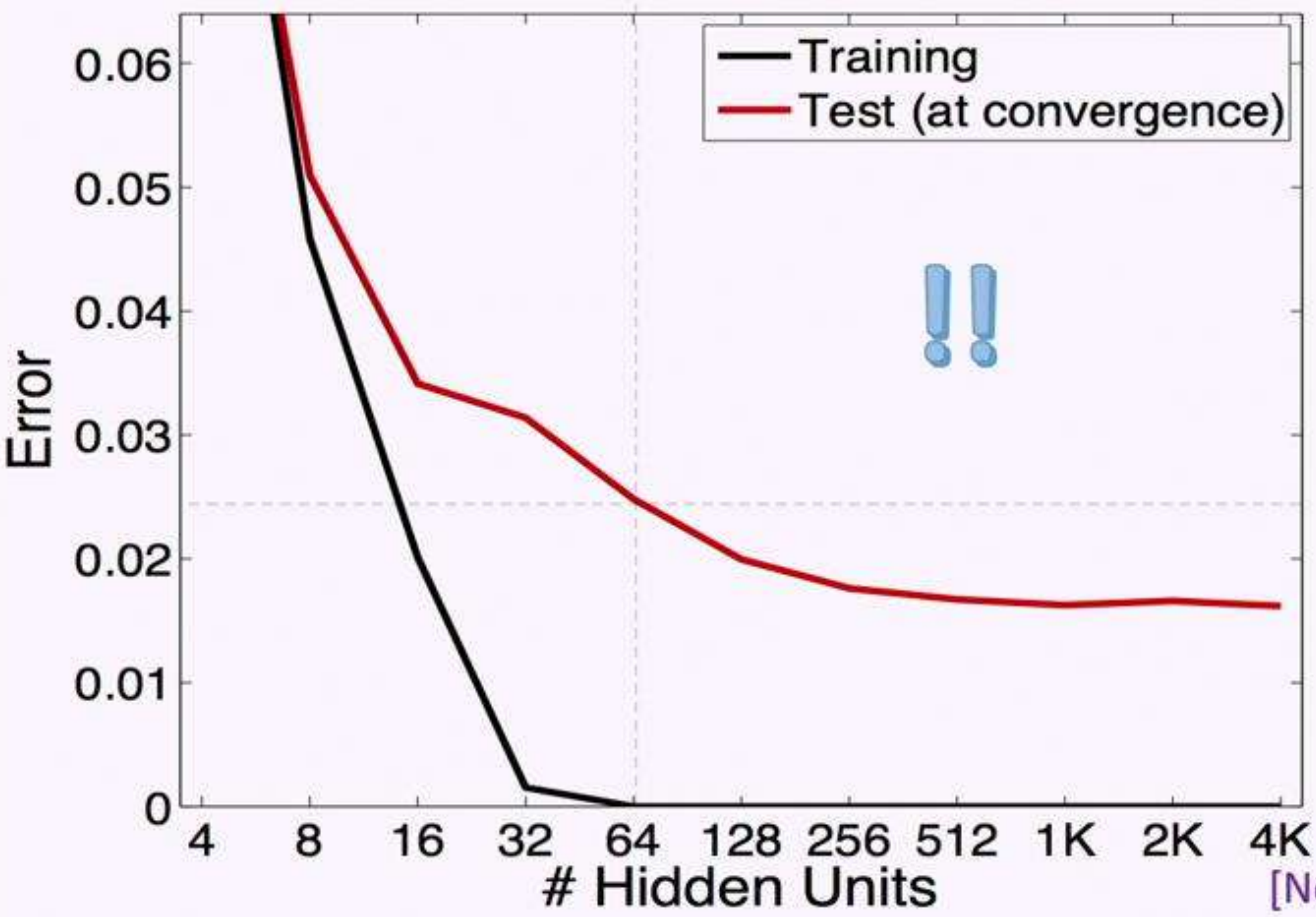

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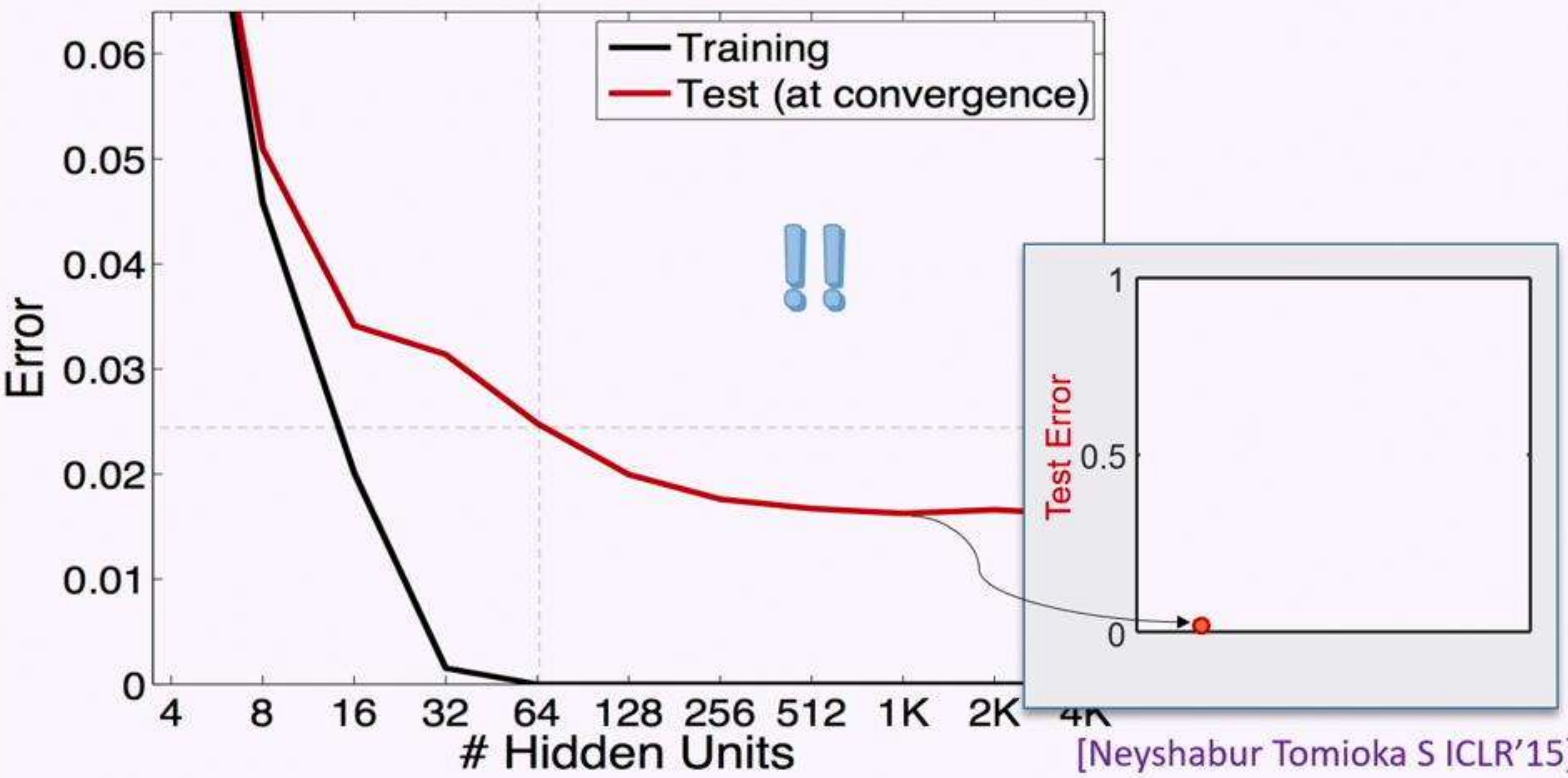

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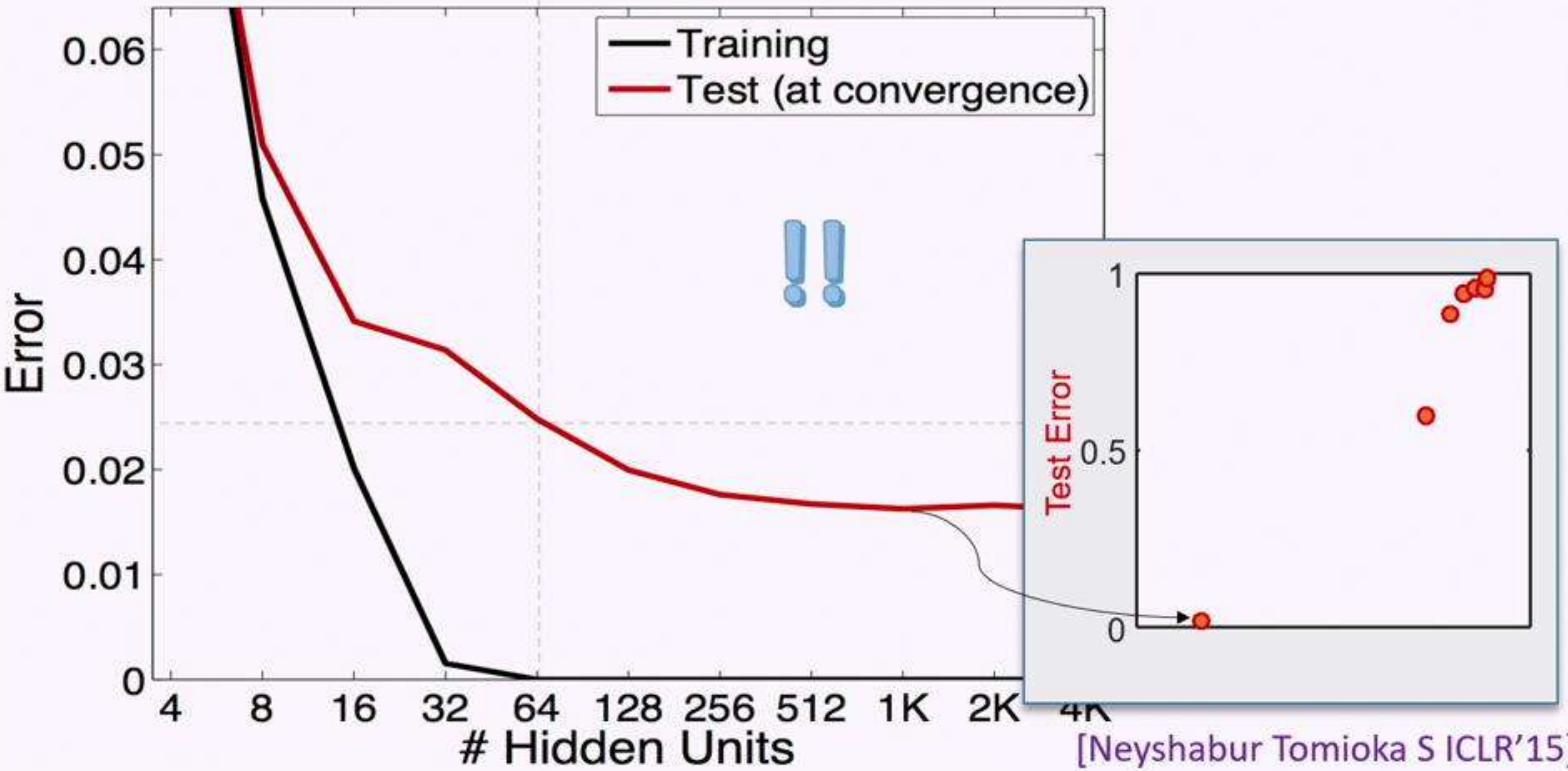
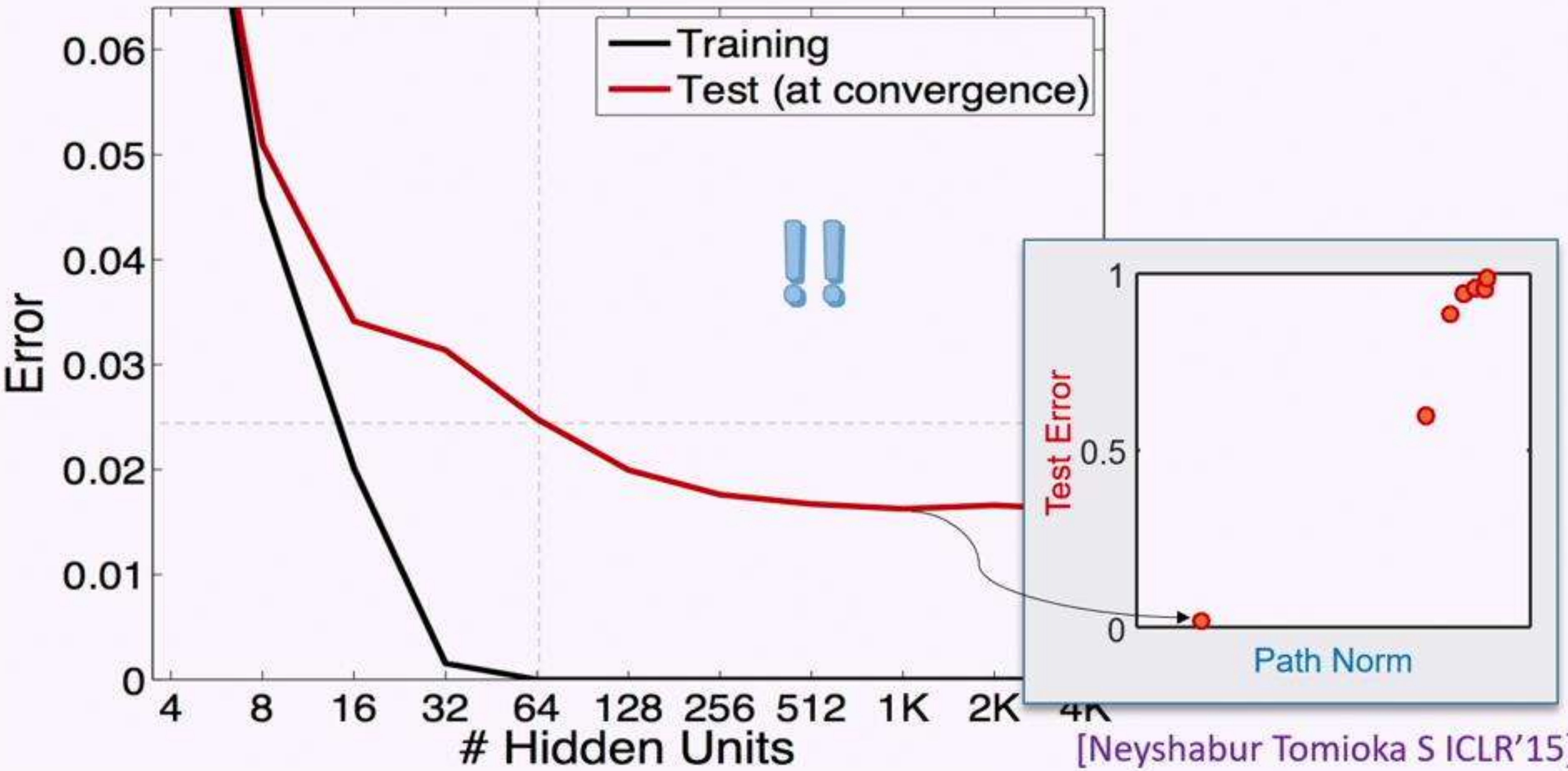


[Neyshabur Tomioka S ICLR'15]

For valid generalization, the size of the weights is more important than the size of the network

1997

Peter L. Bartlett



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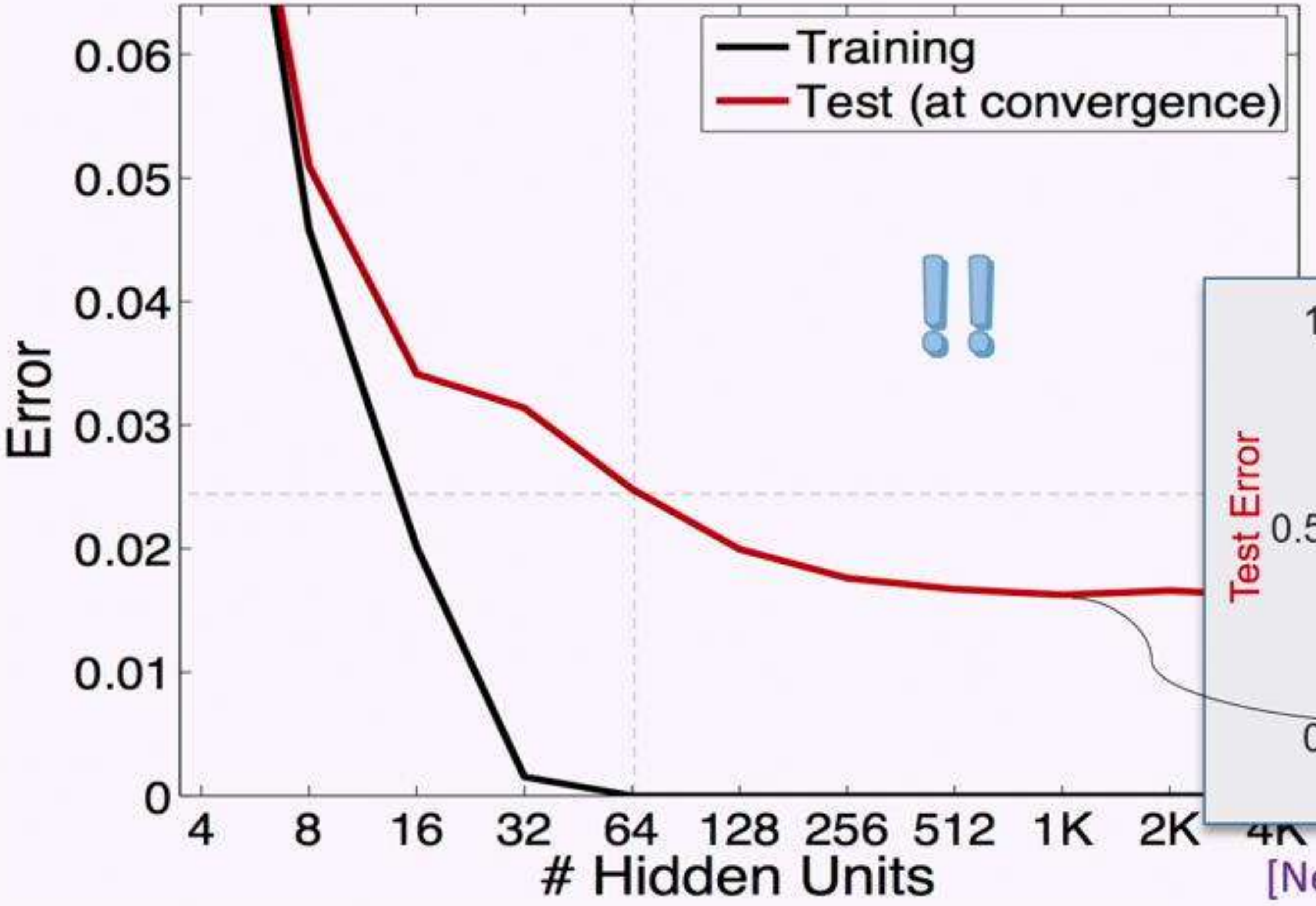

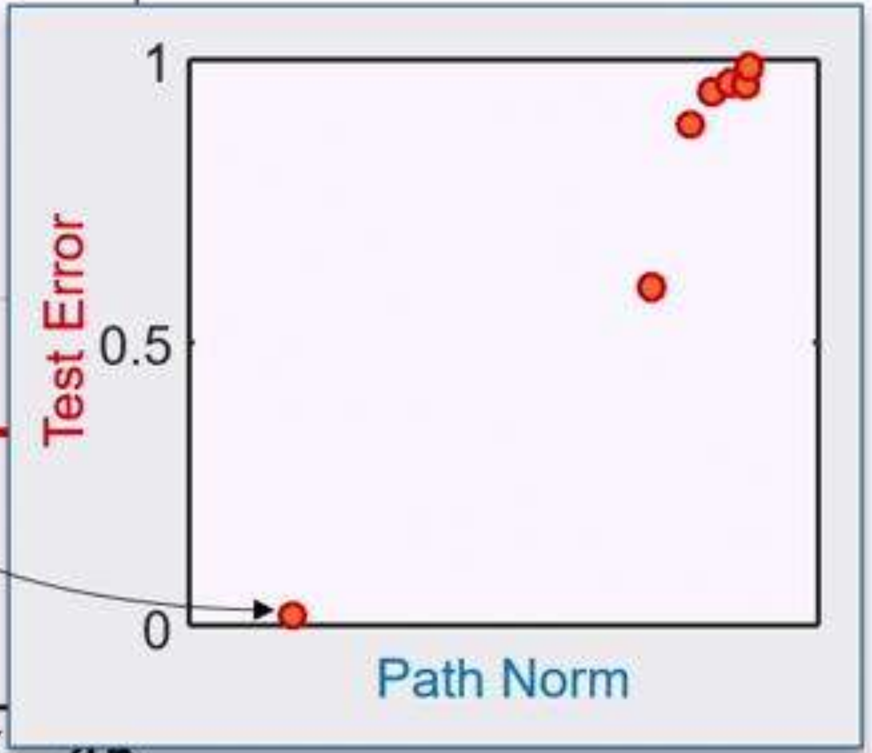

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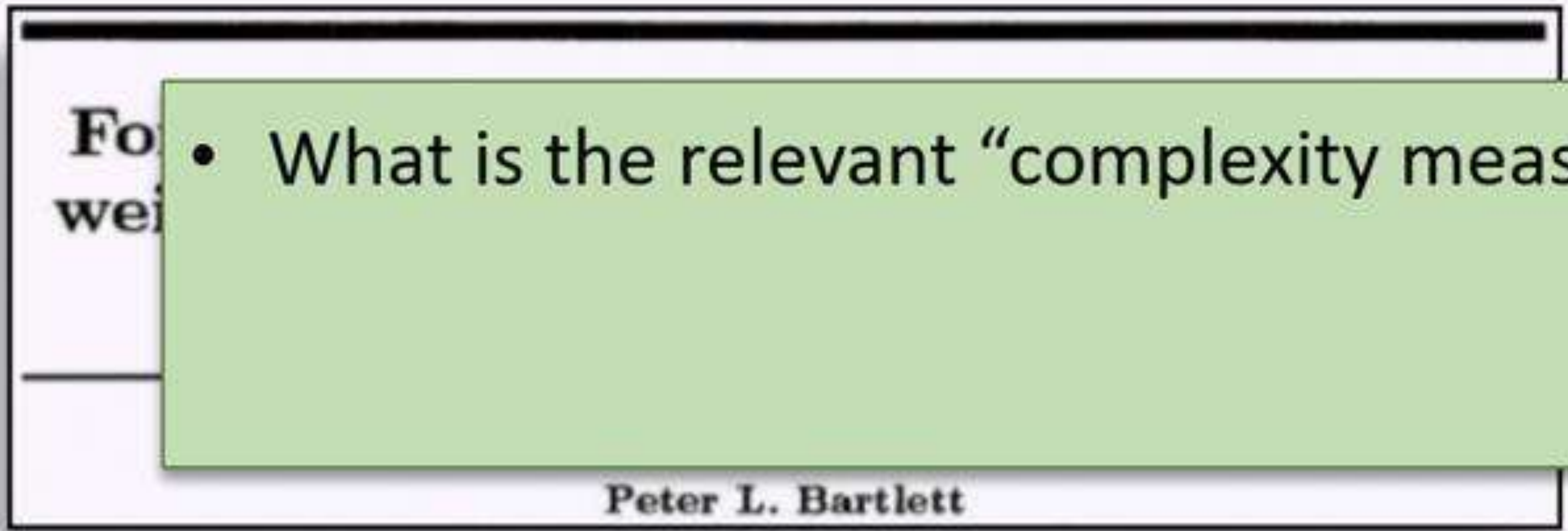
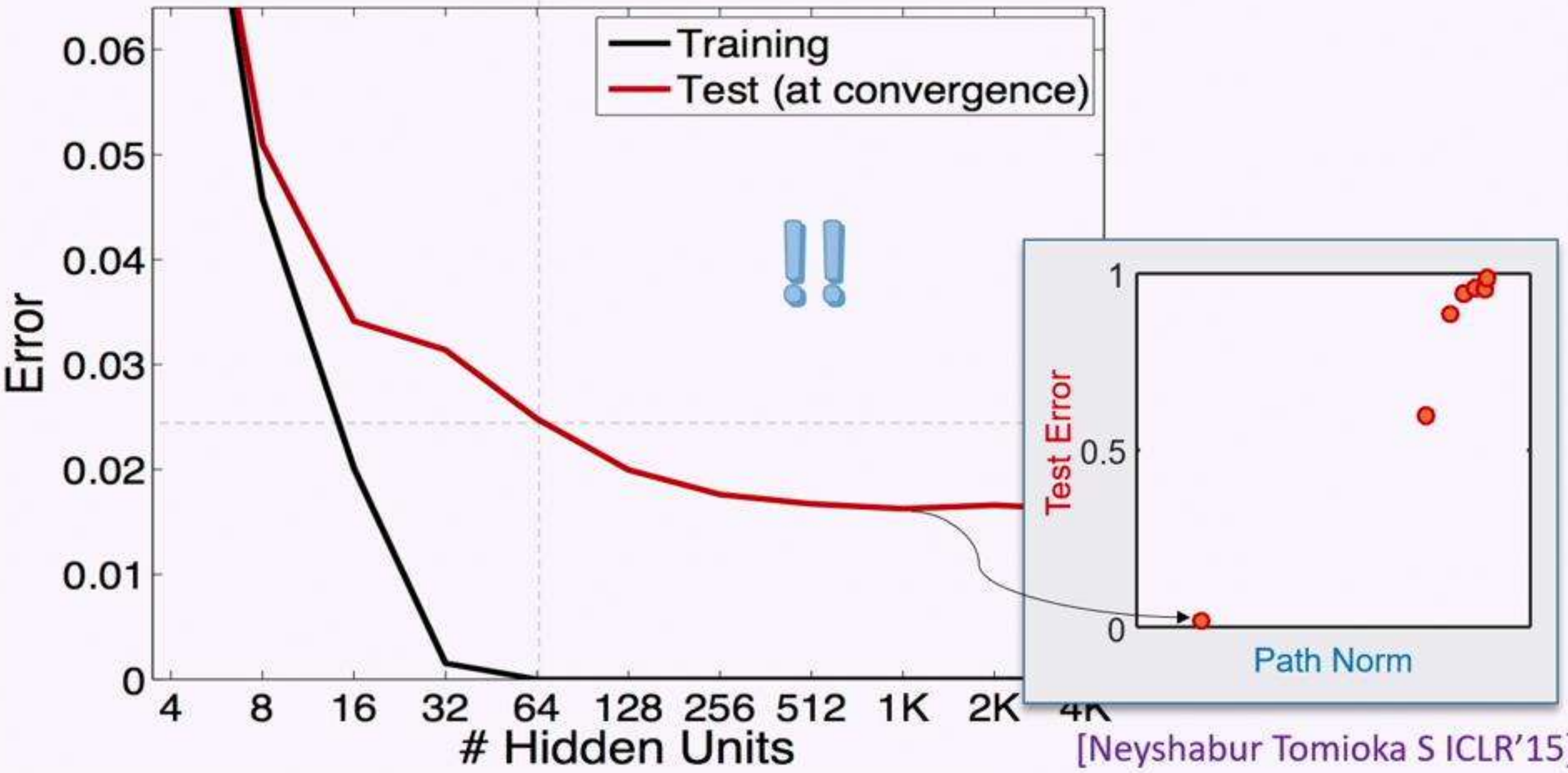


- What is the relevant “complexity measure” (eg norm)?



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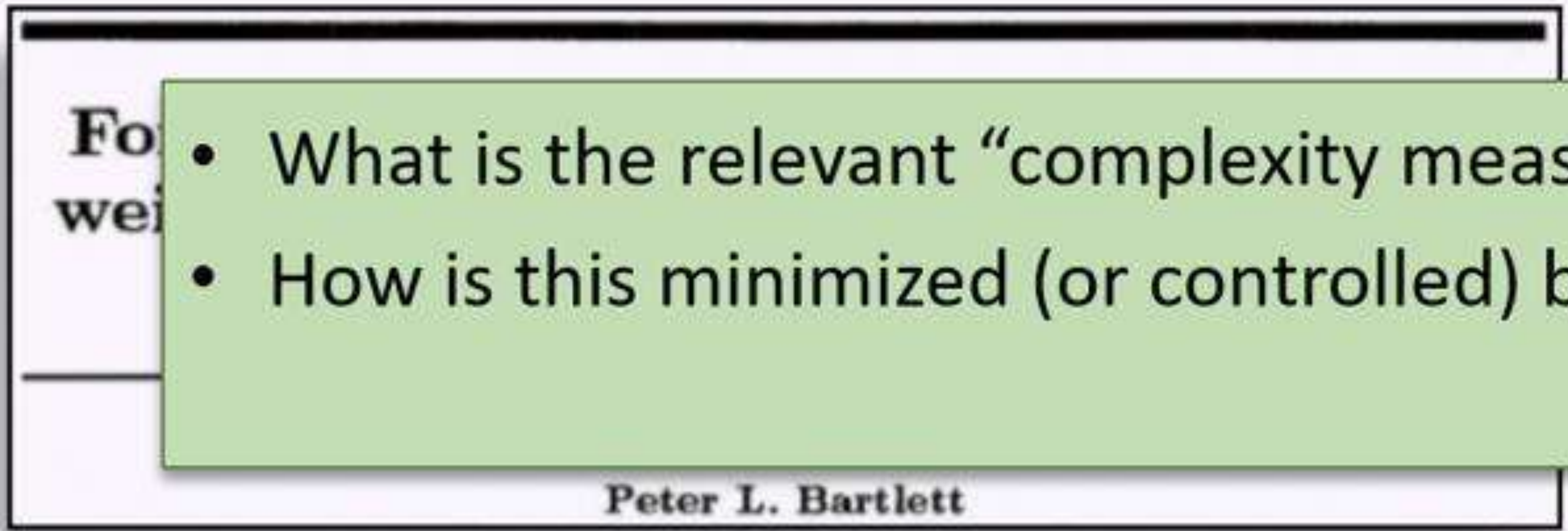

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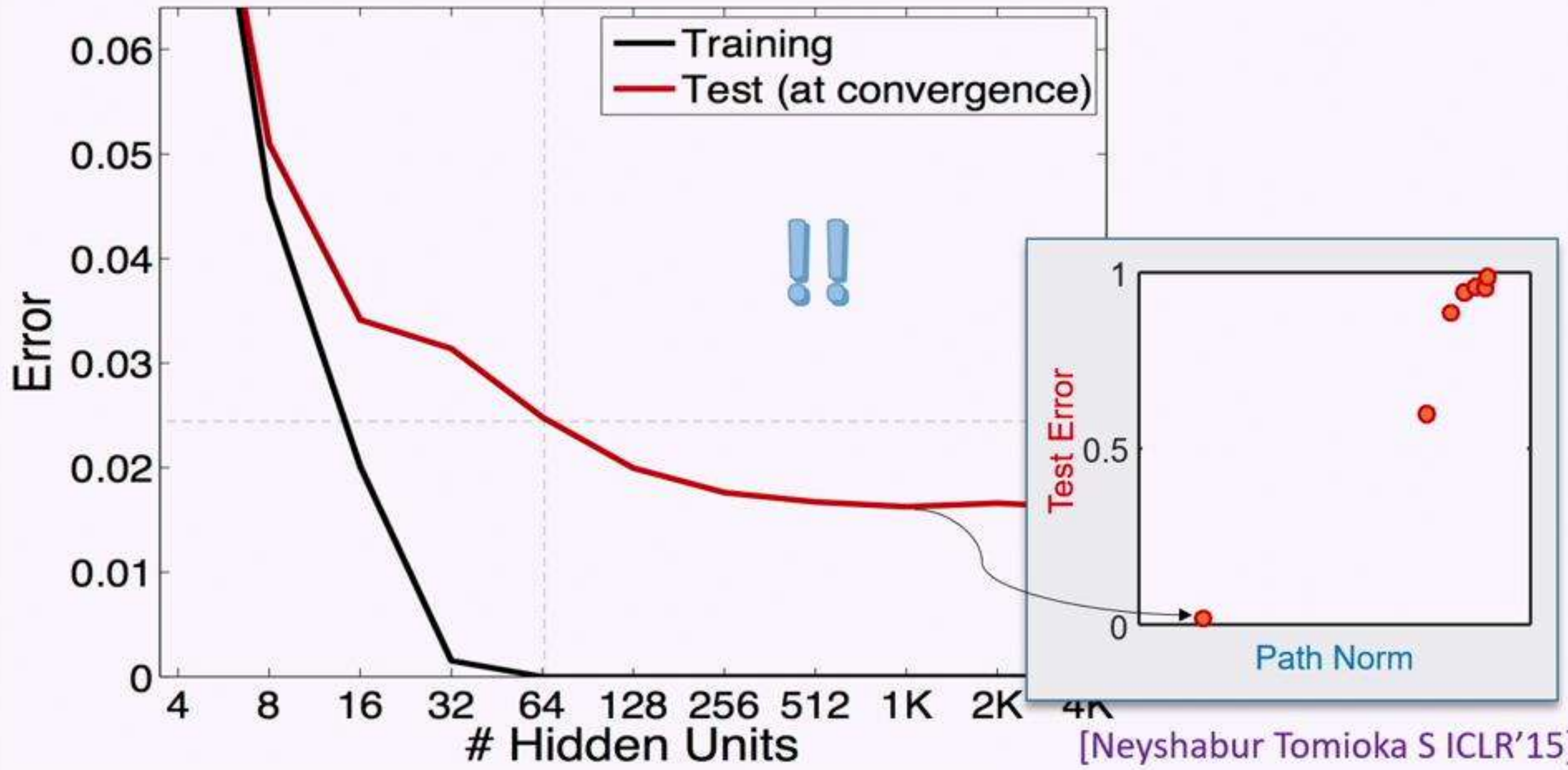

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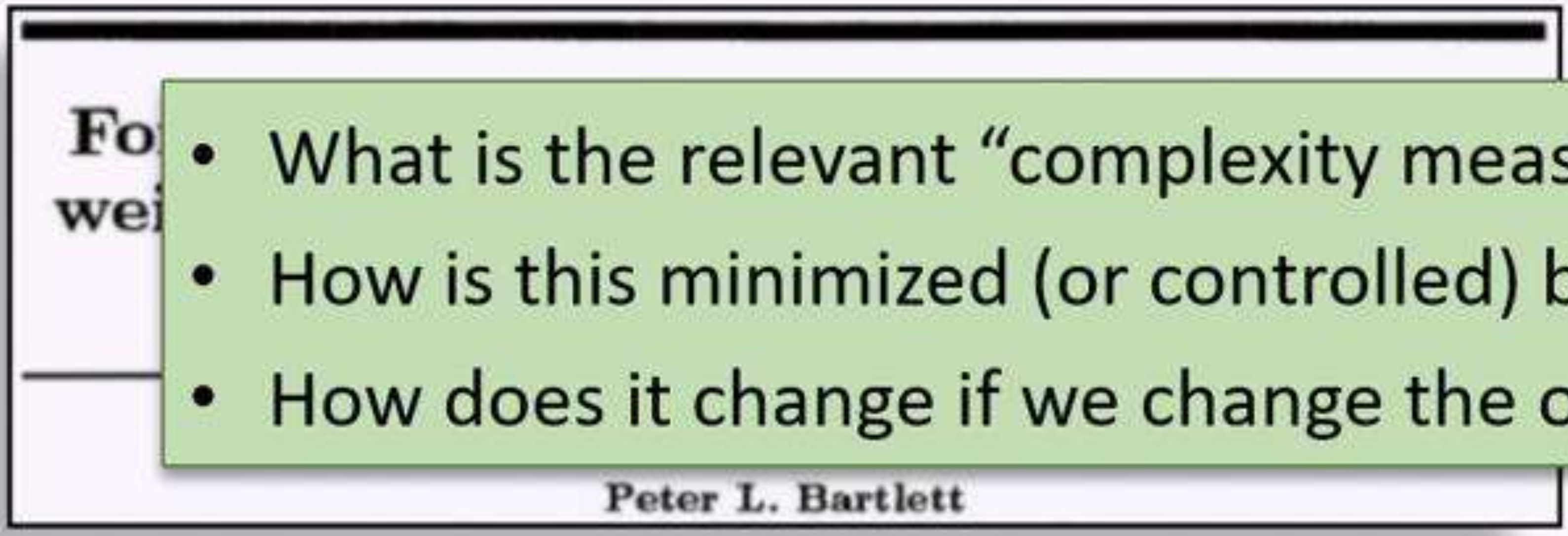
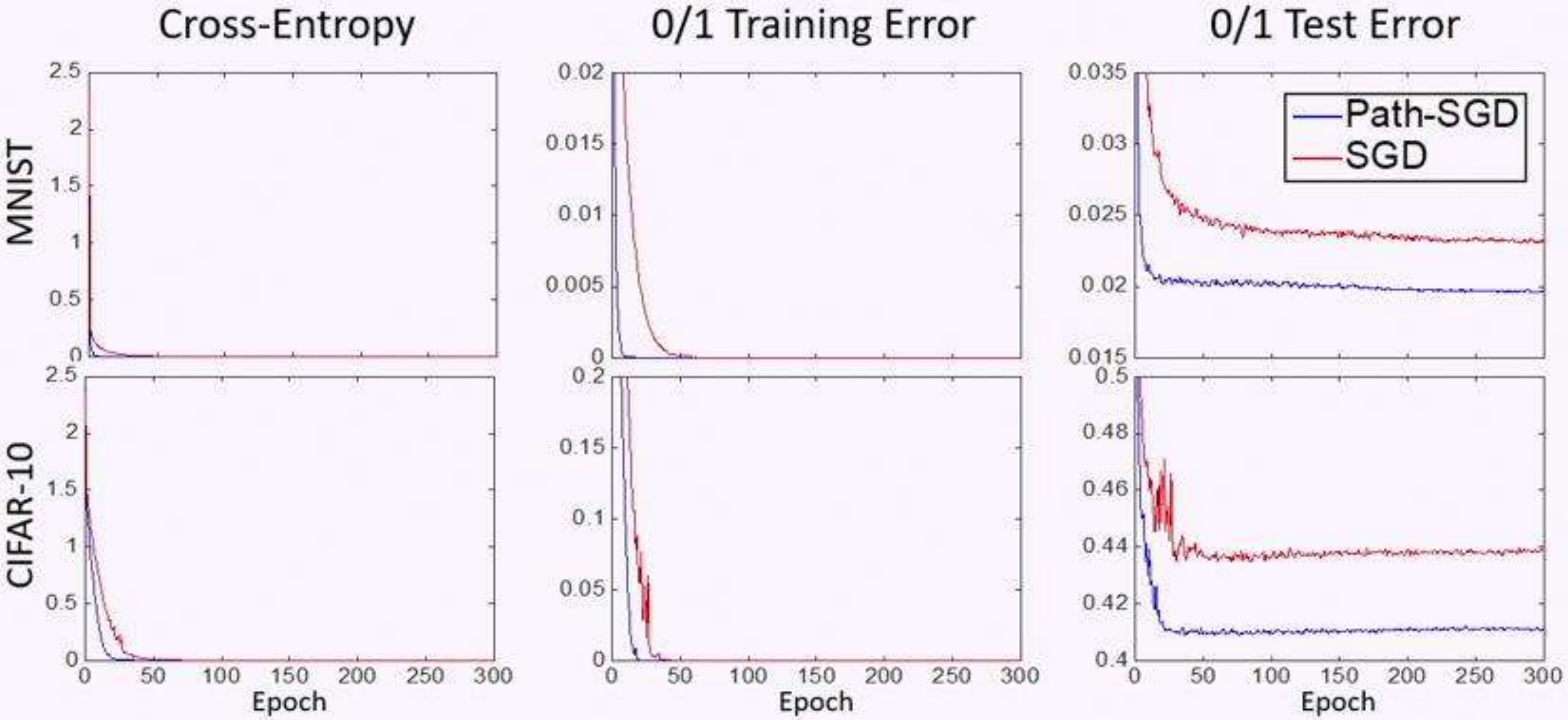
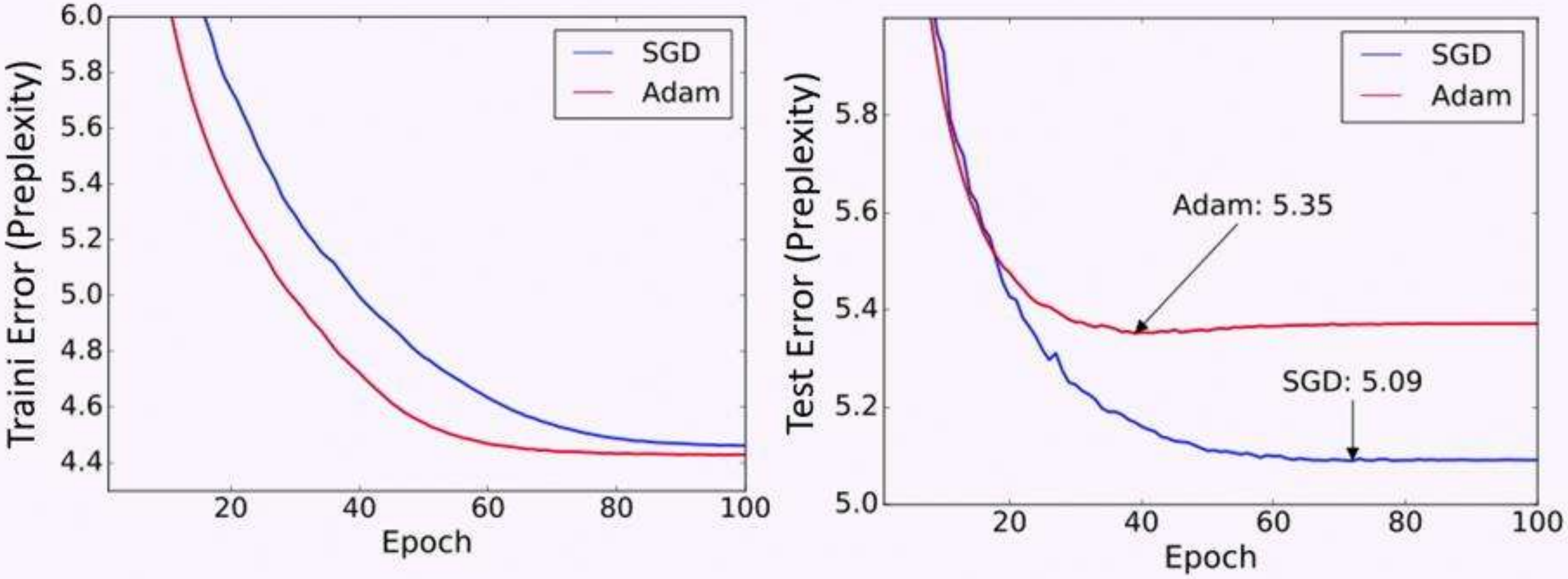

Fo
wei
Peter L. Bartlett

- What is the relevant "complexity measure" (eg norm)?
- How is this minimized (or controlled) by the opt algorithm?
- How does it change if we change the opt algorithm?



[Neyshabur Salakhudtinov S NIPS'15]

SGD vs ADAM



Results on Penn Treebank using 3-layer LSTM

[Wilson Roelofs Stern S Recht, “The Marginal Value of Adaptive Gradient Methods in Machine Learning”, NIPS’17]

The Deep Recurrent Residual Boosting Machine

Joe Flow, DeepFace Labs

Section 1: Introduction

We suggest a new amazing architecture and loss function that is great for learning. All you have to do to learn is fit the model on your training data

Section 2: Learning Contribution: our model

The model class h_w is amazing. **Our learning method is:**

$$\mathbf{arg\,min}_{\boldsymbol{w}} \frac{\mathbf{1}}{\boldsymbol{m}} \sum_{\boldsymbol{i}=\mathbf{1}}^{\boldsymbol{m}} \boldsymbol{loss}(\boldsymbol{h}_{\boldsymbol{w}}(\boldsymbol{x}); \boldsymbol{y}) \qquad (*)$$

Section 3: Optimization

This is how we solve the optimization problem (*): [...]

Section 4: Experiments

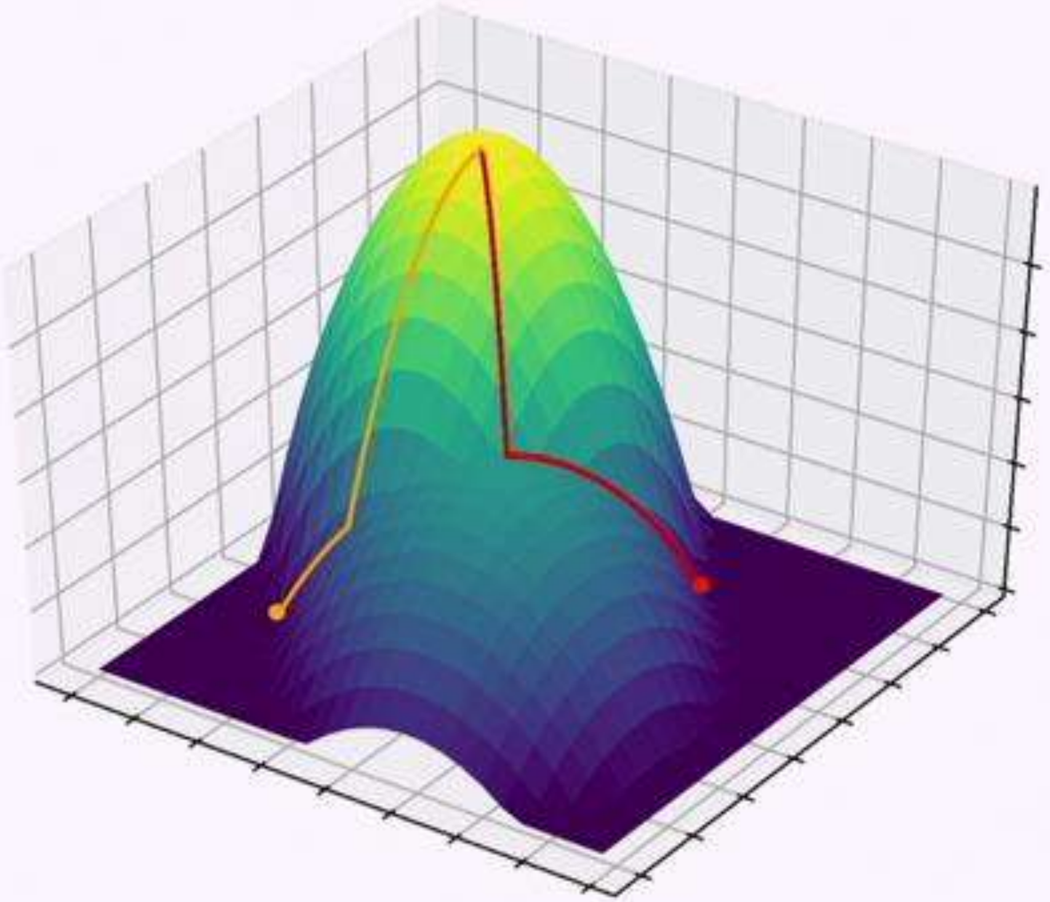
It works!

Different optimization algorithm

➔ Different bias in optimum reached

➔ Different Inductive bias

➔ Different generalization properties



Need to understand optimization alg. not just as reaching ***some*** (global) optimum, but as reaching a ***specific*** optimum

Effect of Optimization Geometry

- Gradient descent on underspecified linear regression $\min_w \|Xw - y\|^2$

  ➔ $w \to \arg\min_{Xw=y} \|w\|_2$

Effect of Optimization Geometry

- Gradient descent on underspecified linear regression $\min_w \|Xw - y\|^2$

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- Natural Gradient/Mirror Descent w.r.t. $\Psi(w)$ on $\min_w \|Xw - y\|^2$

  ➔ $w \to \arg\min_{Xw=y} \Psi(w)$

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  with init→0 and stepsize→0
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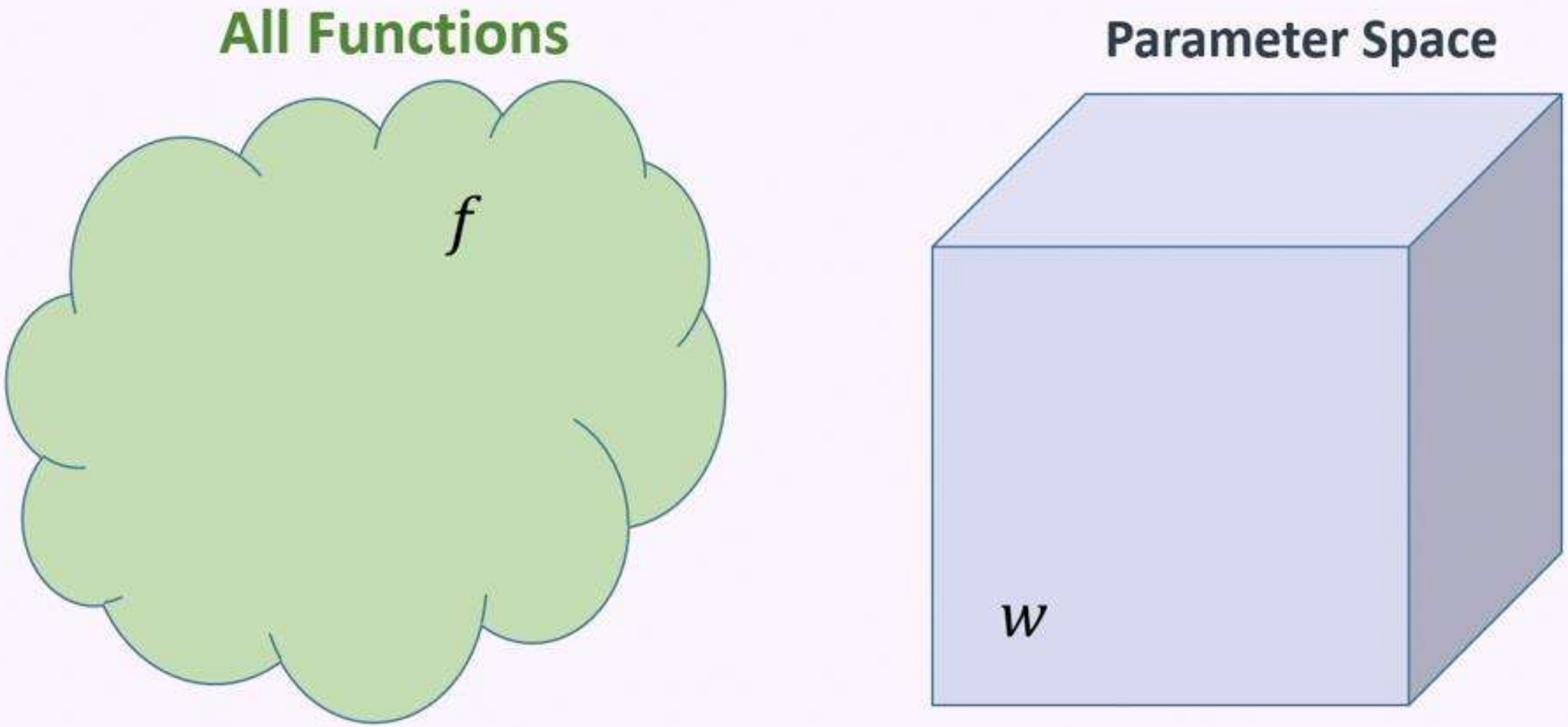
$$\max\left(\int |\boldsymbol{f''}| \boldsymbol{dx} \ , |f'(-\infty) + f'(+\infty)| \right)$$

[Savarese Evron Soudry S 2019]



Optimization Geometry and hence Inductive Bias effected by:

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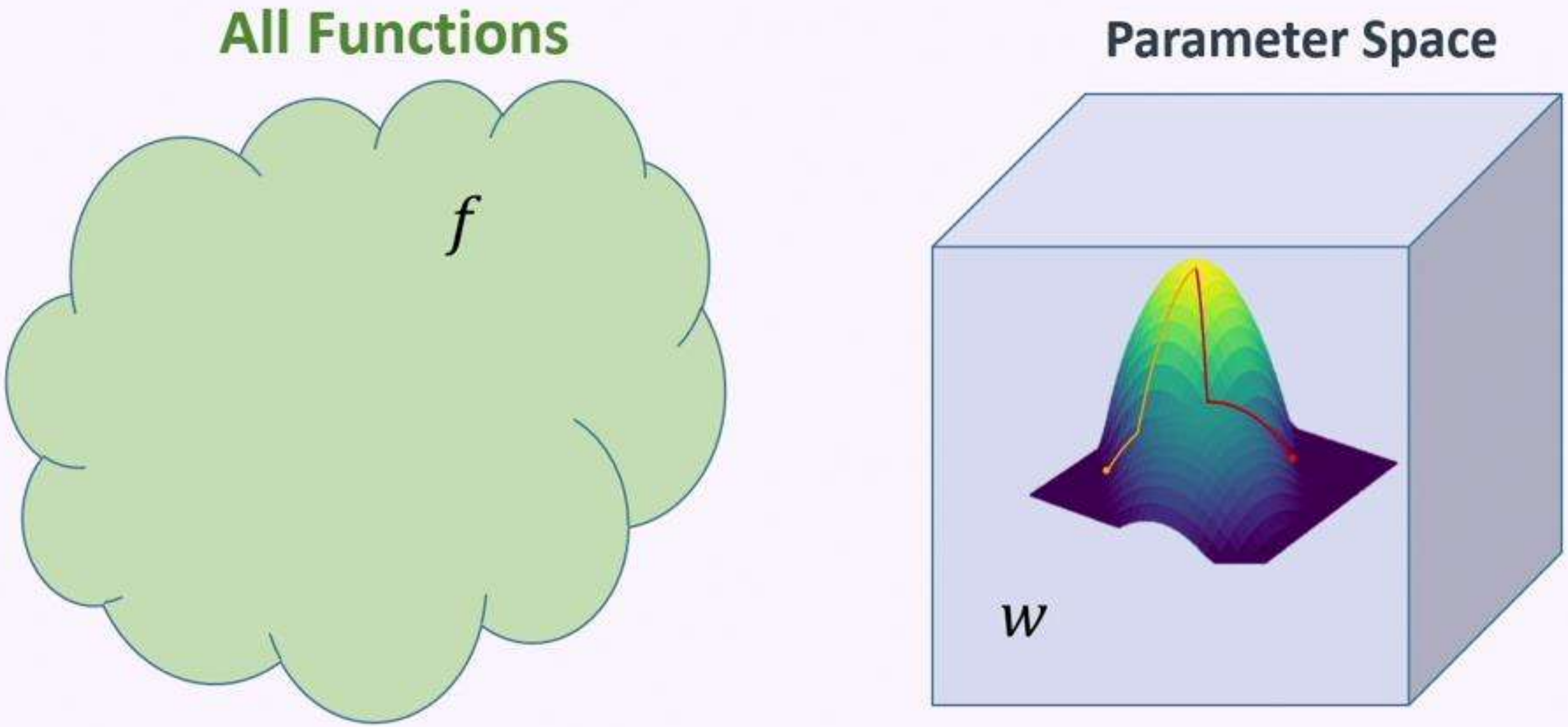

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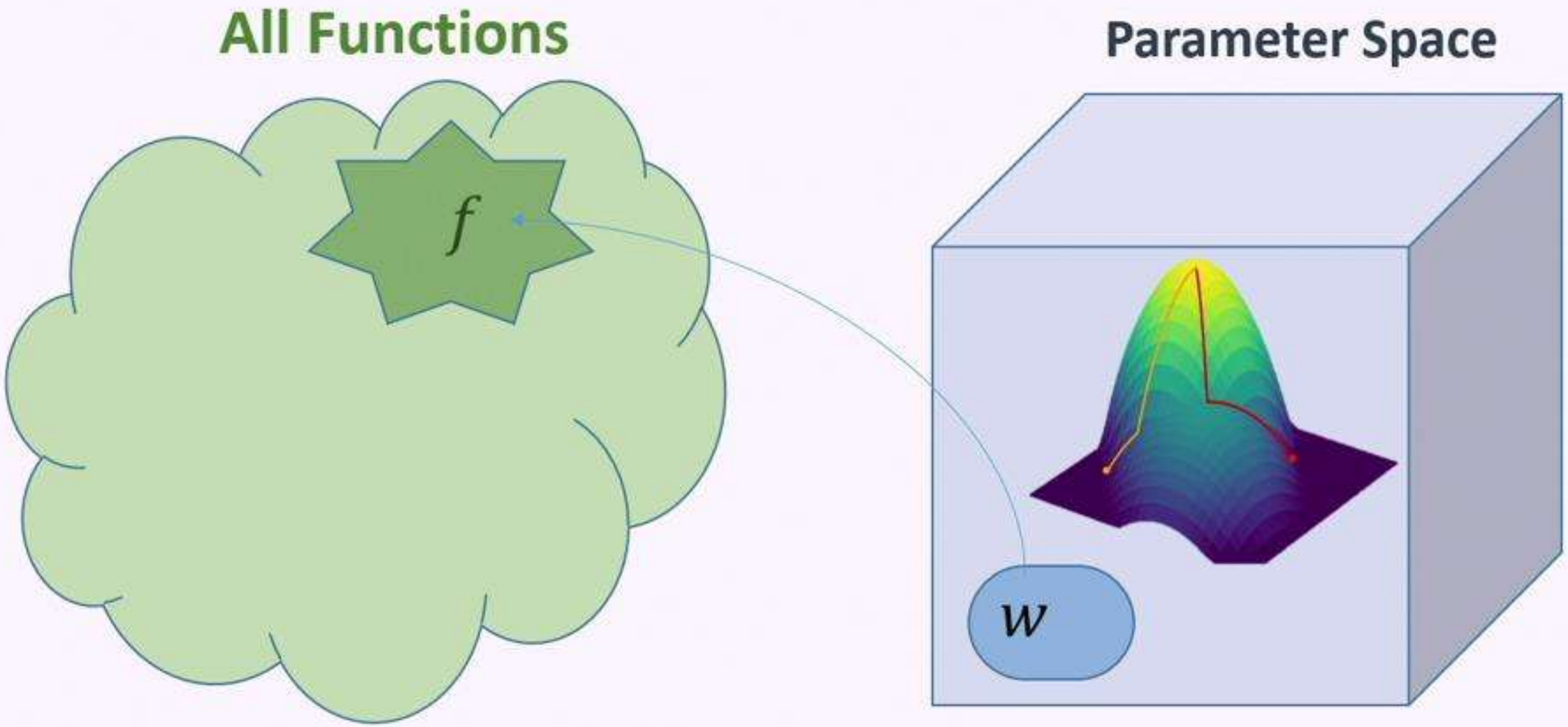

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$f(w, x) = h_w(x) =$ prediction on x with params ("weights") w

Linear models: $f(w, x) = \langle \beta_w, x \rangle$ $F(w) = \beta_w$

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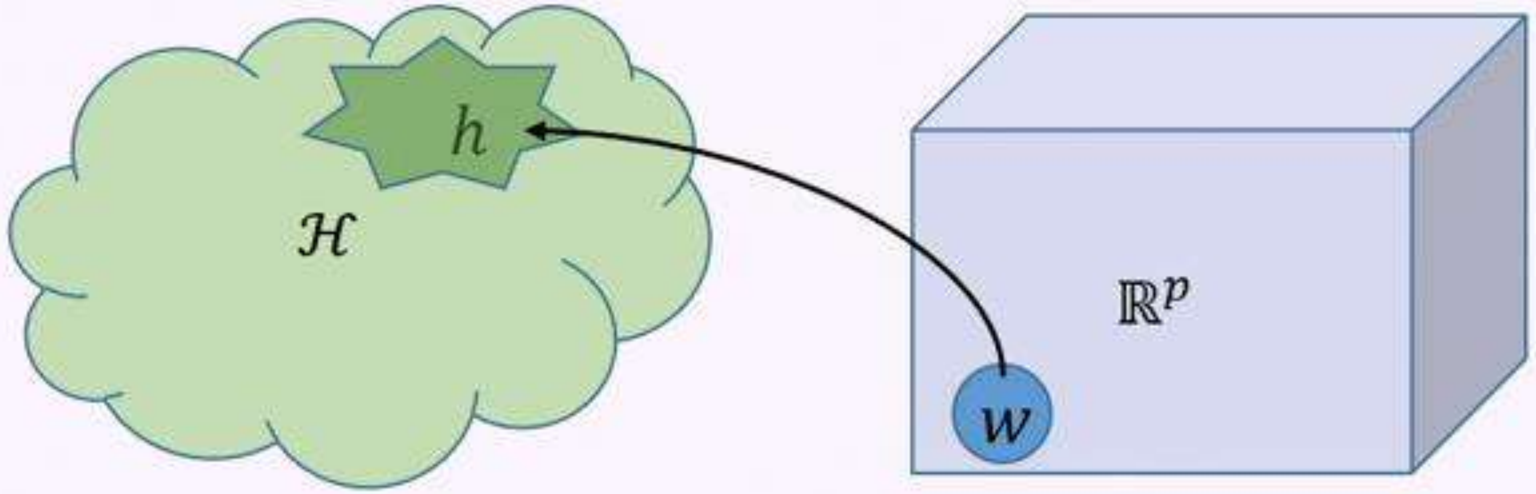

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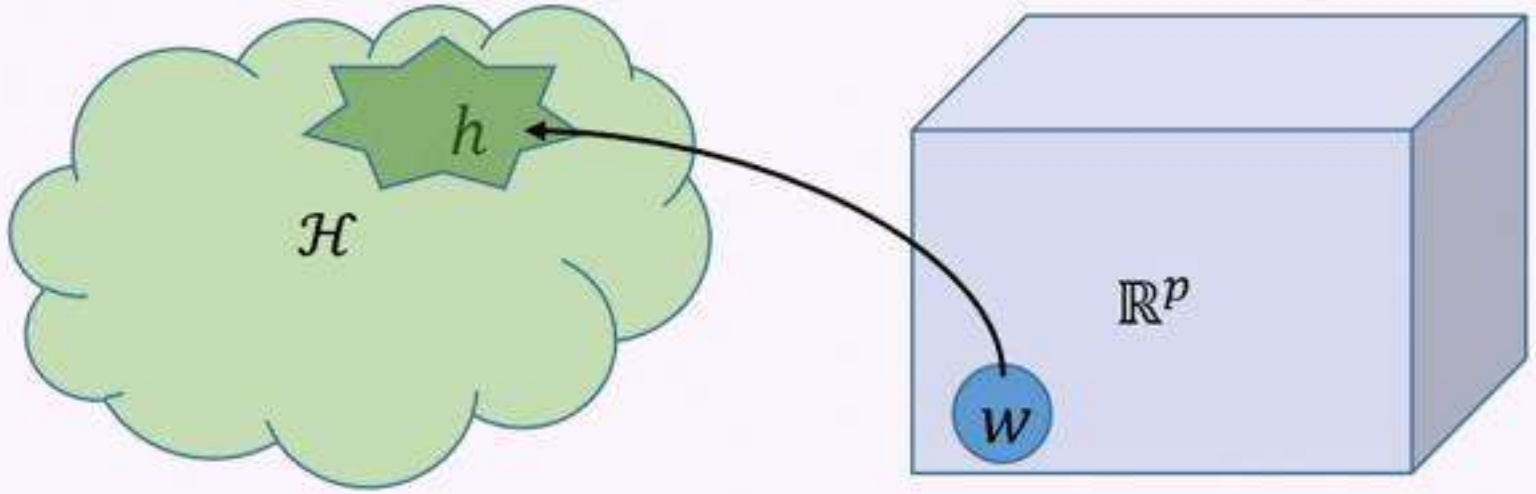

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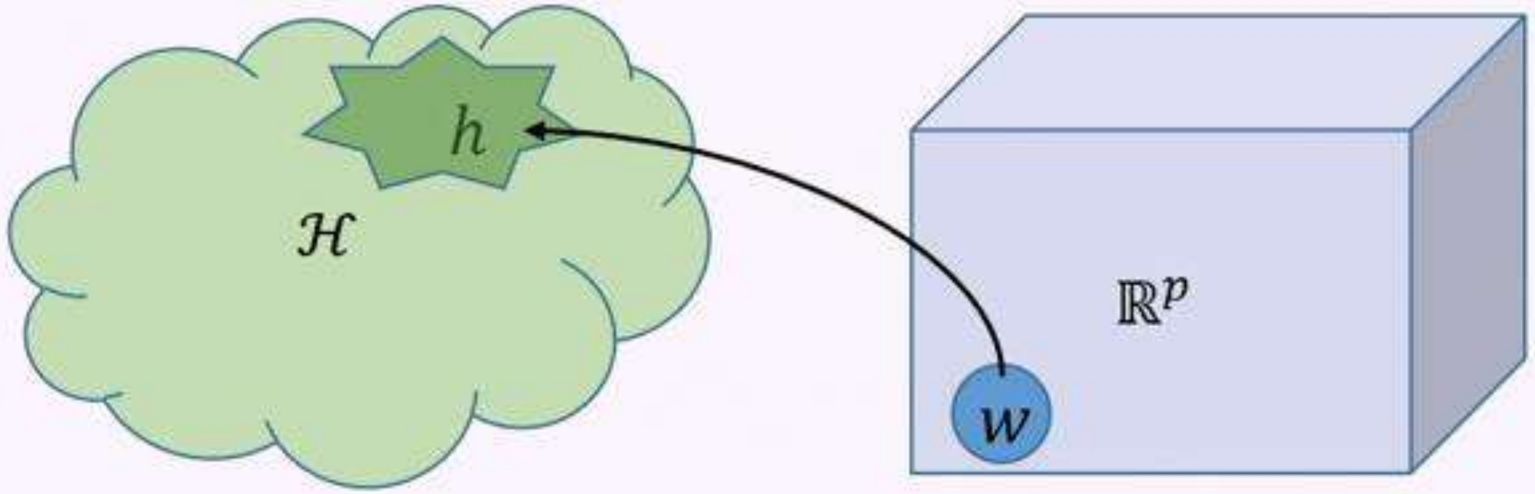

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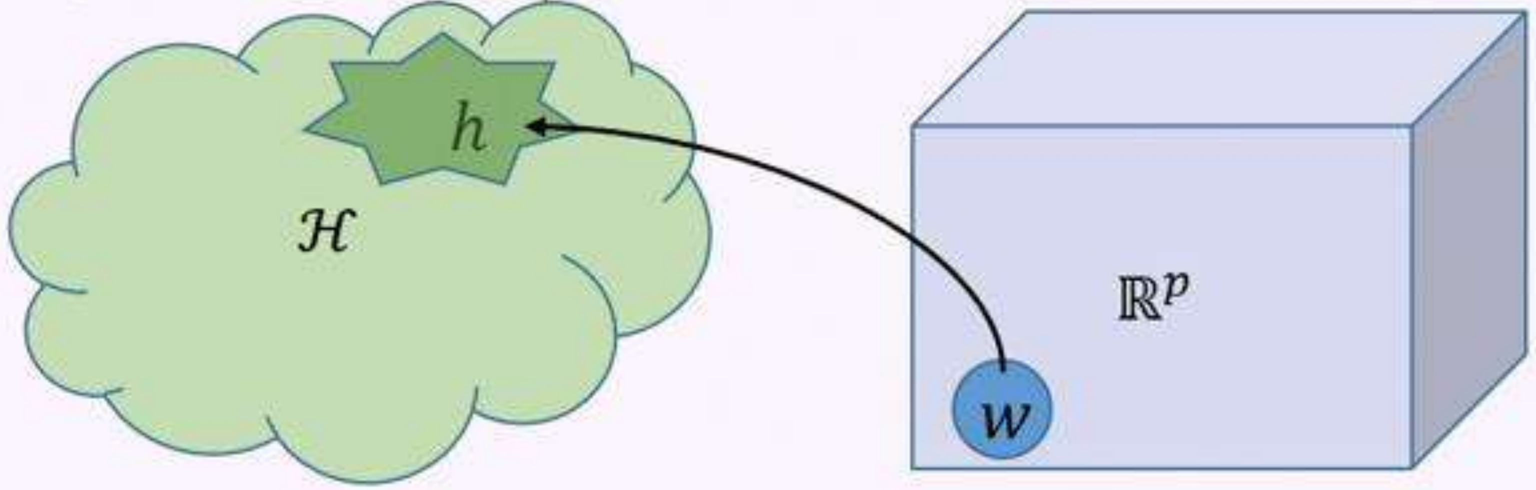

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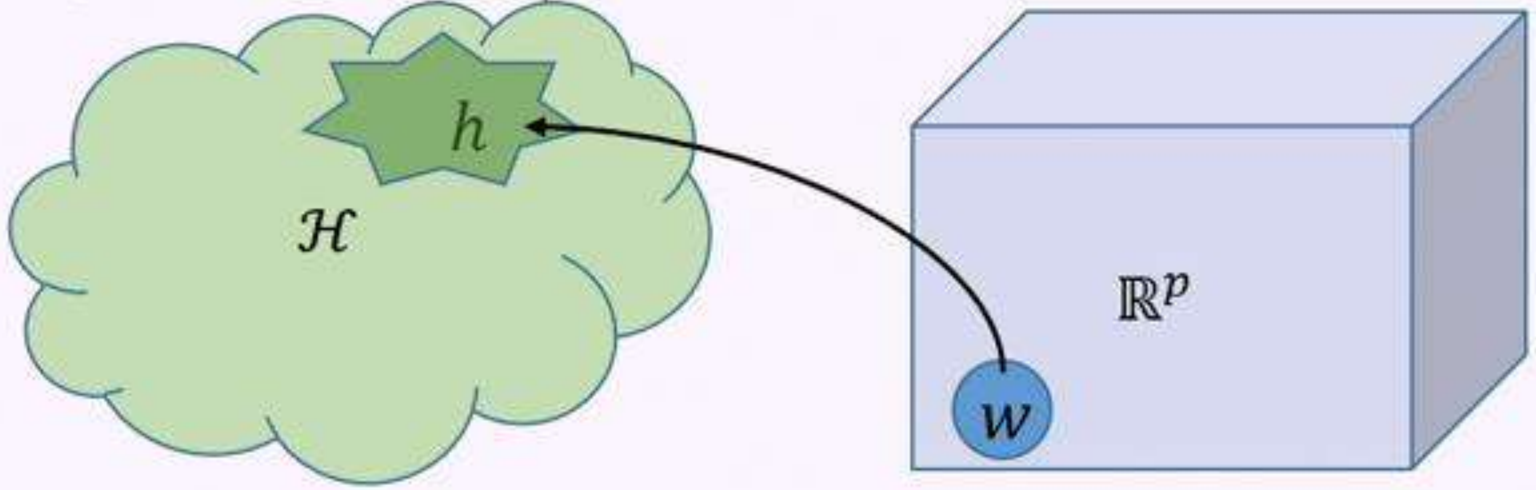

Consider gradient descent w.r.t. logistic loss $L_s(w) = \sum_i g\big(y_i f(w, x_i)\big)$ (or other loss exp-tail loss) on a D-homogenous model $f(w, x)$:

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If $L_s(w) \to 0$, with stepsize→0 (or finite but ensures convergence in direction):

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But need to be careful: f.o.s.p of **(*)** does ***not*** imply f.o.s.p of **(**)**

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- Maybe yes? Implicit bias given by $R(h) = \arg\min_{F(w)=h} \|w\|_2$?
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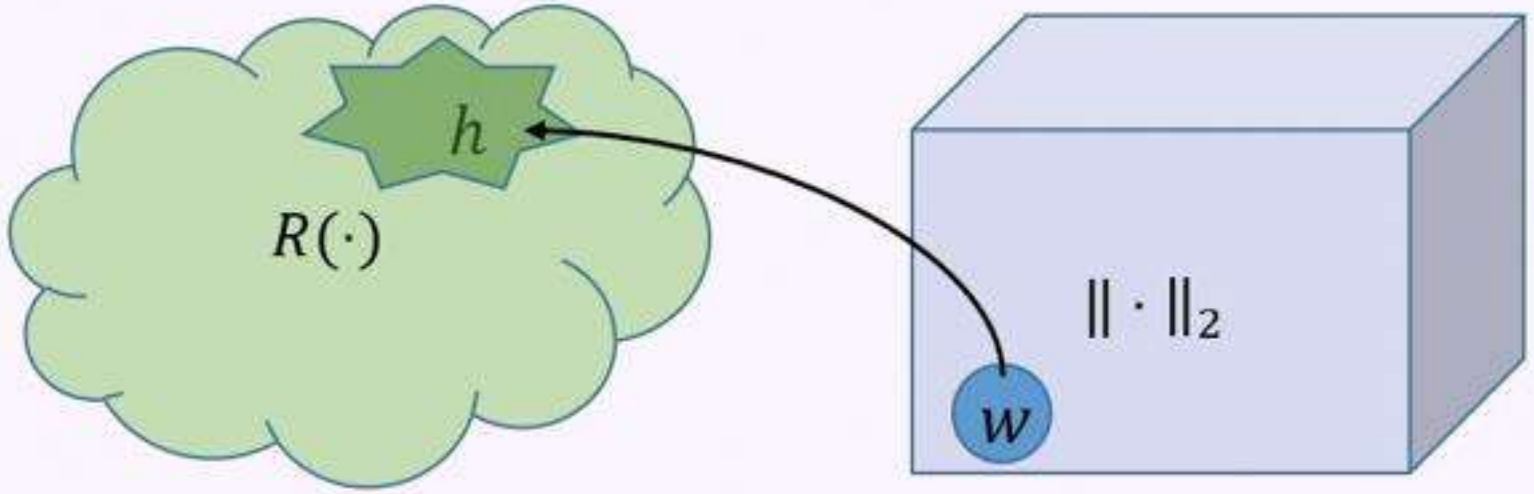

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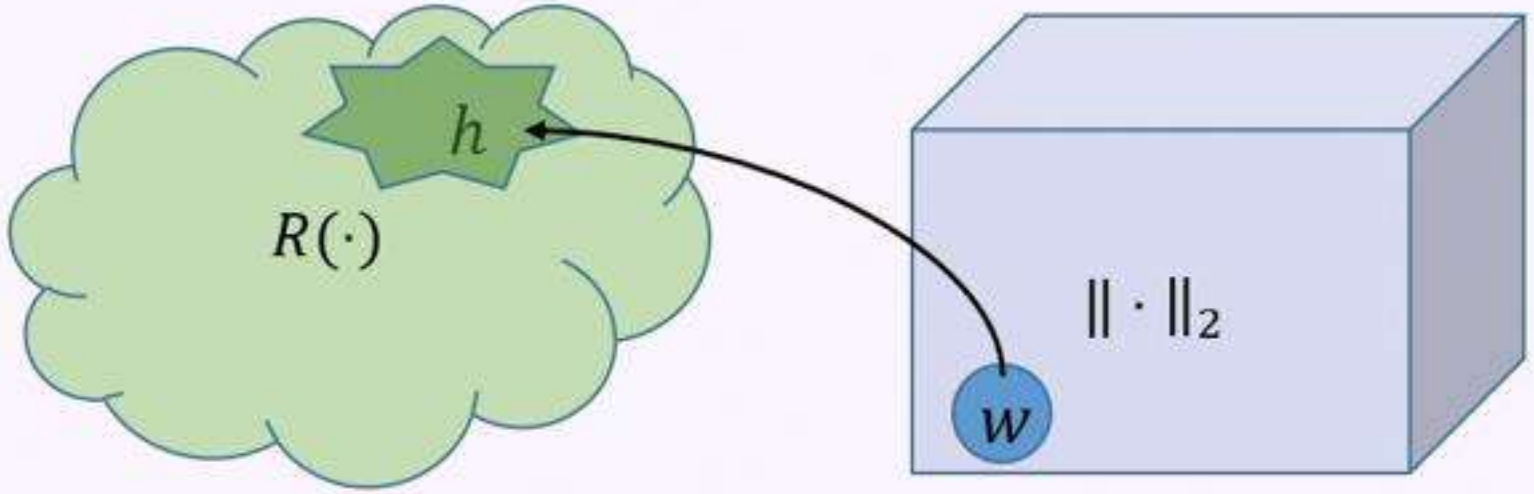

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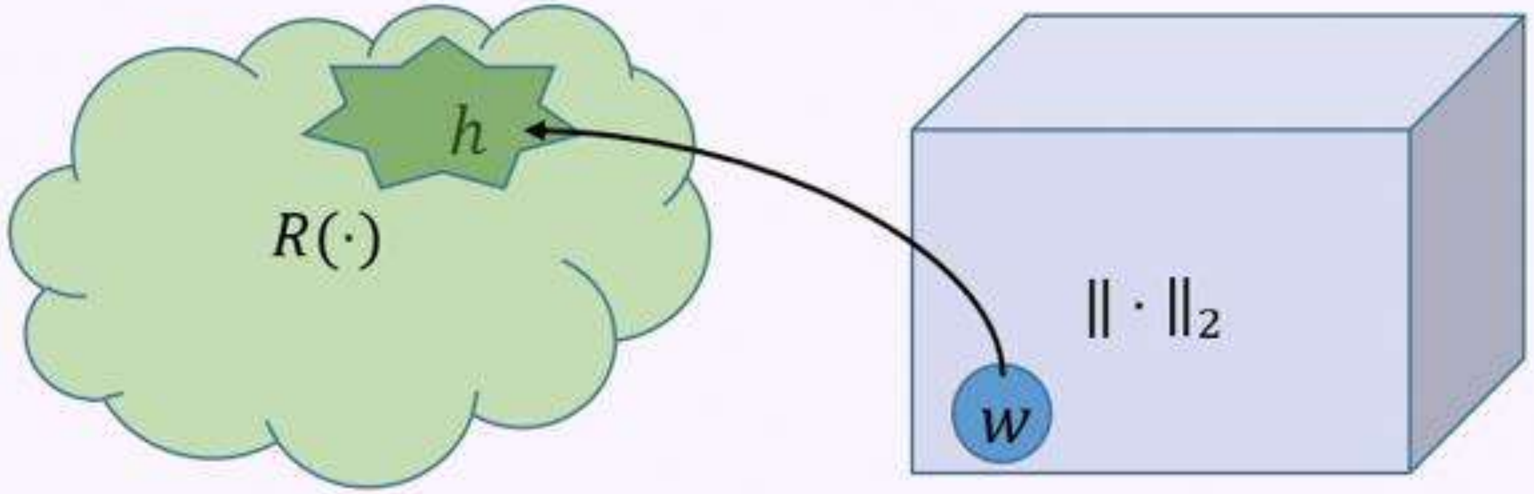

Doesn’t it all boil down to the NTK?

Is it all just a Kernel?

In kernel regime, training behaves according to 1st order approximation about $w^{(0)}$:

$$\boldsymbol{f}(\boldsymbol{w}, \boldsymbol{x}) \approx \boldsymbol{h}_{\boldsymbol{w}^{(0)}}(\boldsymbol{x}) + \langle \boldsymbol{w}, \boldsymbol{\phi_0}(\boldsymbol{x}) \rangle$$

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$$\Rightarrow \frac{1}{\alpha} h_\alpha(\infty) \to \hat{h}_{K_0} = \arg\min \|h\|_{K_0} \text{ s.t. } h(x_i) = y_i$$

Kernel Regime and Scale of Init

- For D-homogenous model, consider gradient flow with:

$$\dot{w}_\alpha = -\nabla L_S(w) \quad \text{and} \quad w_\alpha(0) = \alpha w_0 \text{ with unbiased } F(w_0) = 0$$

We are interested in $w_\alpha(\infty) = \lim_{t\to\infty} w_\alpha(t)$ and $h_\alpha(\infty) = F\big(w_\alpha(\infty)\big)$

- When will this behave like the kernel gradient flow:

$$\dot{w}_K = -\nabla L_S(x \mapsto \langle w, \phi_0(x)\rangle) \quad \text{and} \quad w(0) = w_0$$

where $\phi_0(x) = \nabla f(w_0, x)$ with associated kernel K_0

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➔ $\frac{1}{\alpha} h_\alpha(\infty) \to \hat{h}_{K_0} = \arg\min \|h\|_{K_0} \text{ s.t. } h(x_i) = y_i$

- But: when $\alpha \to 0$, we got interesting, non-RKHS inductive bias (e.g. nuclear norm, sparsity)

Scale of Init: Kernel vs Deep

Consider linear regression with squared parametrization:

$$f(w, x) = \sum_j \left(w_+[j]^2 - w_-[j]^2\right) x_i \quad \text{i.e.} \quad F(w) = \beta = w_+^2 - w_-^2$$

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What's the implicit bias of grad flow w.r.t square loss $L_S(w) = \|XF(w) - y\|_2^2$?

$$\beta_\alpha(\infty) = \lim_{t \to \infty} F(w_\alpha(t))$$

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In Kernel Regime $\alpha \to \infty$: $K_0(x,x') = 4\langle x,x'\rangle$ and so

$$\beta_\alpha(\infty) \to \hat{\beta}_{L2} = \arg\min_{X\beta=y} \|\beta\|_2$$

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In Deep Regime $\alpha \to 0$: special case of MF with commutative measurements

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In Deep Regime $\alpha \to 0$: special case of MF with commutative measurements

$$\beta_\alpha(\infty) \to \hat{\beta}_{L1} = \arg\min_{X\beta=y} \|\beta\|_{\mathbf{1}}$$

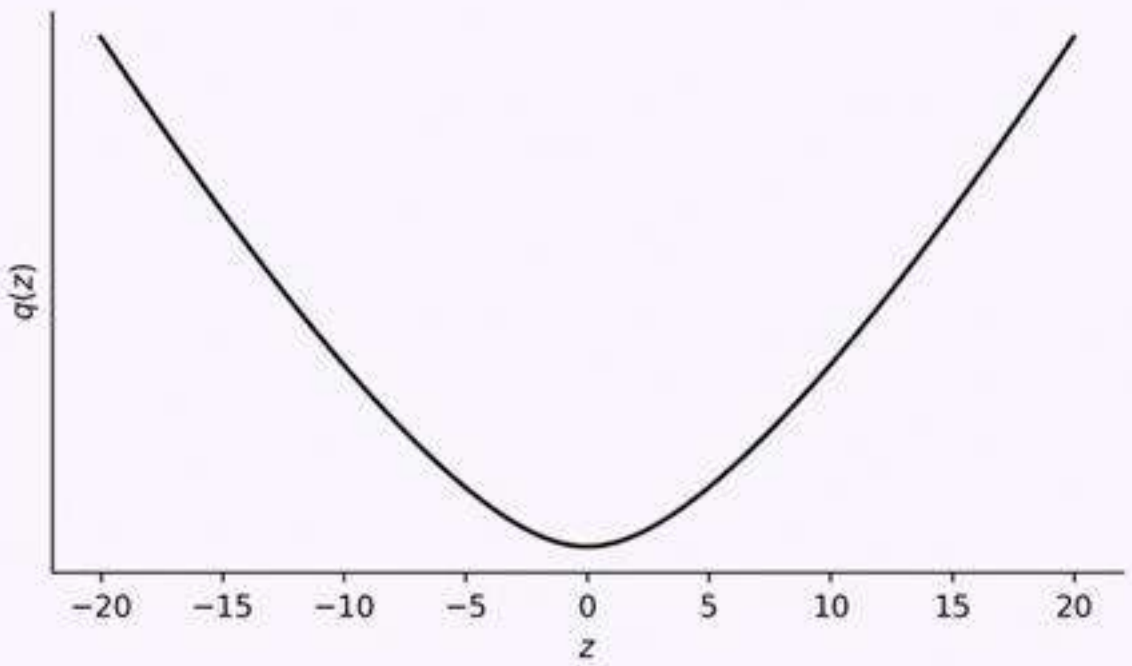
For any α: $\quad \beta_\alpha(\infty) = \arg\min_{X\beta=y} Q_\alpha(\beta)$

where $Q_\alpha(\beta) = \sum_j q\left(\frac{\beta[j]}{\alpha^2}\right)$ and $q(b) = 2 - \sqrt{4-b^2} + b\sinh^{-1}\left(\frac{b}{2}\right)$

Interpolating between Kernel and Deep

$$\beta_\alpha(\infty) = \arg\min_{X\beta=y} Q_\alpha(\beta)$$

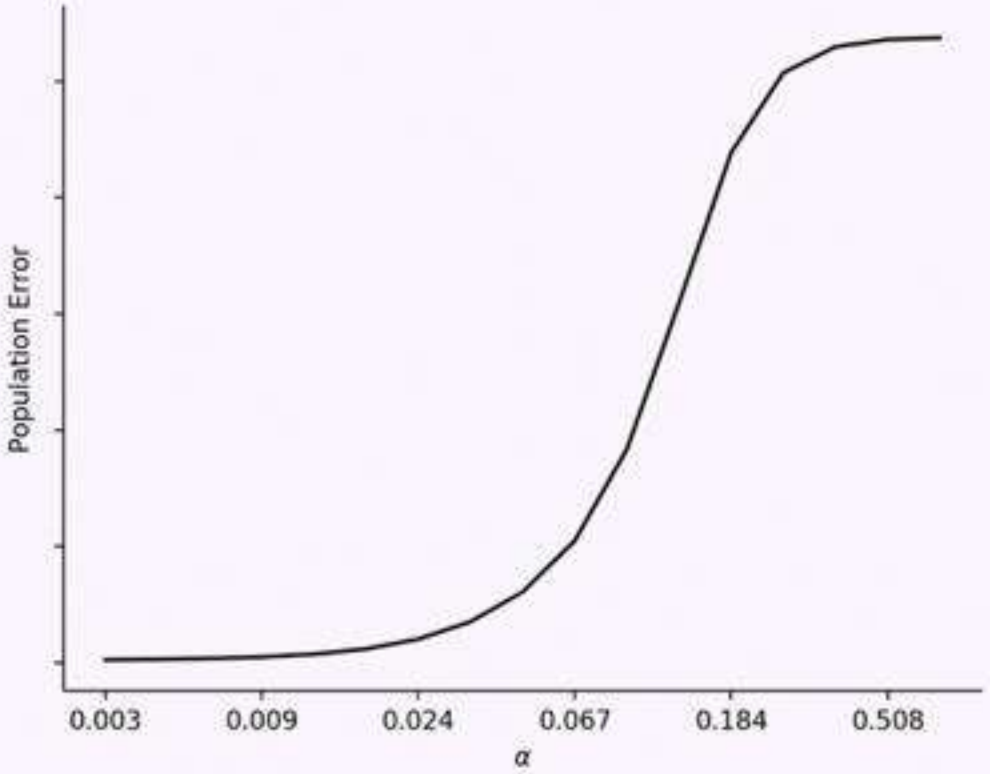
where $Q_\alpha(\beta) = \sum_j q\left(\frac{\beta[j]}{\alpha^2}\right)$ and $q(b) = 2 - \sqrt{4 - b^2} + b\sinh^{-1}\left(\frac{b}{2}\right)$

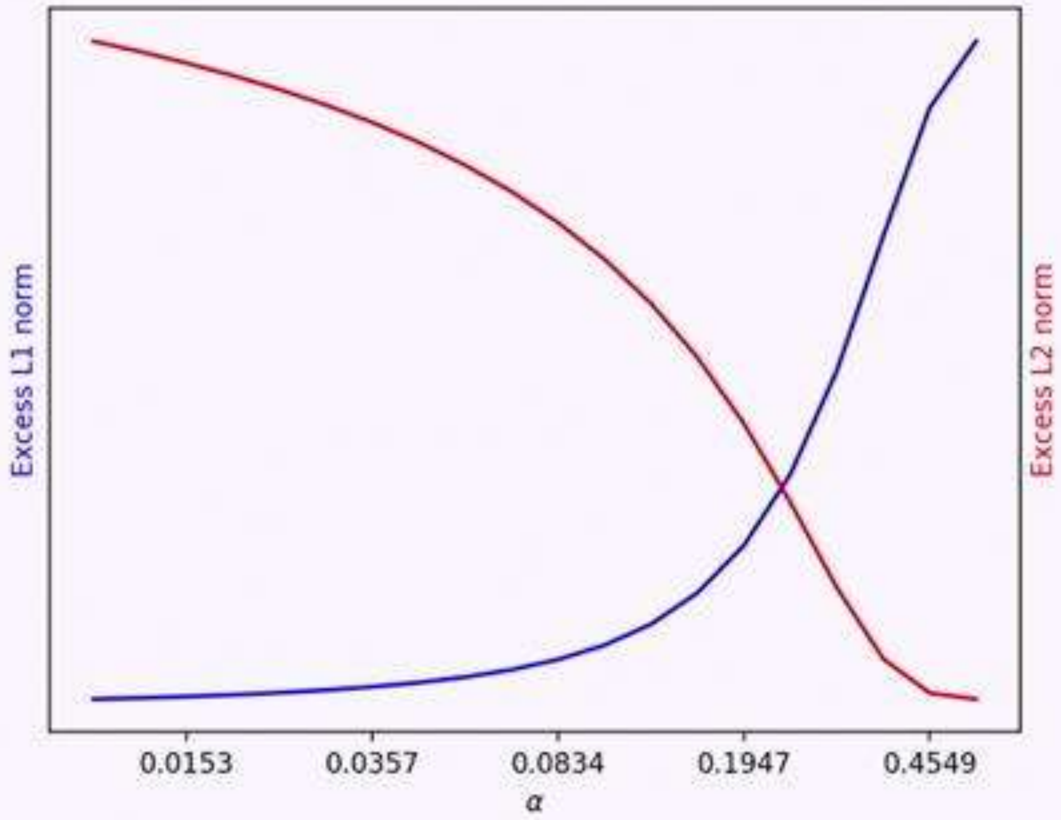


Induced dynamics: $\dot{\beta}_\alpha = -\sqrt{\beta_\alpha^2 + 4\alpha^4} \odot \nabla L_s(\beta_\alpha)$

Sparse Learning

$$y_i = \langle \beta^*, x_i \rangle + N(0,0.01)$$
$$d = 1000, \qquad \|\beta^*\|_0 = 5, \qquad m = 100$$

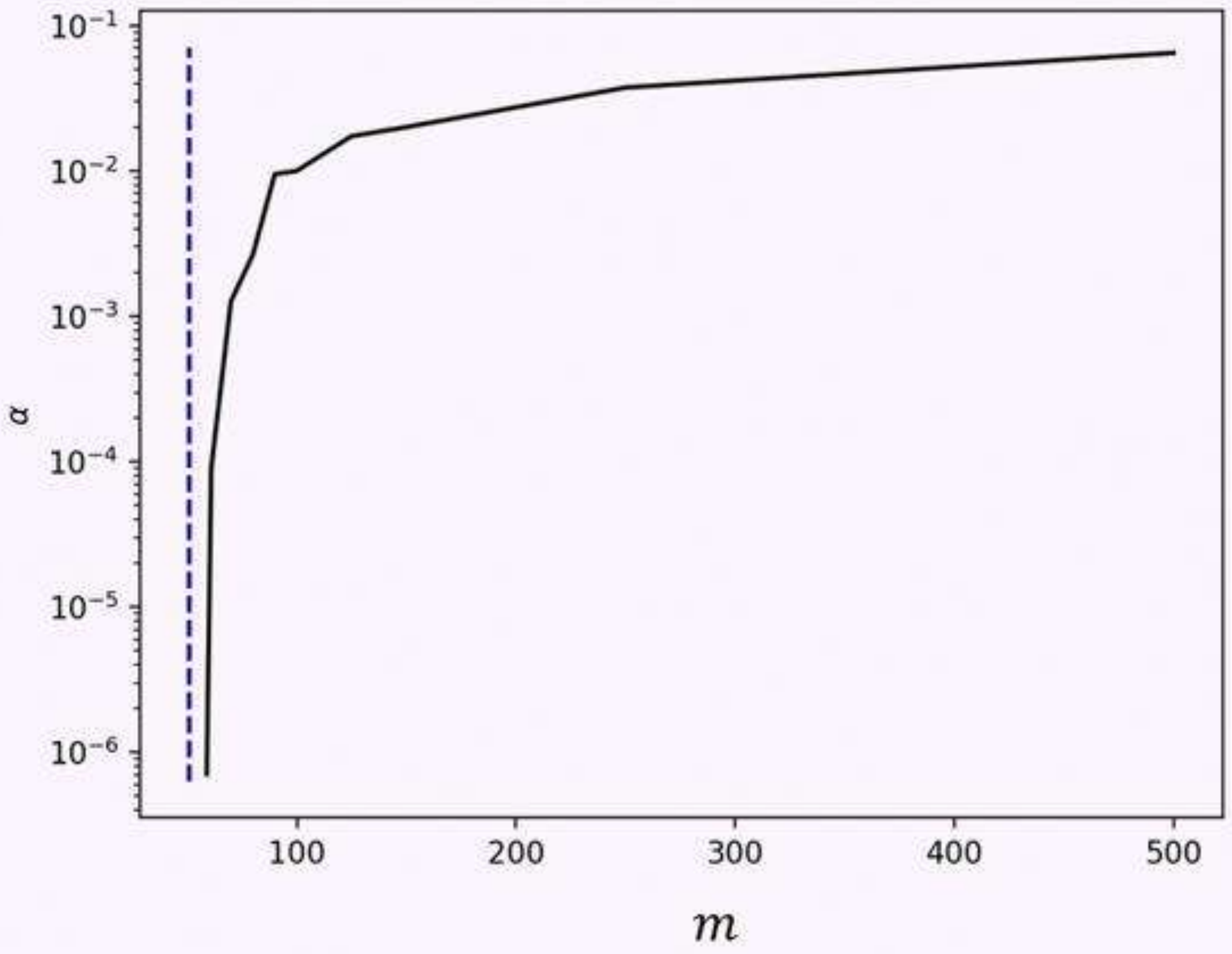




Sparse Learning

$$y_i = \langle \beta^*, x_i \rangle + N(0,0.01)$$
$$d = 1000, \qquad \|\beta^*\|_0 = k$$

How small does α need to be to get $L\big(\beta_\alpha(\infty)\big) < 0.025$



Relationship to Explicit Reg

Is initializing to $w(0) = \alpha\mathbf{1}$ the same as regularizing distance to $\alpha\mathbf{1}$?

$$\beta_\alpha^R = F\left(\arg\min_{L_S(w)=0} \|w - \alpha\mathbf{1}\|_2^2\right) = \arg\min_{X\beta=y} R_\alpha(\beta)$$

Where $R_\alpha(\beta) = \min_{F(w)=\beta} \|w - \alpha\mathbf{1}\|_2^2$

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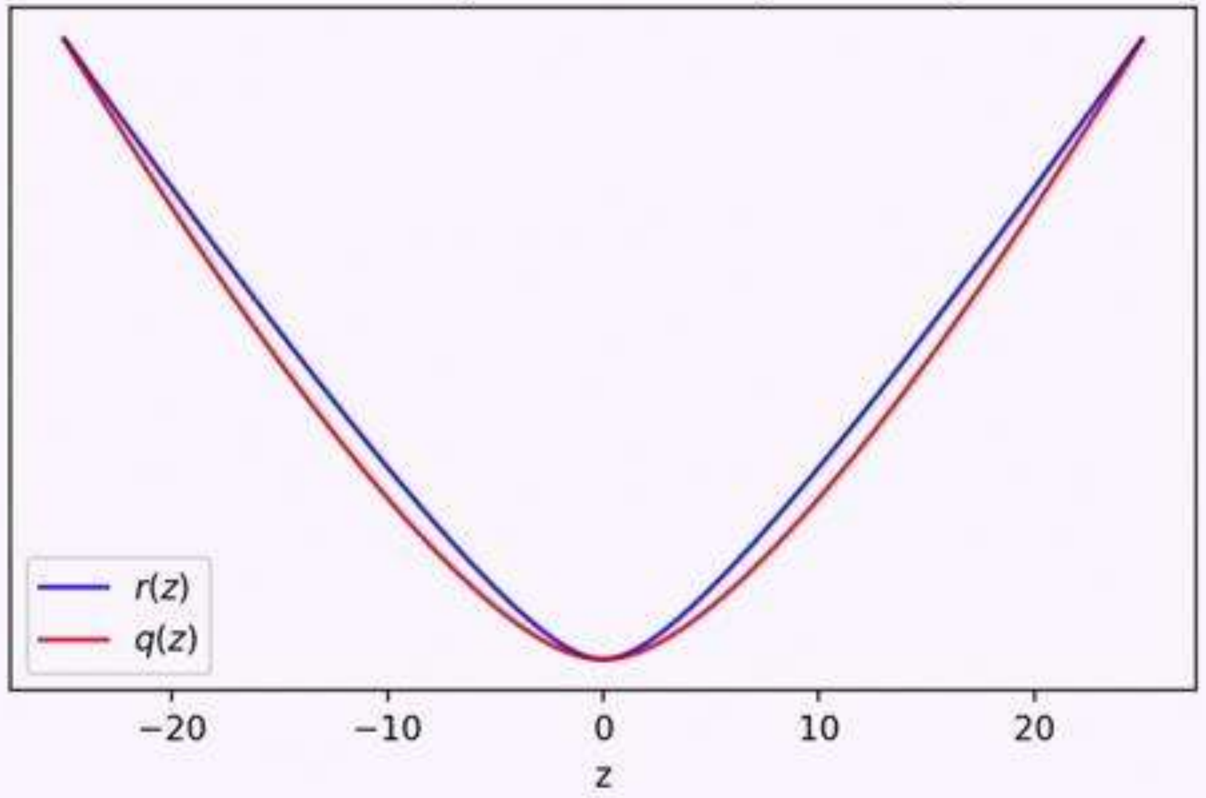
Is initializing to $w(0) = \alpha\mathbf{1}$ the same as regularizing distance to $\alpha\mathbf{1}$?

$$\beta_\alpha^R = F\left(\arg\min_{L_S(w)=0} \|w - \alpha\mathbf{1}\|_2^2\right) = \arg\min_{X\beta=y} R_\alpha(\beta)$$

Where $R_\alpha(\beta) = \min_{F(w)=\beta} \|w - \alpha\mathbf{1}\|_2^2$

$R_\alpha(\beta) = \sum_j r\left(\frac{\beta[j]}{\alpha^2}\right)$ where $r(b)$ is solution of quartic equation:

$$r^4 - 6r^3 + (12 - 2b^2)r^2 - (8 + 10b^2)r + b^2 + b^4 = 0$$

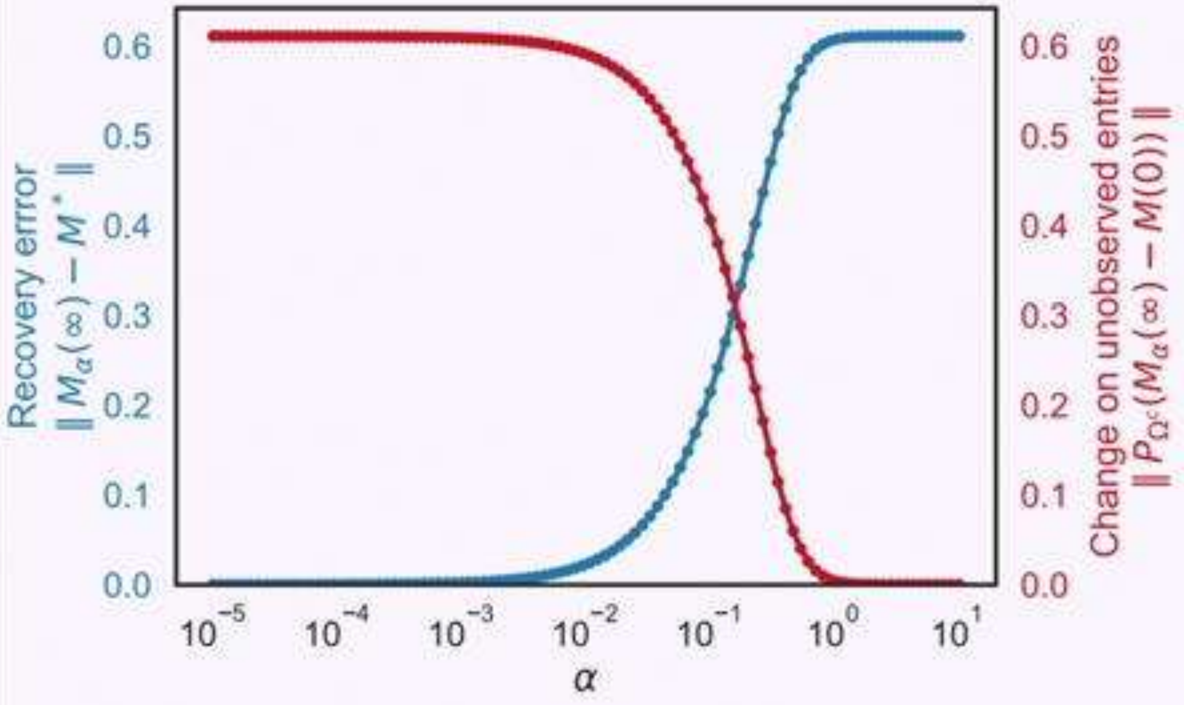


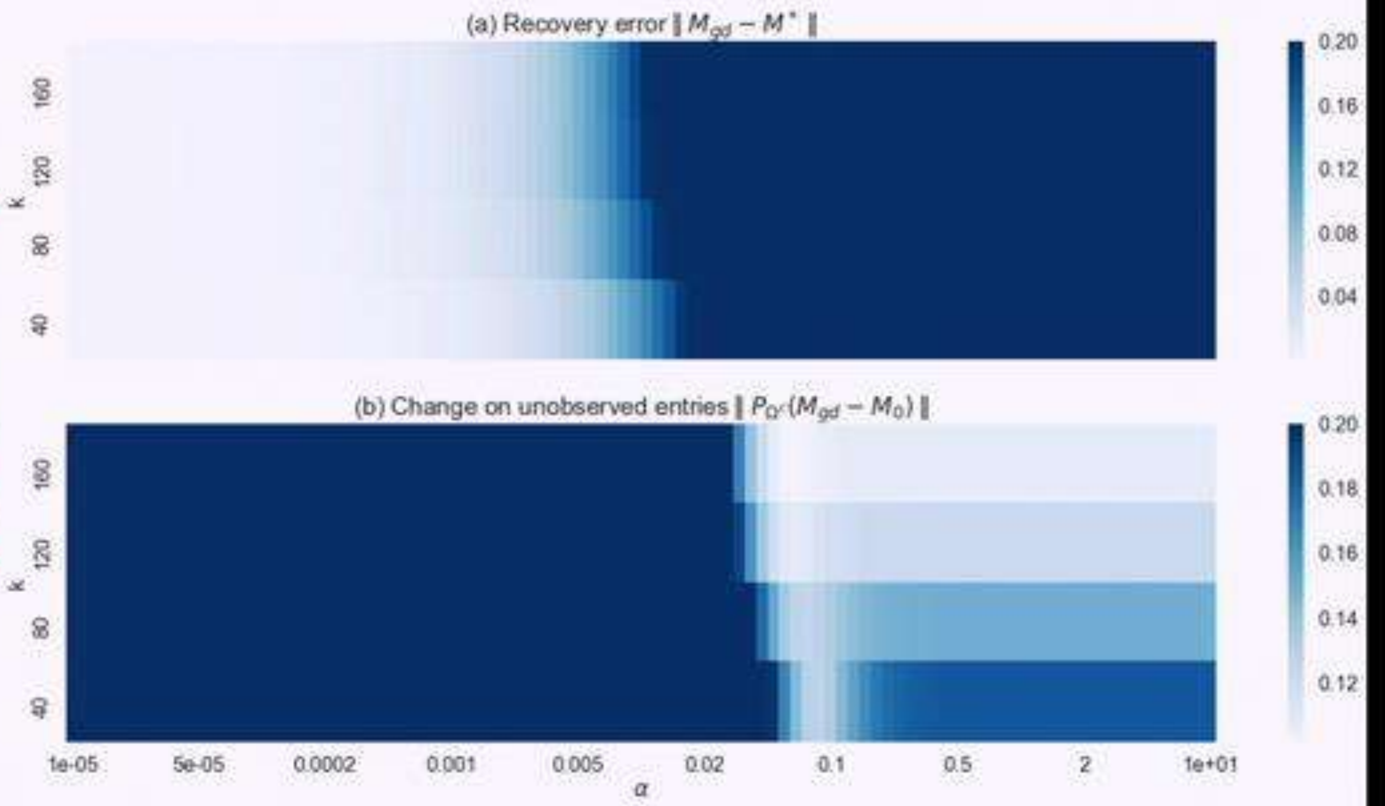
Kernel and Deep Regimes in Matrix Completion

$$f\big((U,V),(i,j)\big) = \big(UV^\top\big)_{ij}$$

Tangent kernel: $K_{U,V}\big((i,j),(i',j')\big) = \delta_{i=i'}\left\langle V_j, V_{j'}\right\rangle + \delta_{j=j'}\langle U_i, U_{i'}\rangle$

For orthogonal initialization: $K_0\big((i,j),(i',j')\big) \propto \delta_{(i,j)=(i',j')}$





Squared Loss vs Exp Loss

- Back to general D-homogenous model

- For squared loss, under some conditions [Chizat and Bach 18]:

$$\lim_{\alpha\to\infty}\sup_t \left\| \frac{1}{\alpha} w_\alpha\left(\frac{1}{\alpha^{D-1}} t\right) - w_K(t) \right\| = 0$$

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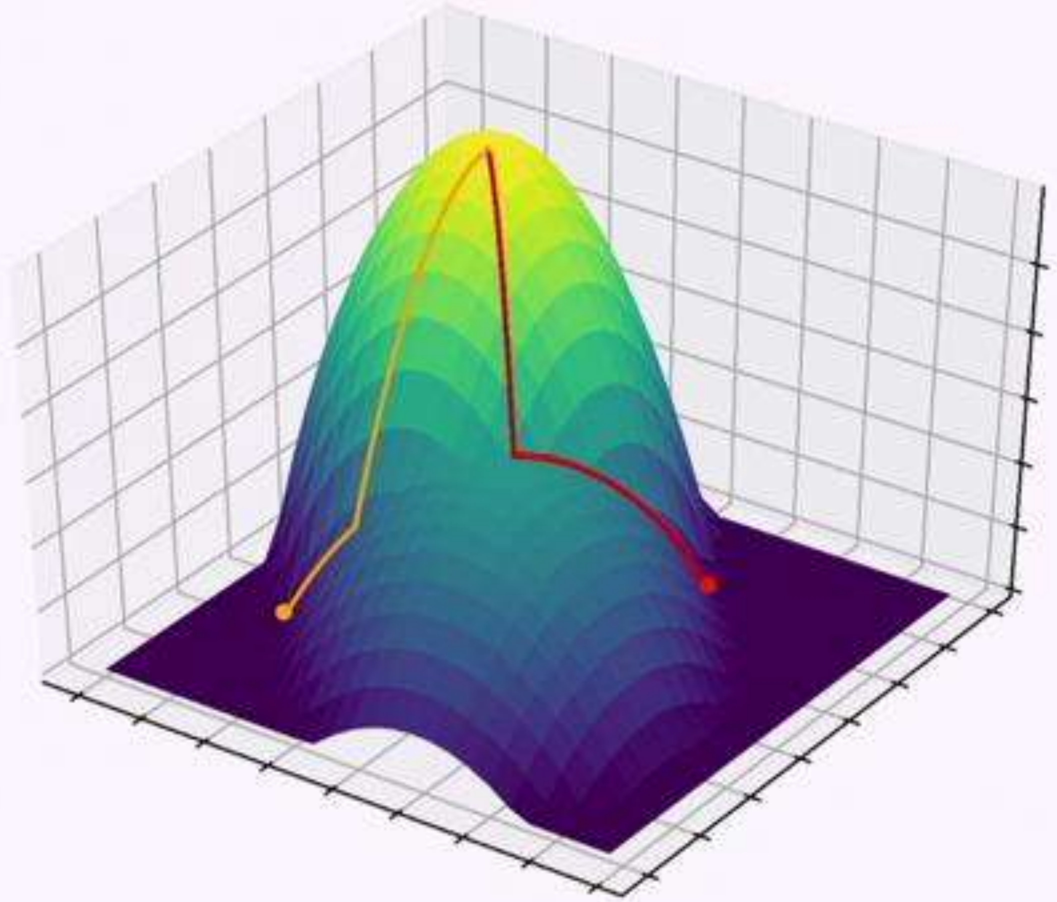
Different optimization algorithm

➔ Different bias in optimum reached

➔ Different Inductive bias

➔ Different generalization properties



Need to understand optimization alg. not just as reaching ***some*** (global) optimum, but as reaching a ***specific*** optimum