Implicit Regularization in Deep Learning May Not Be Explainable by Norms

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based on joint work with Nadav Cohen

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Outline

Generalization via Bias-Variance Tradeoff

In classical learning theory generalization exhibits the bias-variance tradeoff

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Tradeoff can be controlled through regularization:

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1. Limiting model size

Generalization via Bias-Variance Tradeoff

In classical learning theory generalization exhibits the bias-variance tradeoff

Tradeoff can be controlled through regularization:

1. Limiting model size
2. Adding term to loss (typically a norm)

Generalization in Deep Learning (DL)

DNNs In Practice

Generalize without explicit regularization:

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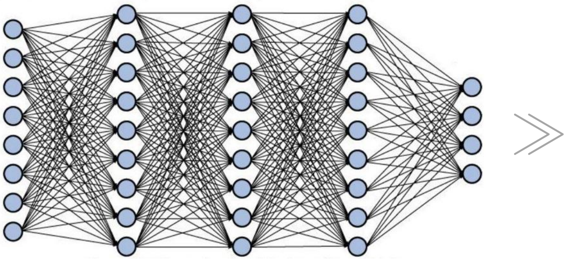
DNNs In Practice

Generalize without explicit regularization:

1. # of learned weights   # of training examples



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DNNs In Practice

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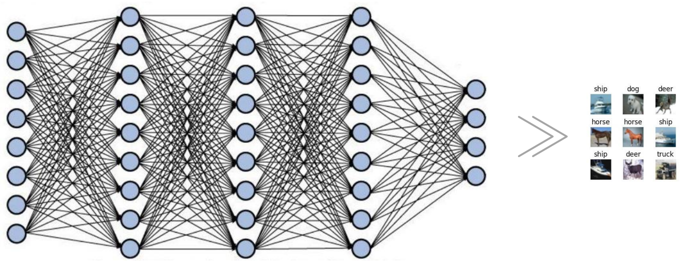

2. Loss unchanged (e.g. no weight decay/dropout)

Optimization Induces an Implicit Regularization

Multiple global minima: some generalize well, others don't

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Conventional Wisdom

Gradient-based optimization induces an implicit regularization

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Question

Can we mathematically understand this e ect in concrete settings?

Linear Regression

When # parameters > # training examples:

Linear Regression

When # parameters $>$ # training examples:

GD initialized at 0 converges to min ℓ_2 norm solution

$$\underset{w}{\operatorname{argmin}} \|w\|_2 \text{ s.t. } Xw = y$$

Widespread Hope

GD in DL finds solutions with minimal norm (or quasi-norm)

$$\operatorname*{argmin}_{w} \|w\| \ \text{ s.t. } w \text{ is global min}$$

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Demonstrated in various settings, e.g.:

Neyshabur et al. 2015
Gunasekar et al. 2017
Soudry et al. 2018
Gunasekar et al. 2018a
Gunasekar et al. 2018b
Li et al. 2018
Jacot et al. 2018
Mei et al. 2019
Ji & Telgarsky 2019a
Ji & Telgarsky 2019b
Wu et al. 2019
Oymak & Soltanolkotabi 2019
Nacson et al. 2019a
Nacson et al. 2019b
Woodworth et al. 2020
Lyu & Li 2020
Ali et al. 2020
Chizat & Bach 2020
Belabbas 2020

Matrix completion: recover low-rank matrix given subset of entries

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observed entries ! training data

unobserved entries ! test data

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observed entries $\rightarrow$ training data

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Denote observations by $\{b_{ij}\}_{(i,j)\in\Omega}$

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Convex Programming Approach

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Find minimal nuclear norm solution:

$$\min \|W\|_{nuclear} \quad s.t. \quad W_{ij} = b_{ij} \quad \forall (i,j) \in$$

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$$\min \|W\|_{nuclear} \quad s.t.: \; W_{ij} = b_{ij} \quad \forall (i,j) \in$$

Perfectly recovers if observations are sufficiently many (Candes & Recht 2008)

Deep Learning Approach

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GD is run w.r.t. $W_1, \ldots, W_L$ over:

$$\ell(W_{L:1}) = \frac{1}{2}\sum_{(i,j)\in\Omega}\left((W_{L:1})_{ij} - b_{ij}\right)^2$$

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To which solutions does product matrix $W_{L:1}$ converge?

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To which solutions does product matrix $W_{L:1}$ converge?

Empirical phenomenon: low-rank matrix often recovered accurately

Conjecture (Gunasekar et al. 2017)

With small learning rate and init close to the origin, GD over depth 2 matrix factorization converges to min nuclear norm solution.

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- Experiments
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Conjecture established under other restricted conditions:

- Li et al. 2018
- Belabbas 2020

Conjecture (Arora et al. 2019)

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Open Question

Does the implicit regularization in matrix factorization minimize a norm?

Theorem (informal)

There exist matrix factorization settings where:

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Result stronger than conjecture:

Settings jointly disqualify all norms

Norms driven towards 1

Common surrogate for GD with small learning rate and init[1]

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Common surrogate for GD with small learning rate and init:[1]

Gradient flow (GF) is a continuous version of GD (step size $\to 0$):

$$\frac{d}{dt}w(t) = -\nabla f(w(t)) \quad , t \in \mathbb{R}_{\geq 0}$$

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$\Uparrow$

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Closely matches GD in practice for linear neural networks

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Consider the following 2-by-2 matrix completion problem:

$$\begin{pmatrix} & 1 \\ 1 & 0 \end{pmatrix}$$

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Schatten-p (quasi-)norms are minimized () = 0

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Arbitrary norms (or quasi-norms):

Proposition

For minimal k k solutions, is bounded

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Contradiction between norm and rank minimization

Theorem

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Implicit regularization $\neq$ norm minimization!

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Proof Sketch[1]

[1] based on singular values differential equations from Arora et al. 2019

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GF trajectory analysis: $\det(W_{L:1}(t))$ does not change sign[1]

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$$\det(W_{L:1}(t)) = w_{1,1}(t)w_{2,2}(t) - w_{1,2}(t)w_{2,1}(t) > 0$$

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$\Longrightarrow |w_{1,1}(t)| \to \infty$ (behaves as $\Omega(1/\sqrt{\ell(t)})$)

Bound on $|w_{1,1}(t)|$ implies bounds for norms and rank suboptimality

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- Experiments: GD consistently finds global min
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If at init $W_{L:1}(0) = \quad I$, for depth $L = 2$ and $0 < \quad 1$, then $\ell(t) \to 0$

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Proof Approach

Careful analysis of GF differential equations

What happens when observations are perturbed?

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1 0

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$$\begin{matrix} & 1 \\ 1 & 0 \end{matrix} \implies \begin{matrix} & z \\ z' & \end{matrix} \qquad \text{non-zero } z; z' \text{ arbitrary}$$

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Theorem (original setting)

If $\det(W_{L:1}(0)) > 0$ at init, then for any (quasi-)norm $\|\cdot\|$:

1. $\|W_{L:1}(t)\| = \Omega(1/\sqrt{\ell(t)})$
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Theorem (original setting)

If $\mathrm{sign}(\det(W_{L:1}(0))) = -\mathrm{sign}(1 \cdot 1)$ at init, then for any (quasi-)norm $\|\cdot\|$:

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Theorem (intermediate)

If $\mathrm{sign}(\det(W_{L:1}(0))) = -\mathrm{sign}(z \cdot z')$ at init, then for any (quasi-)norm $\|\cdot\|$:

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Theorem (intermediate)

If $\mathrm{sign}(\det(W_{L:1}(0))) = -\mathrm{sign}(z \cdot z')$ at init, then for any (quasi-)norm $\|\cdot\|$:

1. $\|W_{L:1}(t)\| = \Omega\left(\min\{|z|, |z'|\} / (|\;| + \sqrt{2\ell(t)})\right)$
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2. $\text{rank-subopt}(W_{L:1}(t)) = O(| \; | + \sqrt{2\ell(t)}) = \min\{|z|, |z'|\}$

What happens when observations are perturbed?

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1. $\|W_{L:1}(t)\| = \Omega\left(\min\{|z|, |z'|\} / \left(|\epsilon| + \sqrt{2\ell(t)}\right)\right)$
2. $\text{rank-subopt}(W_{L:1}(t)) = \mathcal{O}\left(\left(|\epsilon| + \sqrt{2\ell(t)}\right) / \min\{|z|, |z'|\}\right)$

$\epsilon = 0 \implies$ all norms driven to ∞ and rank is minimized

What happens when observations are perturbed?

$$\begin{pmatrix} * & 1 \\ 1 & 0 \end{pmatrix} \Longrightarrow \begin{pmatrix} * & z \\ z' & \epsilon \end{pmatrix} \qquad \begin{array}{l} z, z' \text{ non-zero} \\ \epsilon \text{ arbitrary} \end{array}$$

Theorem

If $\mathrm{sign}(\det(W_{L:1}(0))) = -\,\mathrm{sign}(z \cdot z')$ at init, then for any (quasi-)norm $\|\cdot\|$:

1. $\|W_{L:1}(t)\| = \Omega\left(\min\{|z|, |z'|\} \,/\, (|\epsilon| + \sqrt{2\ell(t)}) \right)$
2. $\text{rank-subopt}(W_{L:1}(t)) = O\left((|\epsilon| + \sqrt{2\ell(t)}) \,/\, \min\{|z|, |z'|\} \right)$

$\epsilon = 0 \Longrightarrow$ all norms driven to ∞ and rank is minimized

Phenomenon gracefully recedes as ϵ perturbed from 0

What happens when observations are perturbed?

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Same results hold when changing unobserved entry location

!
1
1 0

!
1
1 0

!
1
1 0

!
2
0:5

!
1
1 0

!
2
0:5

!
1
1 0

!
2
0:5

Theory transfers to practice: unobserved entry ! 1

Analyzed Setting (our work)

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Contrast between norm and rank minimization

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Implicit regularization drives norms to 1 to minimize rank

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Contrast between norm and rank minimization

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Past Work

Analyzed Setting (our work)

Contrast between norm and rank minimization

Implicit regularization drives norms to 1 to minimize rank

Past Work

Empirical evidence: low-rank tendency in matrix factorization

Analyzed Setting (our work)

- Contrast between norm and rank minimization
- Implicit regularization drives norms t01 to minimize rank

Past Work

- Empirical evidence: low-rank tendency in matrix factorization
- Theoretical analysis: sparsity in singular values (Arora et al. 2019)

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Better interpretation $\neq$ rank minimization?

Analyzed Setting (our work)

Contrast between norm and rank minimization

Implicit regularization drives norms to1 to minimize rank

Past Work

Empirical evidence: low-rank tendency in matrix factorization

Theoretical analysis: sparsity in singular values (Arora et al. 2019)

Better interpretation rank minimization?

Does this interpretation extend beyond matrix factorization?

ConvACs are competitive in practice, and admit algebraic structure

Extensively studied (e.g. Cohen et al. 2016, Cohen & Shashua 2016, Cohen & Shashua 2017)

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Tensor factorizations correspond to non-linear NN

Tensor completion : recover low-rank tensor given subset of entries

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Natural extension of matrix completion

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Tensor Basics

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Natural extension of matrix completion

Tensor Basics

Tensor N-dimensional array (N = order of tensor)

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Natural extension of matrix completion

Tensor Basics

Tensor $\rightarrow$ N-dimensional array (N = order of tensor)

Tensor rank $\rightarrow$ minimal R s.t. $W = \sum_{r=1}^{R} w_r^{(1)} \otimes \cdots \otimes w_r^{(N)}$

$\otimes$:= outer product , $w_r^{(i)} \in \mathbb{R}^{d_i}$

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Tensor   N-dimensional array (N = order of tensor)

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:= outer product , $w_r^{(i)} \in \mathbb{R}^{d_i}$

For $N = 2$ this is exactly matrix rank

Parameterize solution as tensor factorization :

$$W = \sum_{r=1}^{R} w_r^{(1)} \qquad\qquad w_r^{(N)}$$

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R taken large enough to not constrain rank

Does W converge to low-rank tensor when running GD w.r.t. $\left\{ w_r^{(n)} \right\}_{r,n}$?

Order 4 Rank 1 Tensor Completion

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"linear" baseline exactly ts observations, 0 elsewhere

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GD drives rank of a non-linear NN towards minimum!

<u>Theory & Experiments</u>: implicit regularization minimizes matrix rank

Theory & Experiments: implicit regularization minimizes matrix rank

Theory & Experiments: implicit regularization minimizes matrix rank

Experiments: implicit regularization minimizes tensor rank

Theory & Experiments: implicit regularization minimizes matrix rank

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Hypothesis
Implicit regularization in DL minimizes rank of input-output mapping

Theory & Experiments: implicit regularization minimizes matrix rank

Experiments: implicit regularization minimizes tensor rank

Hypothesis

Implicit regularization in DL minimizes rank of input-output mapping

If true, may be key to explaining generalization

Implicit Regularization $\neq$ Norm Minimization

Matrix factorization: exist cases where all norms go to ∞

Implicit Regularization $\neq$ Norm Minimization

- Matrix factorization: exist cases where all norms go to ∞
- Unlikely implicit regularization in DL $=$ norm minimization

Implicit Regularization $\neq$ Norm Minimization

- Matrix factorization: exist cases where all norms go to 1
- Unlikely implicit regularization in DL = norm minimization

Better Interpretation: Bias to Low Rank?

Conclusion

Implicit Regularization = Norm Minimization

- Matrix factorization: exist cases where **all norms go to** ∞
- Unlikely implicit regularization in DL = norm minimization

Better Interpretation: Bias to Low Rank?

- Matrix factorization: growing empirical and theoretical evidence

Conclusion

Implicit Regularization = Norm Minimization

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Better Interpretation: Bias to Low Rank?

- Matrix factorization: growing empirical and theoretical evidence
- Extends to certain type of **non-linear NN**

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Looking Forward

Developing notions of rank for input-output mappings of NNs may be key

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Thank You