Generalization in Deep Learning Through the Lens of Implicit Rank Lowering

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Sources

Implicit Regularization in Deep Learning May Not Be Explainable by Norms

R + Cohen

NeurIPS 2020

Implicit Regularization in Tensor Factorization

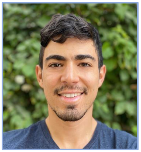
R* + Maman* + Cohen

ICML 2021

Implicit Regularization in Hierarchical Tensor Factorization and Deep Convolutional Neural Networks

R + Maman + Cohen

ICML 2022



Asaf Maman

Nadav Cohen

*Equal contribution

Outline

1 Implicit Regularization in Deep Learning

2 Matrix Factorization

- Implicit Regularization $\neq$ Norm Minimization

3 Tensor Factorization

4 Hierarchical Tensor Factorization

5 Implications for Modern Deep Learning

6 Conclusion

Generalization via Bias-Variance Tradeoff

Classically, generalization is understood via the bias-variance tradeoff

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Tradeoff can be controlled through:

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Tradeoff can be controlled through:

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Generalization via Bias-Variance Tradeoff

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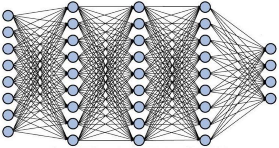
Tradeoff can be controlled through:

- Limiting model size
- Adding regularization (e.g. ℓ_2 penalty)

Generalization in Deep Learning

Neural networks (NNs) generalize with no explicit regularization despite:

# of learned weights



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# of training examples

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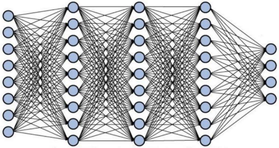

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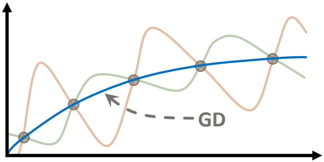
# of training examples

Conventional Wisdom

Gradient descent (GD) induces implicit regularization towards "simplicity"



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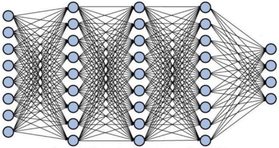
# of learned weights  ≫ 

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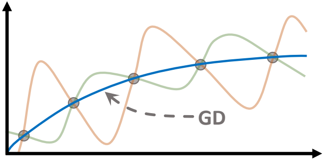
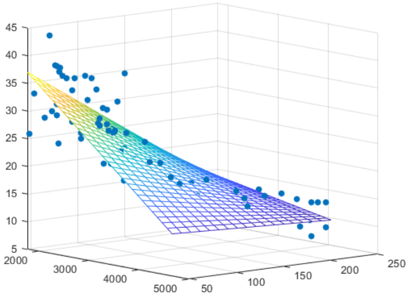


Goal

Mathematically characterize this implicit regularization

Linear Models: Implicit Norm Minimization

Linear Regression



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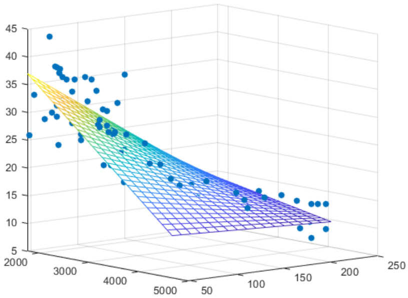

When $\#$ of learned weights $>$ $\#$ of training examples:

Linear Models: Implicit Norm Minimization

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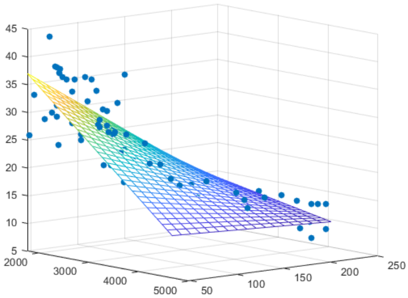

When # of learned weights > # of training examples:

GD initialized at 0 converges to min ℓ_2 norm solution

$$\underset{\mathbf{w}}{\text{argmin}} \|\mathbf{w}\|_2 \text{ s.t. } \mathbf{w} \text{ is global min}$$

Implicit Norm Minimization In Deep Learning?

Widespread Hope

In deep learning, GD finds solution with min norm (possibly not ℓ_2)

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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
- 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
- Lyu et al. 2021

Perspective: Implicit Rank Minimization

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To understand implicit regularization in deep learning:

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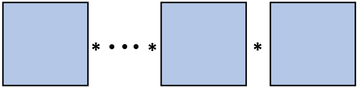
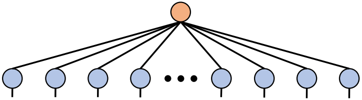
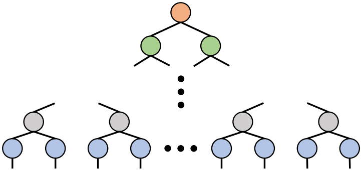
Case will be made via matrix and tensor factorizations







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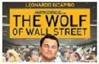
Matrix Completion $\longleftrightarrow$ Two-Dimensional Prediction

Matrix completion: recover unknown matrix given subset of entries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Alice	?	5	4	?
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observations $\{y_{i,j}\}_{(i,j)\in\Omega}$

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				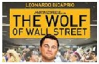
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matrix $\longleftrightarrow$ predictor

MF $\longleftrightarrow$ Linear NN

Matrix Factorization (**MF**):

Parameterize solution as product of matrices and fit observations via GD

$$\min_{W_1,\ldots,W_L} \sum_{(i,j)\in\Omega} \left([W_L W_{L-1} \cdots W_1]_{i,j} - y_{i,j}\right)^2$$

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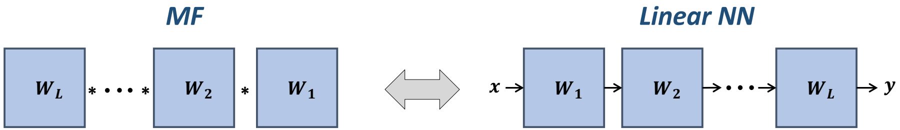

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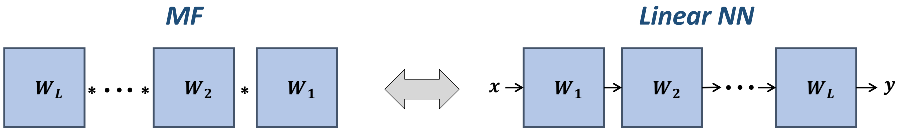

Empirical Phenomenon (Gunasekar et al. 2017)

MF (with small init and step size) accurately recovers low rank matrices

Conjecture: Nuclear Norm Minimization

Classic Result (Candes & Recht 2009)

For low rank ground truth:

$$\min \|W\|_{nuclear} \quad s.t. \quad [W]_{i,j} = y_{i,j} \quad \forall (i,j) \in \Omega$$

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Training MF via gradient flow (GD with step size $\to 0$) with small init $\Longrightarrow$ min nuclear norm solution

Proven in certain restricted cases (Gunasekar et al. 2017, Li et al. 2018, Belabbas 2020)

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Theorem (Arora et al. 2019)

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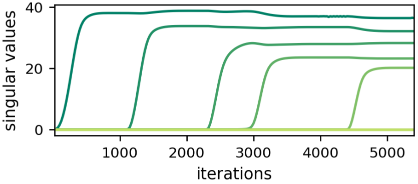

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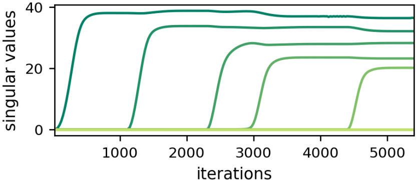

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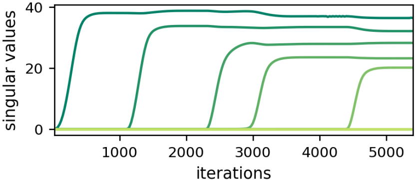

Incremental learning of singular values leads to low rank

Conjecture (Arora et al. 2019)

For any $\|\cdot\|$*, exist observations for which MF* $\not\Longrightarrow$ *min* $\|\cdot\|$ *solution*

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Our Work: Implicit Regularization $\neq$ Norm Minimization

Does the implicit regularization in MF minimize a norm?

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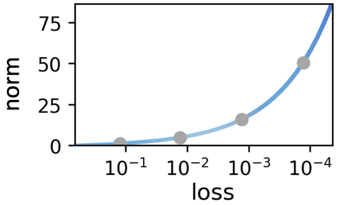

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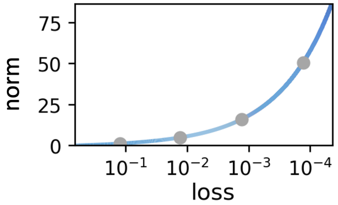

Chou et al. 2020, Li et al. 2021: further support for implicit rank minimization

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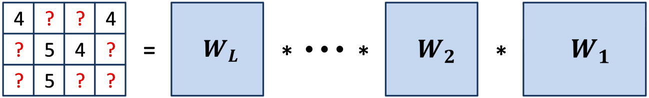
Drawbacks of Studying MF

4	?	?	4
?	5	4	?
?	5	?	?

$$= W_L * \cdots * W_2 * W_1$$

As a surrogate for deep learning, MF is limited:

Drawbacks of Studying MF



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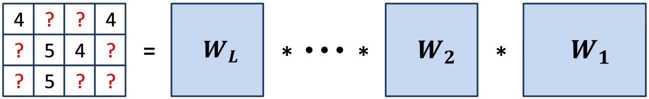

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$$\begin{bmatrix} 4 & ? & ? & 4 \\ ? & 5 & 4 & ? \\ ? & 5 & ? & ? \end{bmatrix} = W_L * \cdots * W_2 * W_1$$

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Tensor factorization accounts for both **(1)** and **(2)**

Tensor Completion $\longleftrightarrow$ Multi-Dimensional Prediction

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

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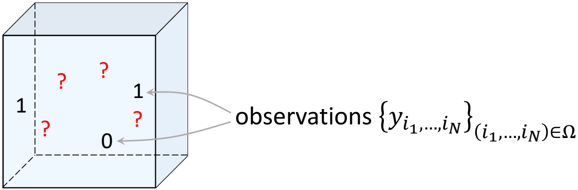
Tensor completion: recover unknown tensor given subset of entries



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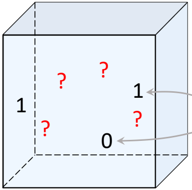

observations $\{y_{i_1,\ldots,i_N}\}_{(i_1,\ldots,i_N)\in\Omega}$

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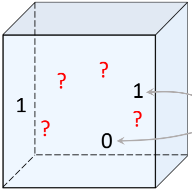

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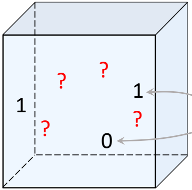

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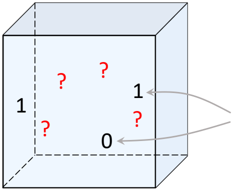

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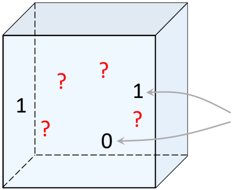

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$d_1 \times \cdots \times d_N$ tensor completion $\longleftrightarrow$ prediction from $[d_1] \times \cdots \times [d_N]$ to $\mathbb{R}$

value of entry $(i_1, \ldots, i_N)$	$\longleftrightarrow$	label of input $(i_1, \ldots, i_N)$
observed entries	$\longleftrightarrow$	train data
unobserved entries	$\longleftrightarrow$	test data
tensor	$\longleftrightarrow$	predictor

TF $\longleftrightarrow$ Shallow Non-Linear Convolutional NN

Tensor Factorization (TF):

Parameterize solution as sum of outer products and fit observations via GD

$$\min_{\{\mathbf{w}_r^n\}_{r,n}} \sum_{(i_1,\ldots,i_N)\in\Omega} \left(\left[\sum_{r=1}^{R} \mathbf{w}_r^1 \otimes \cdots \otimes \mathbf{w}_r^N \right]_{i_1,\ldots,i_N} - y_{i_1,\ldots,i_N} \right)^2$$

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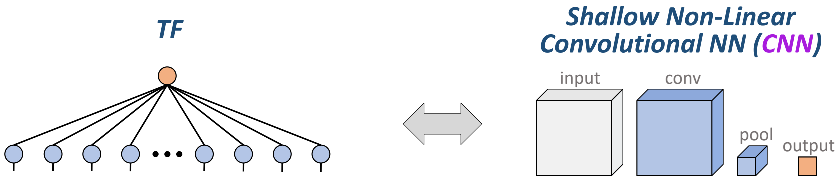

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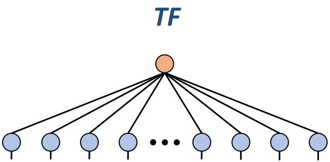

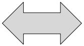

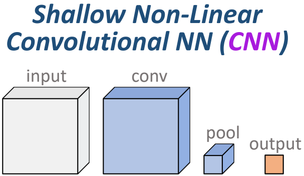

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$\sigma_T^{(r)} := \|\otimes_{n=1}^{N} \mathbf{w}_r^n\|_F$ — Frobenius norm of r'th component

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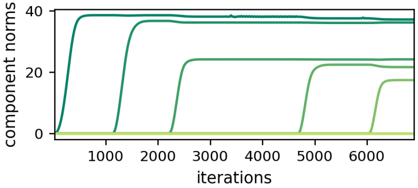

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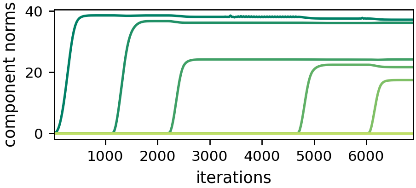

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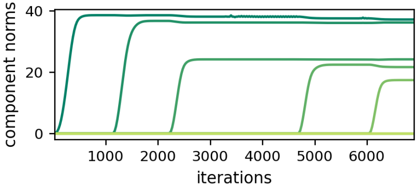

Incremental learning of components leads to low tensor rank!

Theorem (under technical conditions)

If tensor completion has tensor rank 1 solution, then TF will reach it

Analogy Between Implicit Regularizations

	MF	**TF**
Quantity	singular values	component norms
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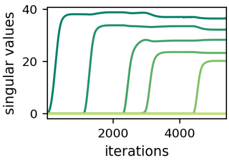

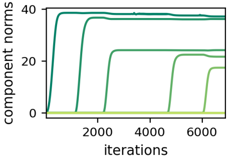

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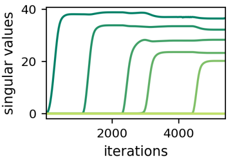
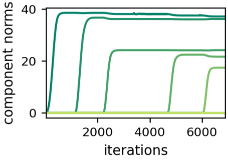
Experiment		
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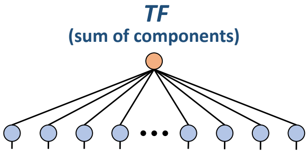
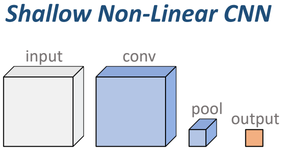
HTF $\longleftrightarrow$ Deep Non-Linear CNN

TF does not account for depth





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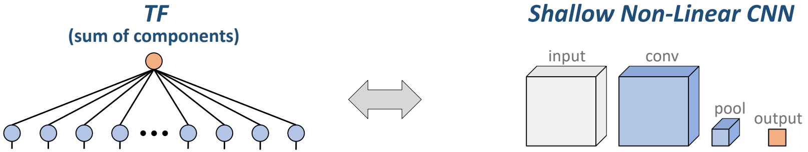

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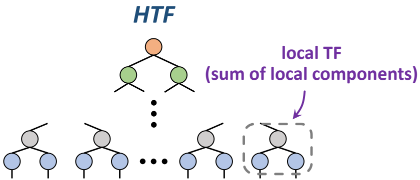

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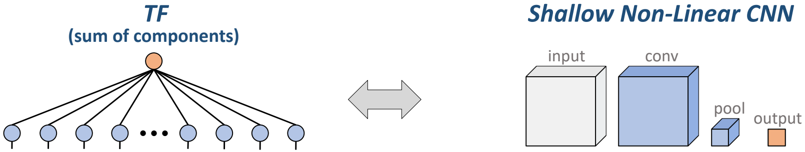

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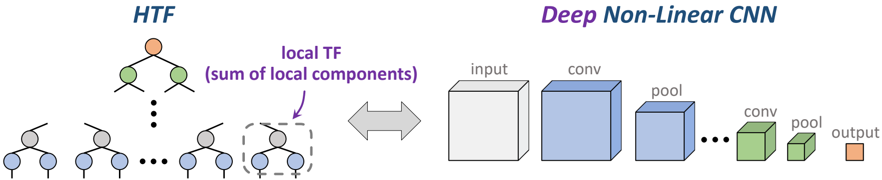

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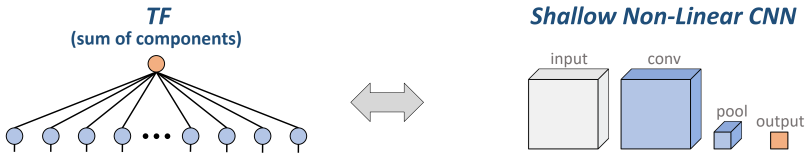

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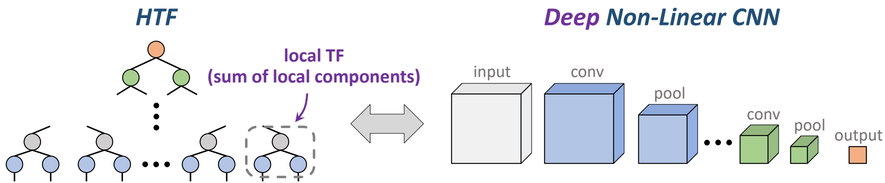

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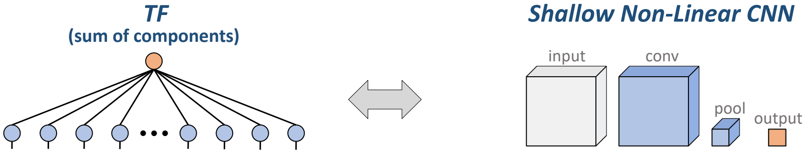

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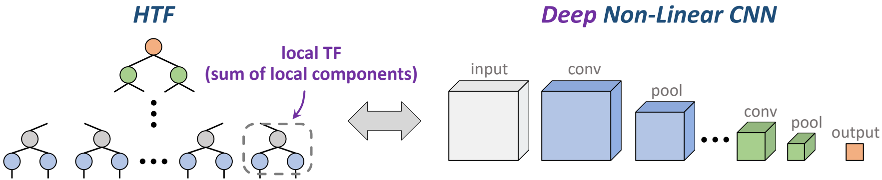

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Representation w/ few local components $\Longrightarrow$ low hierarchical tensor rank

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$\sigma_H^{(r)}$ — Frobenius norm of r'th local component in a location of HTF

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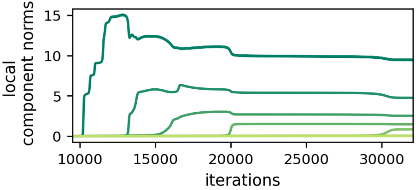

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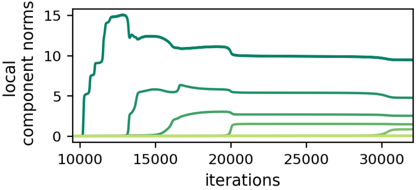

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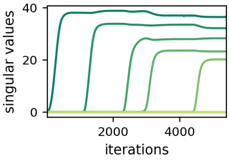
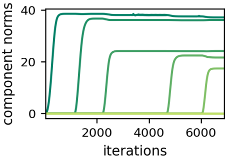
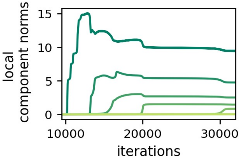
Experiment			
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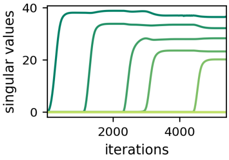

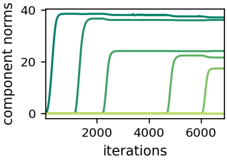

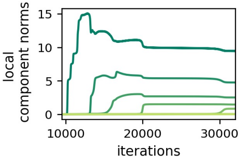

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Practical Application: Rank Lowering in NN Layers

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$\implies$ implicit rank lowering induces compressibility and generalization

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Implicit Rank-Minimizing Autoencoder

Li Jing Facebook AI Research New York
Jure Zbontar Facebook AI Research New York
Yann LeCun Facebook AI Research New York

ExpandNets: Linear Over-parameterization to Train Compact Convolutional Networks

Shuxuan Guo CVLab, EPFL
Jose M. Alvarez NVIDIA
Mathieu Salzmann CVLab, EPFL

THE LOW-RANK SIMPLICITY BIAS IN DEEP NETWORKS

Minyoung Huh MIT CSAIL
Hossein Mobahi Google Research
Richard Zhang Adobe Research
Brian Cheung MIT CSAIL & BCS
Pulkit Agrawal MIT CSAIL
Phillip Isola MIT CSAIL

Understanding Generalization in Deep Learning via Tensor Methods

Jingling Li[1,3] **Yanchao Sun**[1] **Jiahao Su**[4] **Taiji Suzuki**[2,3] **Furong Huang**[1]

[1]Department of Computer Science, University of Maryland, College Park
[2]Graduate School of Information Science and Technology, The University of Tokyo
[3]Center for Advanced Intelligence Project, RIKEN
[4]Department of Electrical and Computer Engineering, University of Maryland, College Park

Potential Explanation for Generalization on Natural Data

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Challenge

Find complexity measures that:

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MNIST & FMNIST can be fit with low (hierarchical) tensor rank

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Implicit lowering of ranks may explain generalization on natural data!

Countering Locality of CNNs via Regularization

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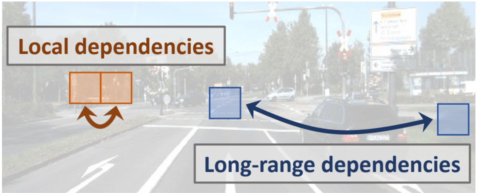
Fact (Cohen & Shashua 2017, Levine et al. 2018)

Hierarchical tensor rank measures long-range dependencies



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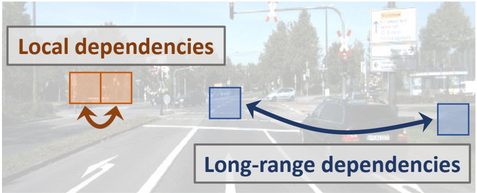

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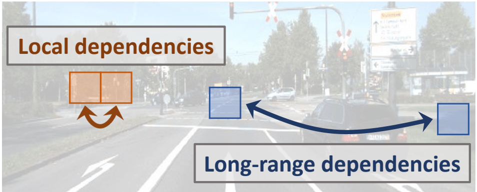

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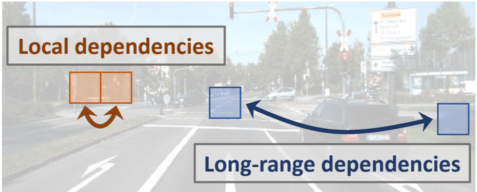

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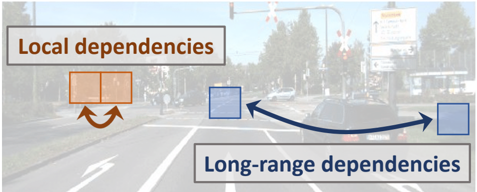

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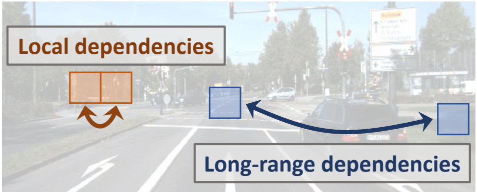
  (Cohen & Shashua 2017, Linsley et al. 2018, Kim et al. 2020)
- *Our analysis:* implicit regularization is also a cause

Countering Locality of CNNs via Regularization

Fact (Cohen & Shashua 2017, Levine et al. 2018)

Hierarchical tensor rank measures long-range dependencies



Implicit lowering of
hierarchical tensor rank in HTF
⇕
Implicit lowering of
long-range dependencies in CNNs!

CNNs are not suitable for long-range tasks

- *Conventional wisdom*: due to expressiveness
  (Cohen & Shashua 2017, Linsley et al. 2018, Kim et al. 2020)
- *Our analysis*: implicit regularization is also a cause

Can explicit regularization improve CNNs on long-range tasks?

Countering Locality of CNNs via Regularization

Experiment

Tasks: "Is Same Class" and Pathfinder (Linsley et al. 2018, Tay et al. 2021)

Countering Locality of CNNs via Regularization

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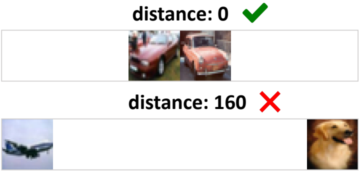

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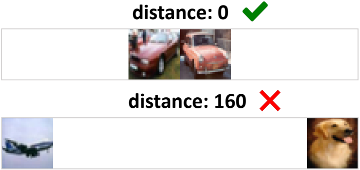

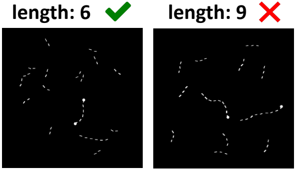

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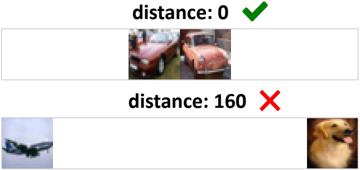

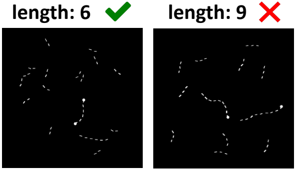

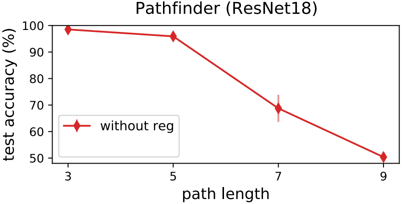

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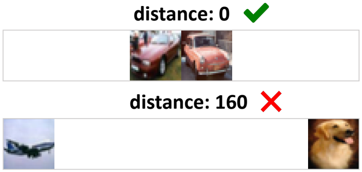
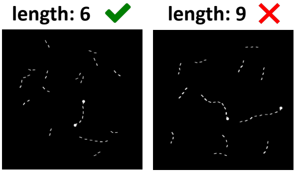
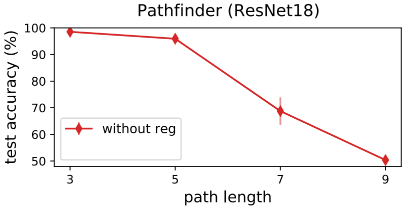




Regularization: promotes high hierarchical tensor rank



Countering Locality of CNNs via Regularization

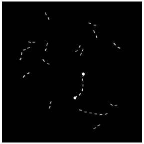
Experiment

Tasks: "Is Same Class" and Pathfinder (Linsley et al. 2018, Tay et al. 2021)

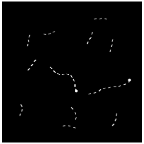
distance: 0 ✓

distance: 160 ✗

length: 6 ✓



length: 9 ✗



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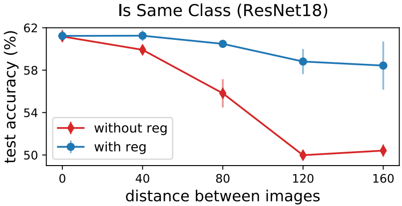

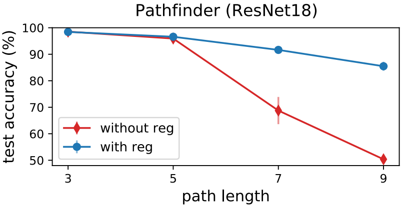

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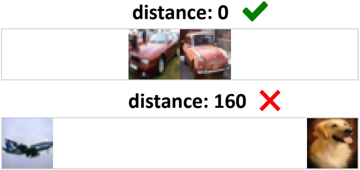

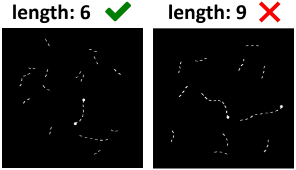

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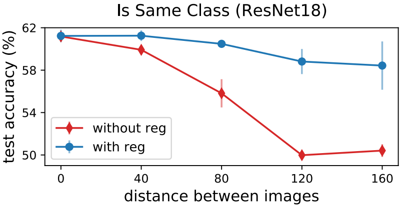

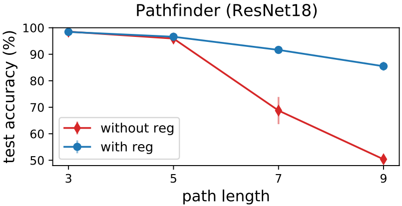

Explicit regularization can improve CNNs on long-range tasks!

Outline

1 Implicit Regularization in Deep Learning

2 Matrix Factorization
- Implicit Regularization $\neq$ Norm Minimization

3 Tensor Factorization

4 Hierarchical Tensor Factorization

5 Implications for Modern Deep Learning

6 Conclusion

Recap

Goal: understand implicit regularization in deep learning

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Matrix Factorization (Linear NN):

- *Existing conjecture:* implicit regularization minimizes norm

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Implications to Modern Deep Learning:

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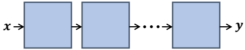
Implications to Modern Deep Learning:

- Parameterizing layers of NN as MF / TF/ HTF $\implies$ compression
- Rank lowering may explain generalization on natural data
- One may counter locality of CNNs via explicit regularization!

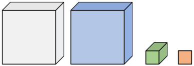
Implicit Rank Minimization in Deep Learning

Linear NN



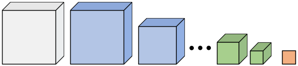
matrix rank lowering

Shallow Non-Linear CNN



tensor rank lowering

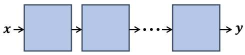
Deep Non-Linear CNN



hierarchical tensor rank lowering

Implicit Rank Minimization in Deep Learning

Linear NN



matrix rank lowering

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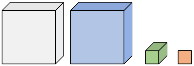

tensor rank lowering

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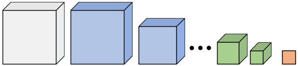
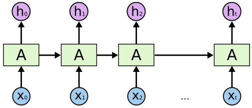
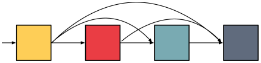


hierarchical tensor rank lowering



??? rank lowering



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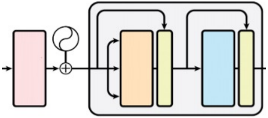
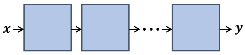
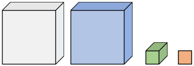
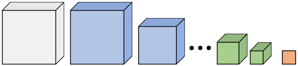
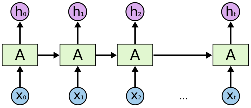
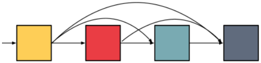
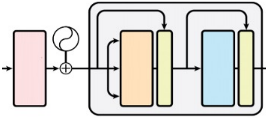


??? rank lowering

Hypothesis: in each NN architecture implicit regularization lowers corresponding notion of rank

Implicit Rank Minimization in Deep Learning

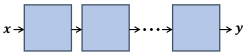
Linear NN	*Shallow Non-Linear CNN*	*Deep Non-Linear CNN*
		
matrix rank lowering	tensor rank lowering	hierarchical tensor rank lowering
		
??? rank lowering	??? rank lowering	??? rank lowering

Hypothesis: in each NN architecture implicit regularization lowers corresponding notion of rank

Discovering lowered notions of rank may pave way to:

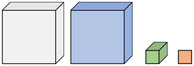
Implicit Rank Minimization in Deep Learning

Linear NN



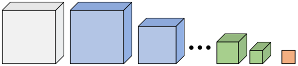
matrix rank lowering

Shallow Non-Linear CNN

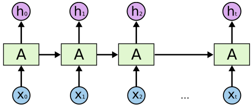


tensor rank lowering

Deep Non-Linear CNN



hierarchical tensor rank lowering



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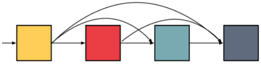

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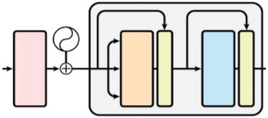


??? rank lowering

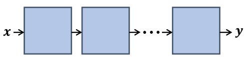
Hypothesis: in each NN architecture implicit regularization lowers corresponding notion of rank

Discovering lowered notions of rank may pave way to:

- Explaining generalization

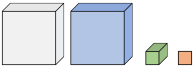
Implicit Rank Minimization in Deep Learning

Linear NN



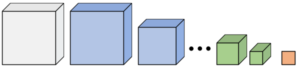
matrix rank **lowering**

Shallow Non-Linear CNN

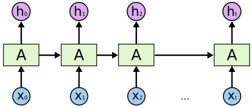


tensor rank **lowering**

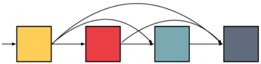
Deep Non-Linear CNN



hierarchical tensor rank **lowering**



??? rank **lowering**



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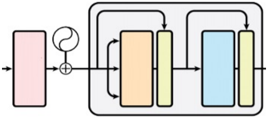

??? rank **lowering**

Hypothesis: in each NN architecture implicit regularization lowers corresponding notion of rank

Discovering lowered notions of rank may pave way to:

- Explaining generalization
- Enhancing performance via regularization and architecture design

Thank You!

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