Generalization in Deep Learning Through the Lens of Implicit Rank Minimization

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Tel Aviv University

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

arXiv 2022

Asaf Maman

Nadav Cohen

*Equal contribution

Outline

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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- Limiting model size

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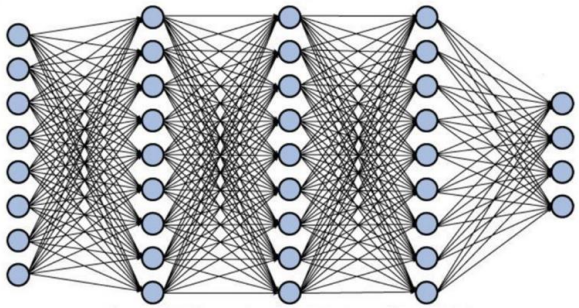
Tradeoff can be controlled through:

- 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



$\gg$

# of training examples

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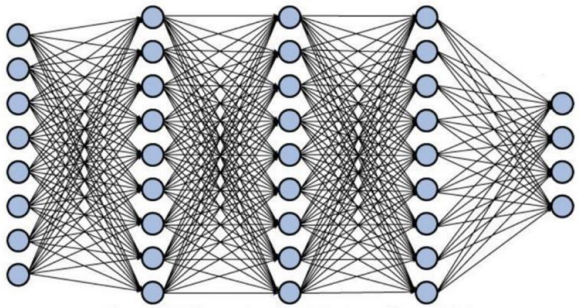
# of learned weights  $\gg$ 

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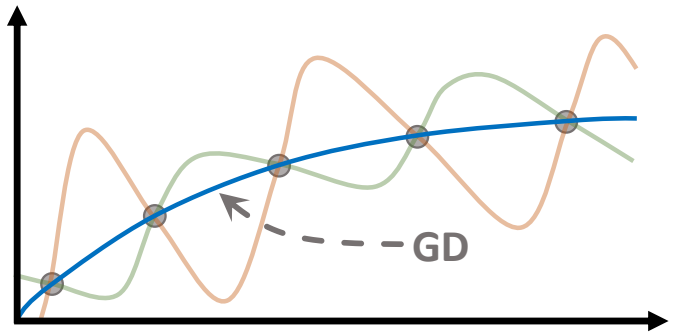
Conventional Wisdom

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



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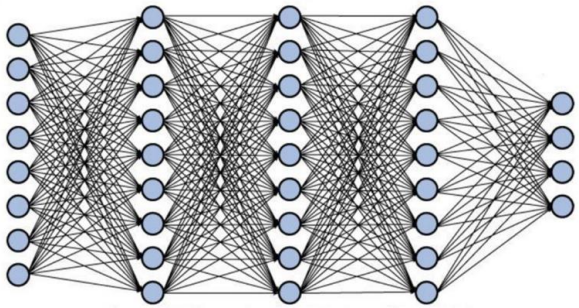
# of learned weights  $\gg$ 

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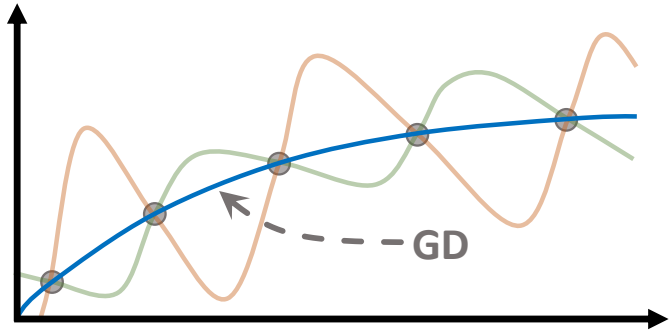
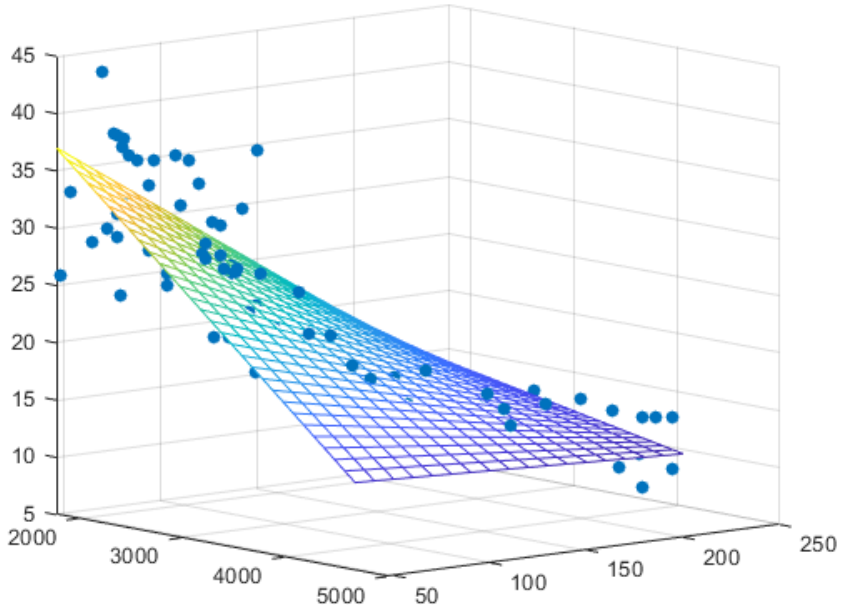


Goal

Mathematically characterize this implicit regularization

Linear Models: Implicit Norm Minimization

Linear Regression



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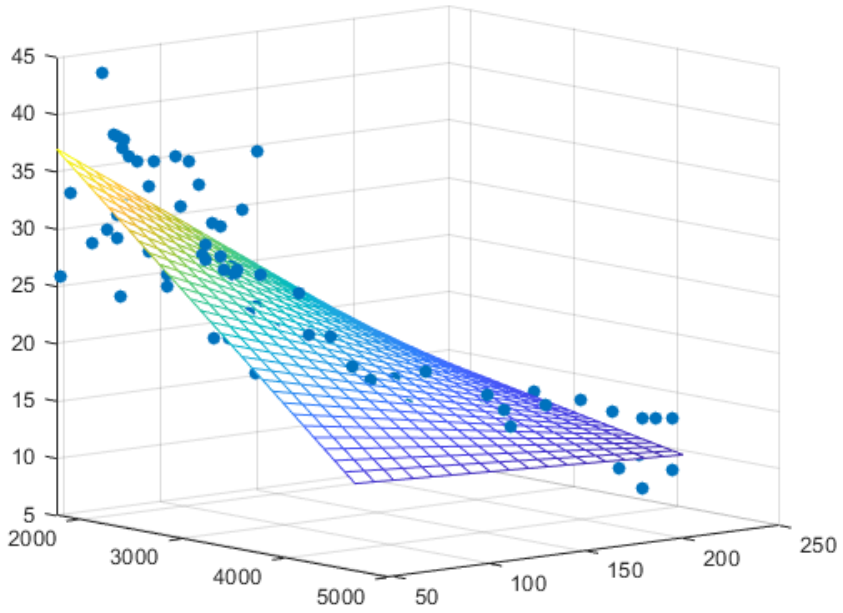

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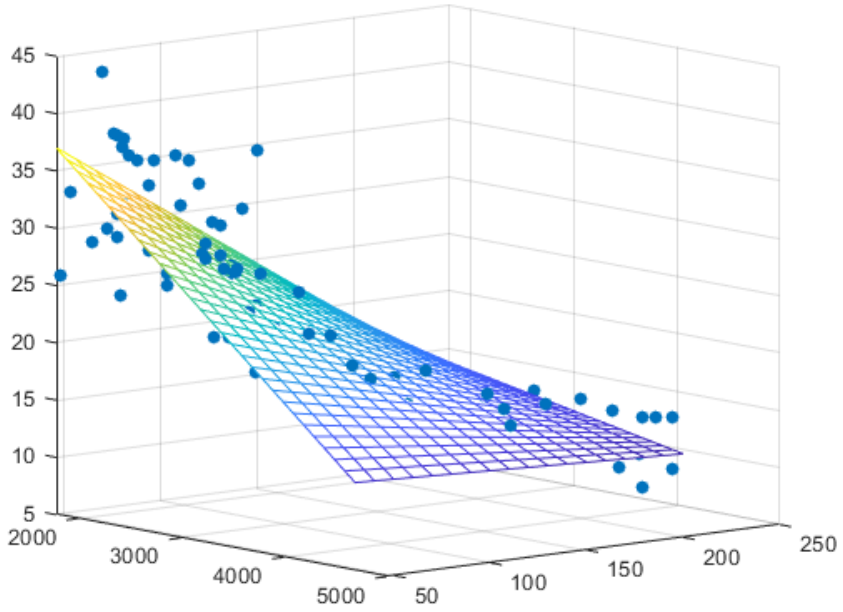

When # of learned weights $>$ # of training examples:

GD initialized at 0 converges to min ℓ_2 norm solution

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

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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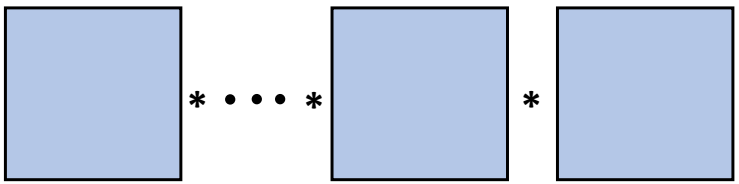
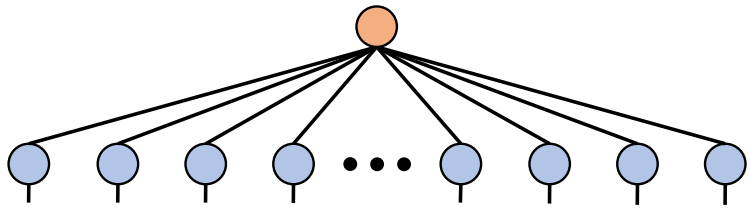
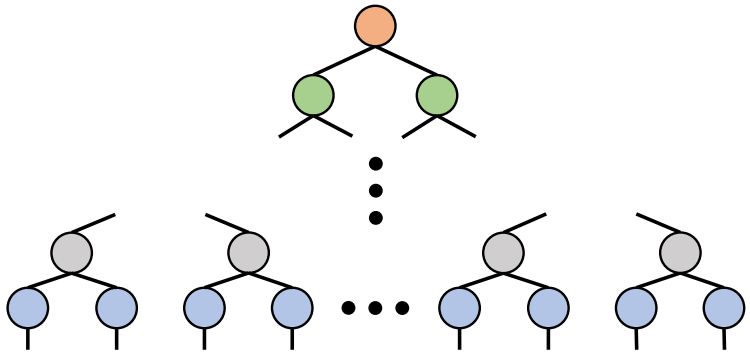
Case will be made via matrix and tensor factorizations



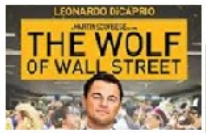




Outline

Matrix Completion $\longleftrightarrow$ Two-Dimensional Prediction

Matrix completion: recover unknown matrix given subset of entries

				
Bob	4	?	?	4
Alice	?	5	4	?
Joe	?	5	?	?

observations $\{y_{i,j}\}_{(i,j)\in\Omega}$

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				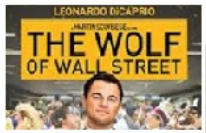
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				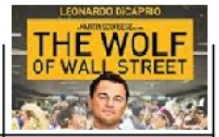
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value of entry (i,j)	$\longleftrightarrow$	label of input (i,j)
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unobserved entries	$\longleftrightarrow$	test data
matrix	$\longleftrightarrow$	predictor

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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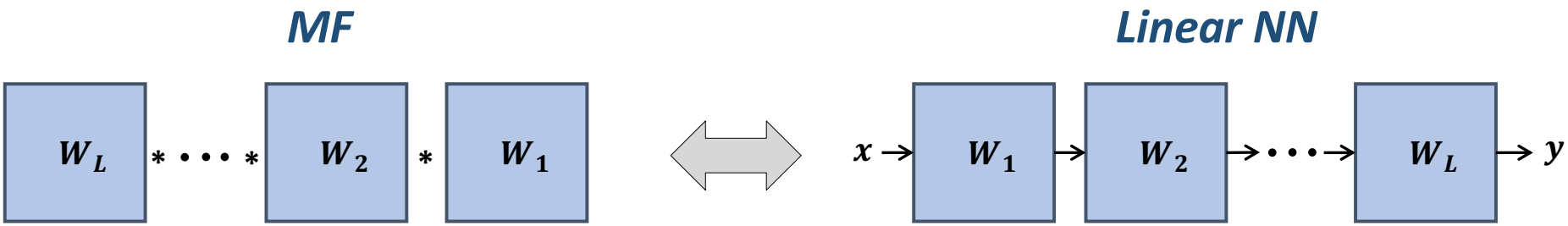

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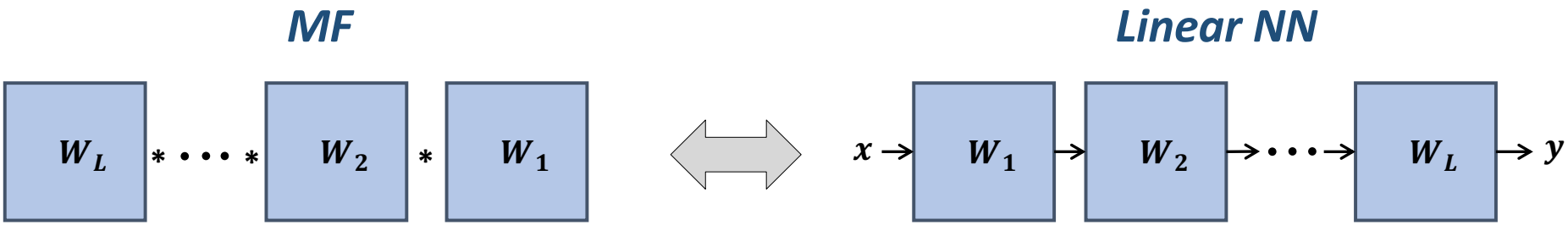

Empirical Phenomenon (Gunasekar et al. 2017)

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

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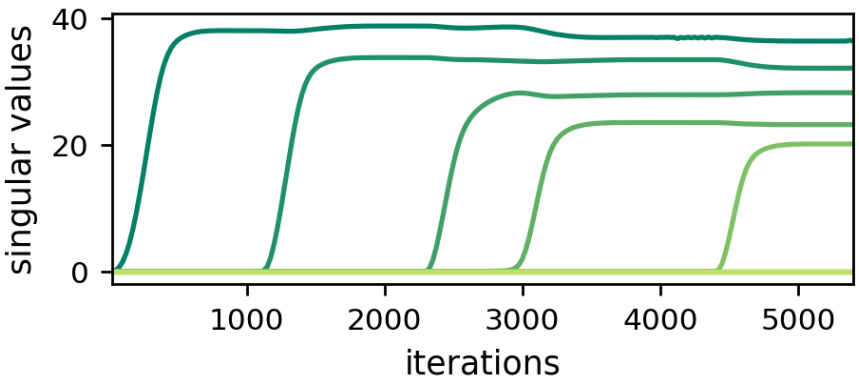

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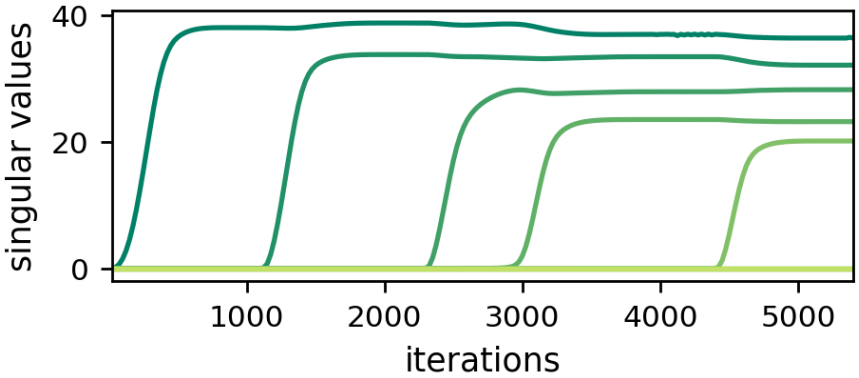

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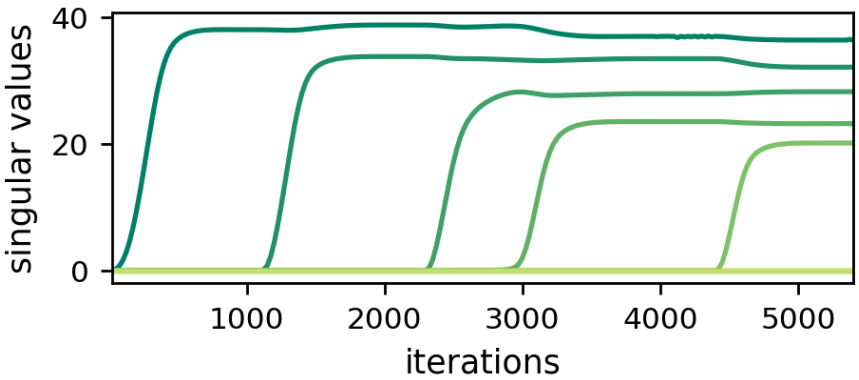

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For any $\|\cdot\|$, *exist observations for which MF* $\not\Rightarrow$ *min* $\|\cdot\|$ *solution*

Outline

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Open question: does implicit regularization in MF minimize a norm?

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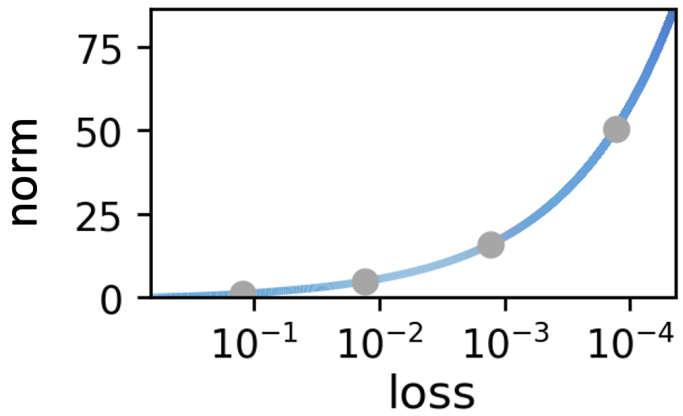

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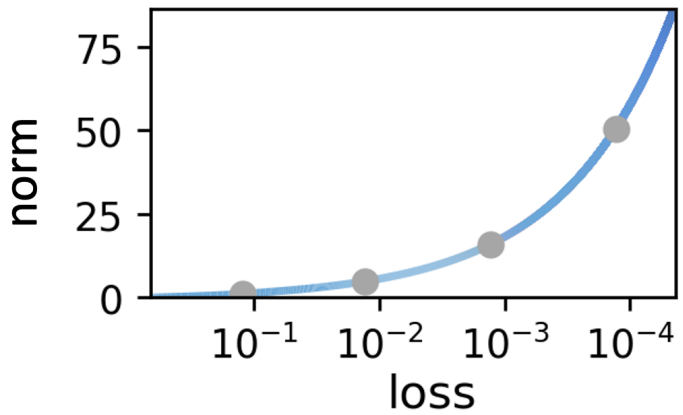
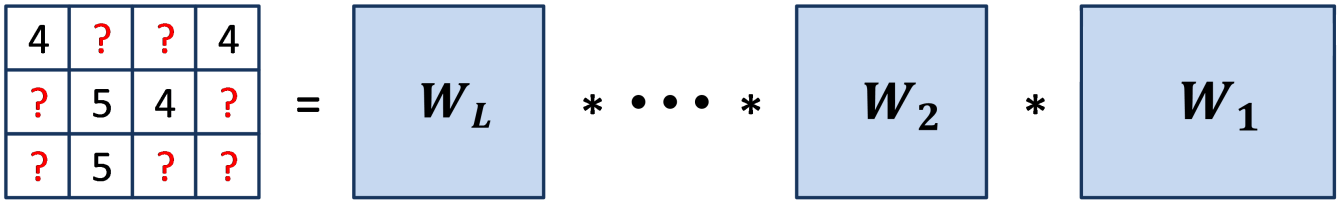


Chou et al. 2020, Li et al. 2021: further support for implicit rank minimization

Outline

Drawbacks of Studying MF



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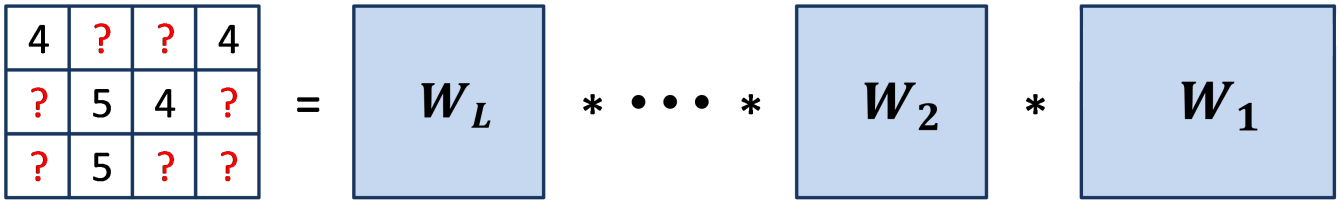

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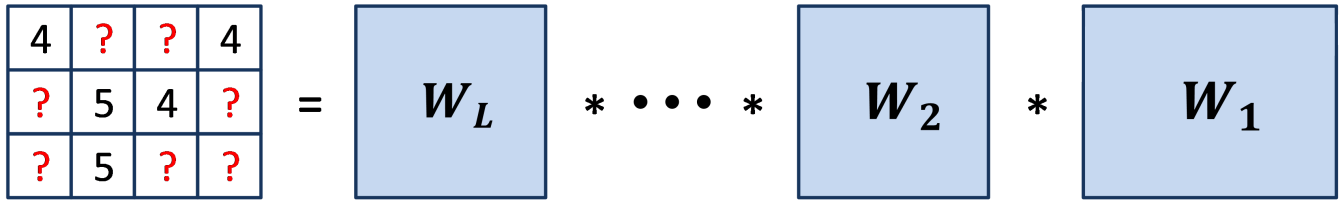

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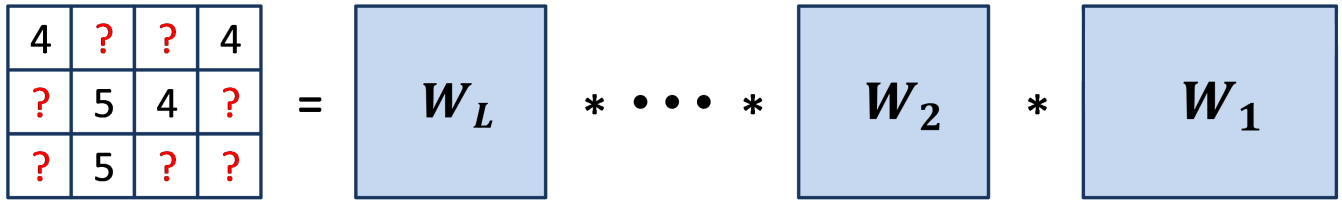

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Tensor factorization accounts for both **(1)** and **(2)**

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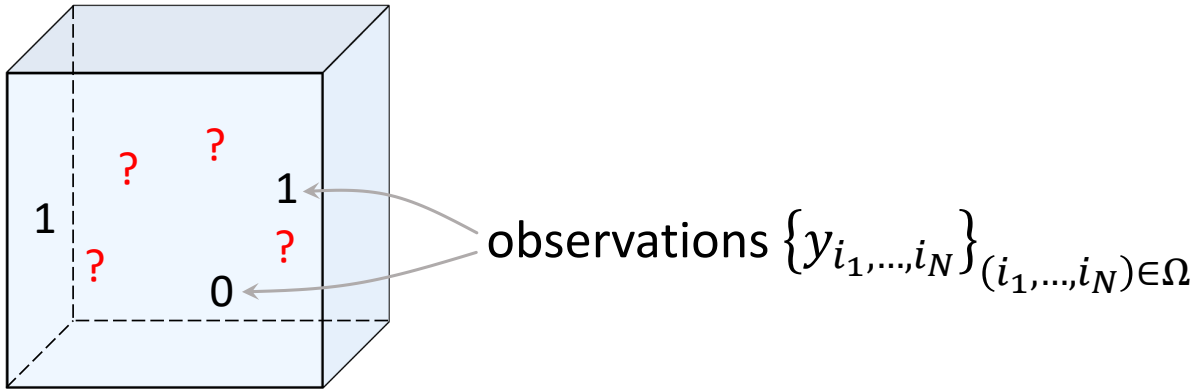

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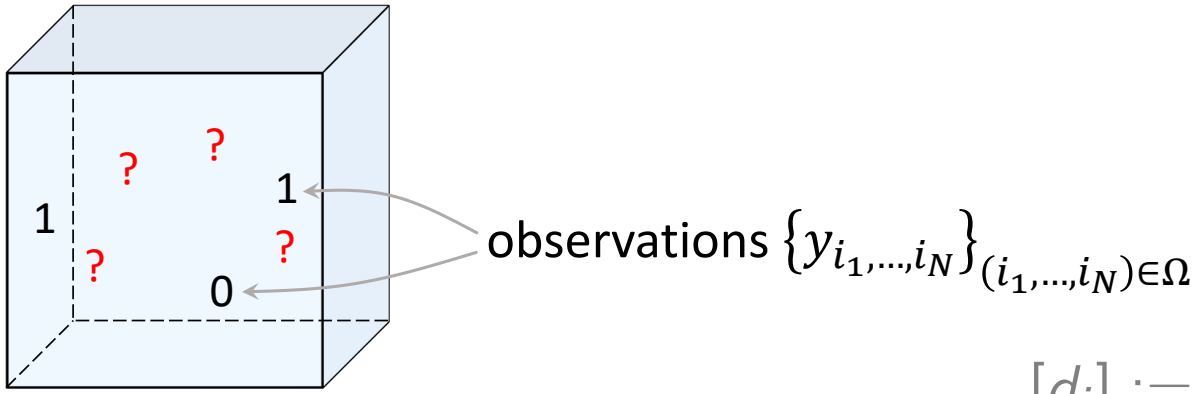

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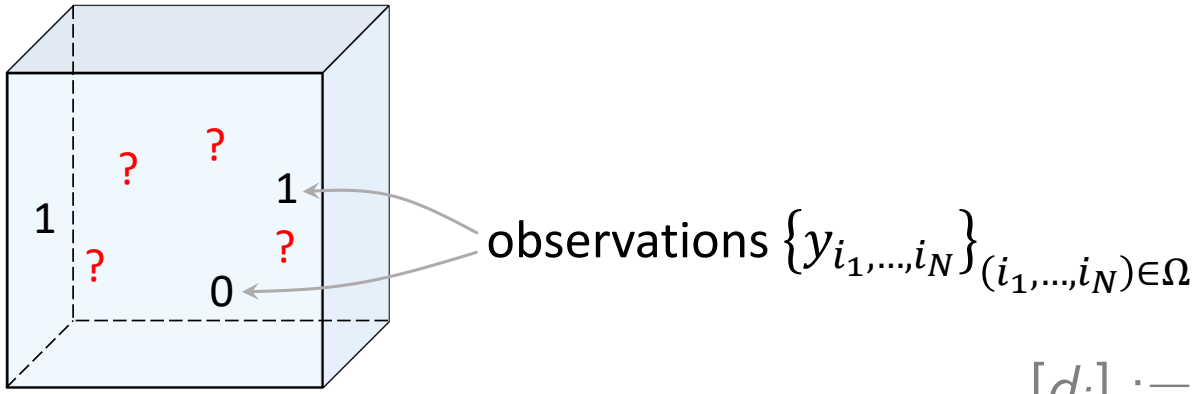

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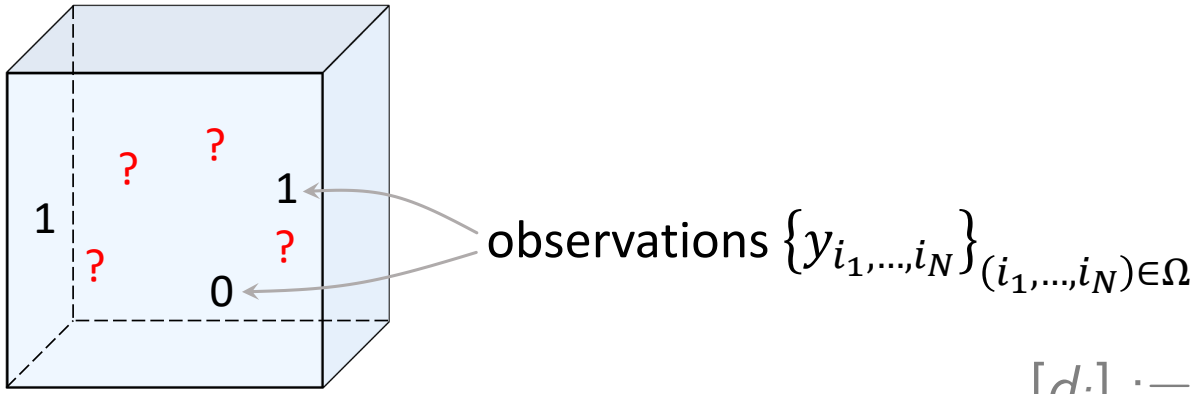

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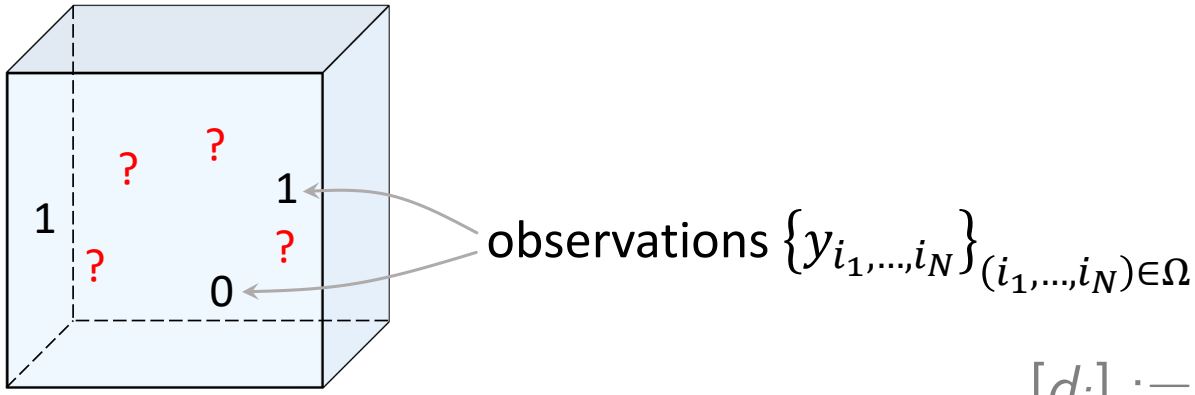

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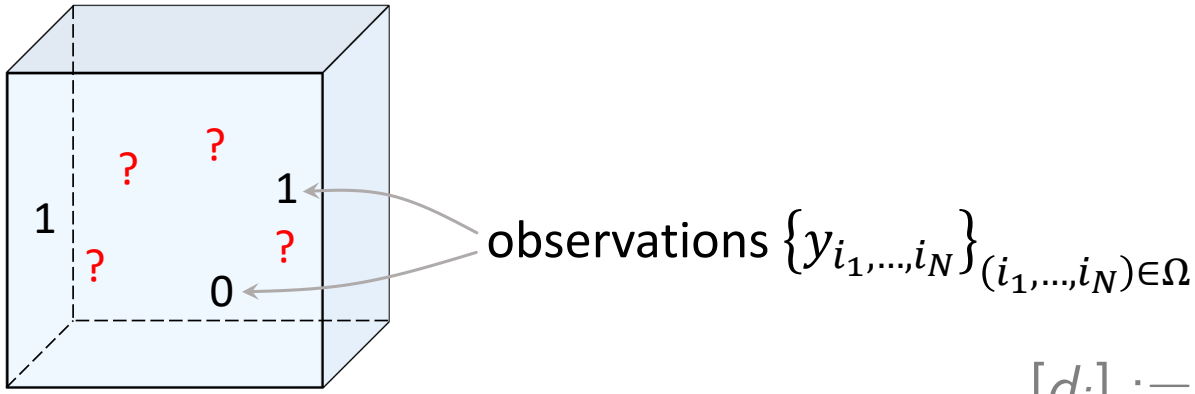

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tensor	$\longleftrightarrow$	predictor

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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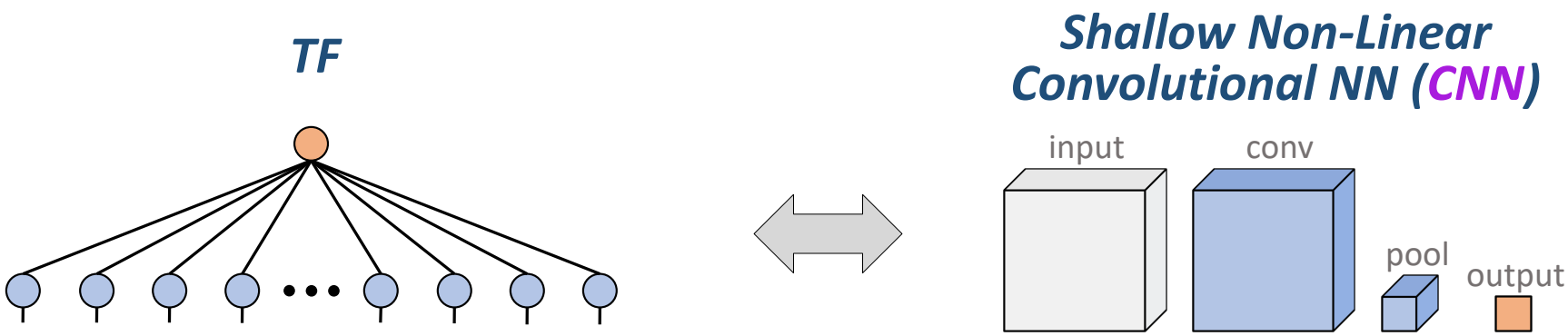

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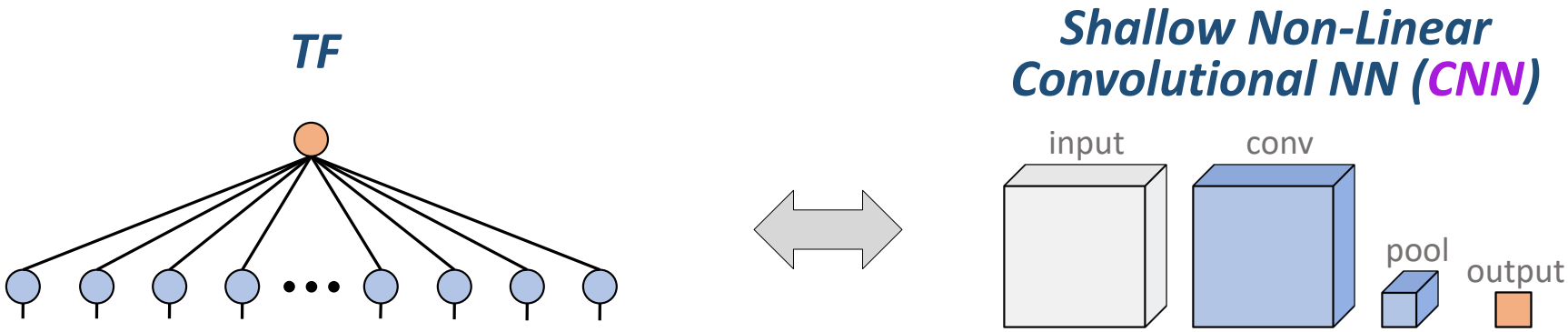

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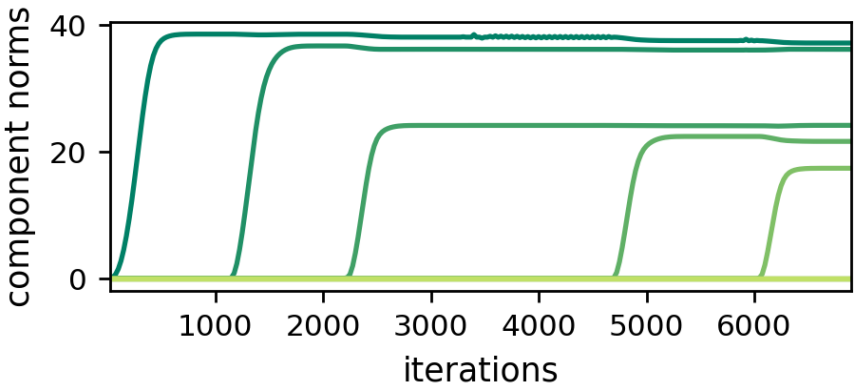

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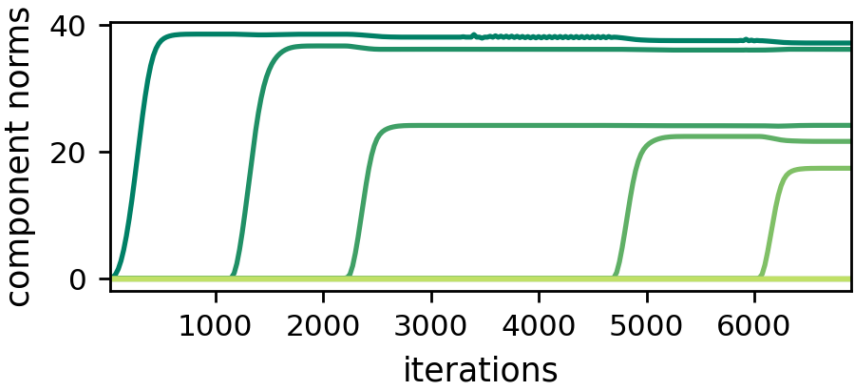

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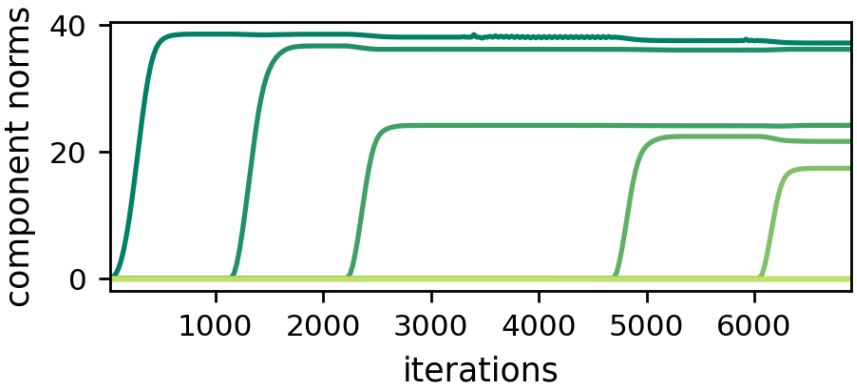
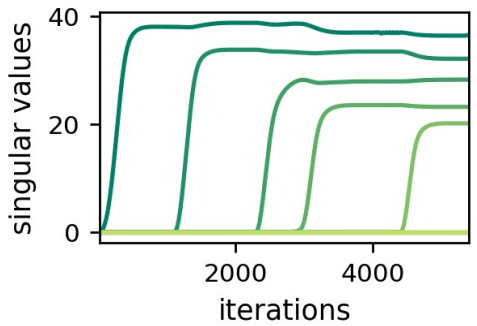
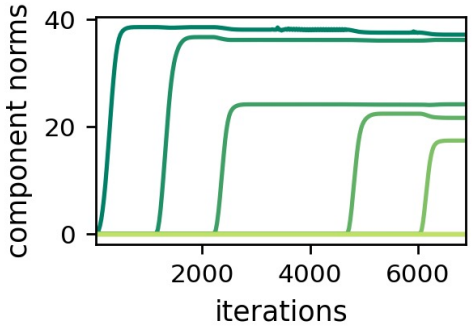


Incremental learning of components leads to low tensor rank!

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
Dynamics	$\frac{d}{dt}\sigma_M^{(r)}(t) \propto \sigma_M^{(r)}(t)^{2-\frac{2}{L}}$	$\frac{d}{dt}\sigma_T^{(r)}(t) \propto \sigma_T^{(r)}(t)^{2-\frac{2}{N}}$
Experiment		
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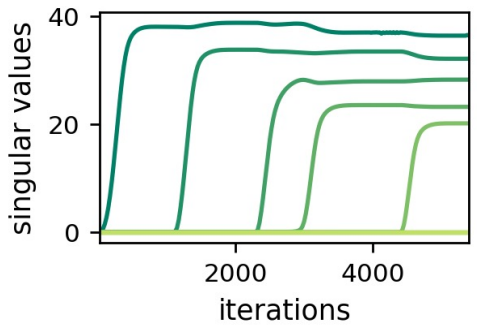
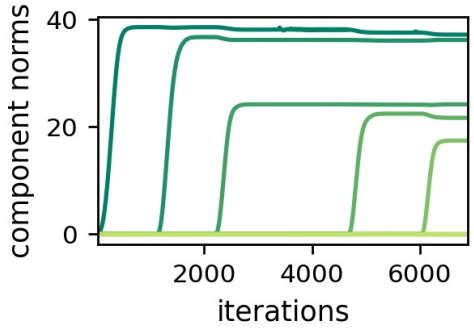
Experiment		
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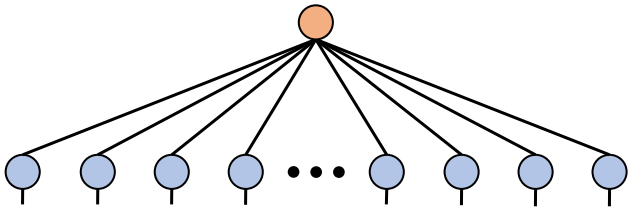
Implicit regularizations in MF and TF have identical structure!

Outline

HTF $\longleftrightarrow$ Deep Non-Linear CNN

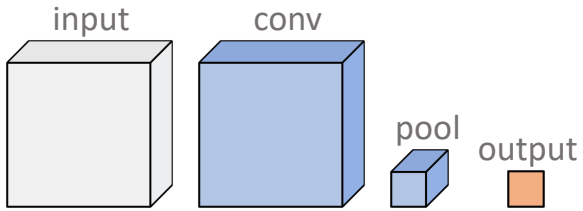
TF does not account for depth

TF
(sum of components)



$\Longleftrightarrow$

Shallow Non-Linear CNN



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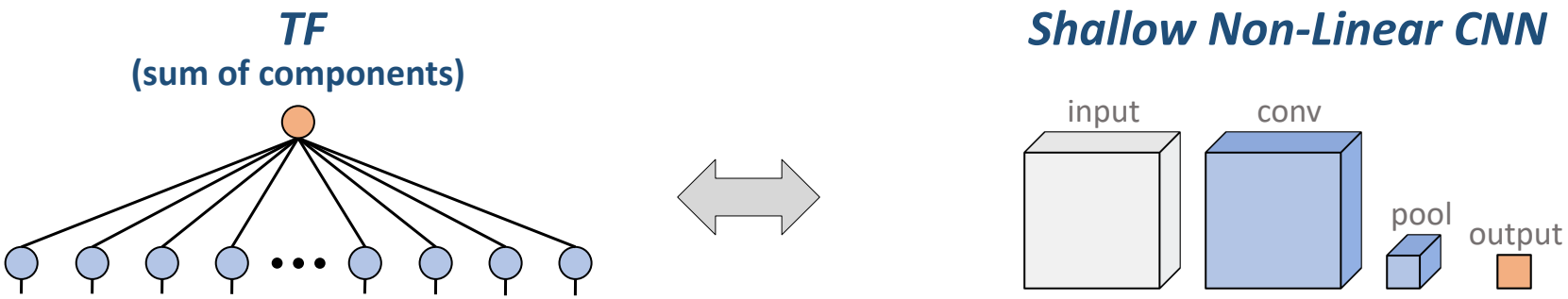
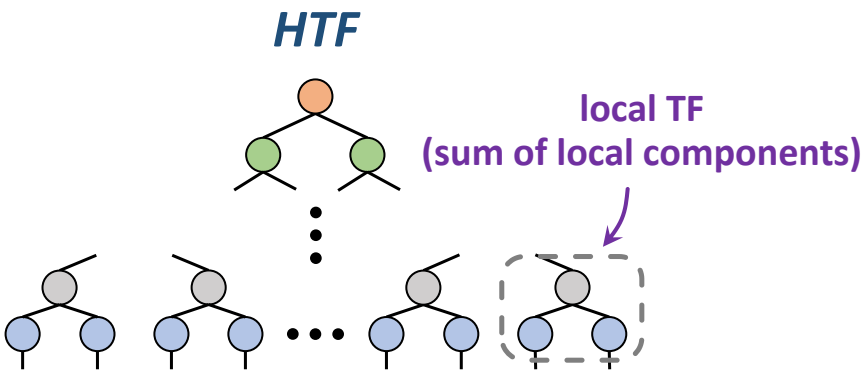


Hierarchical Tensor Factorization (HTF):



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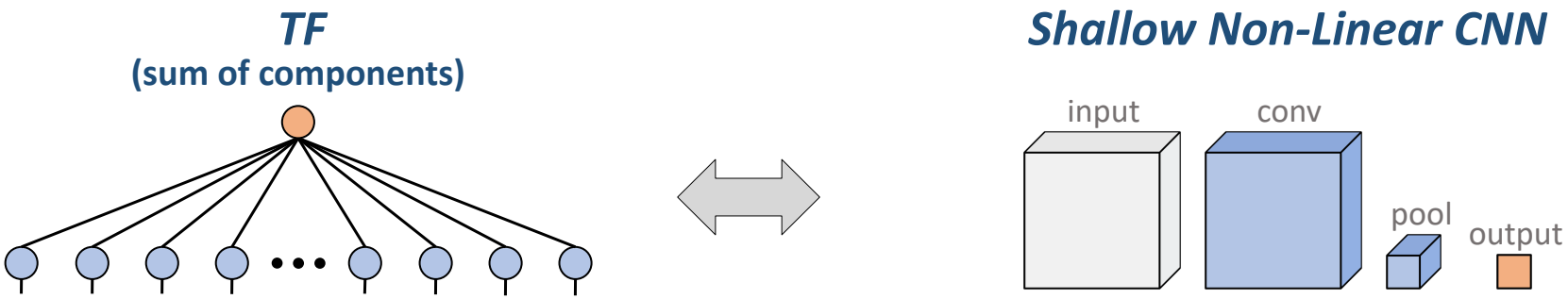

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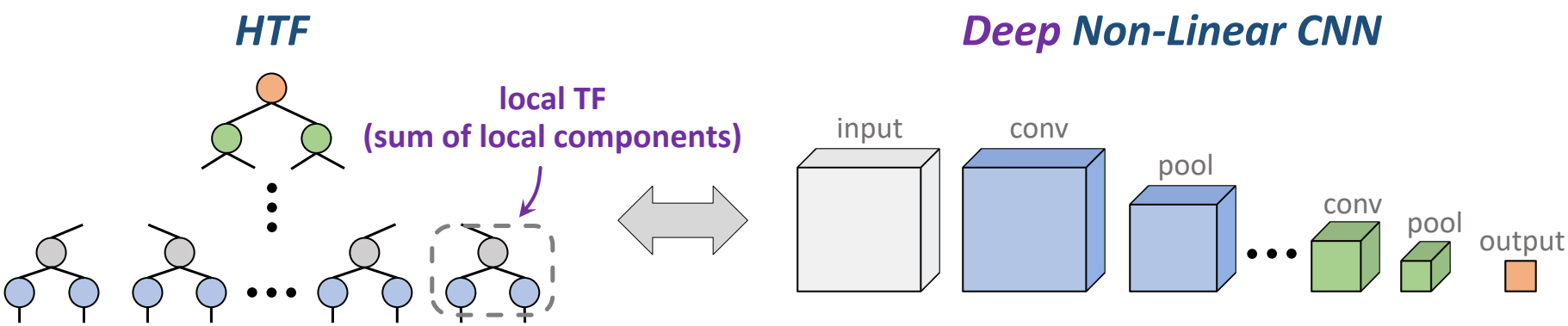

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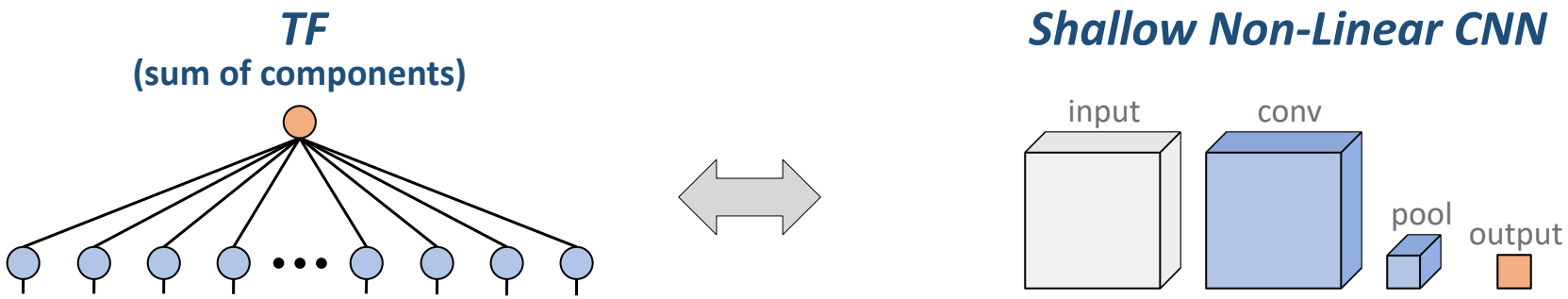

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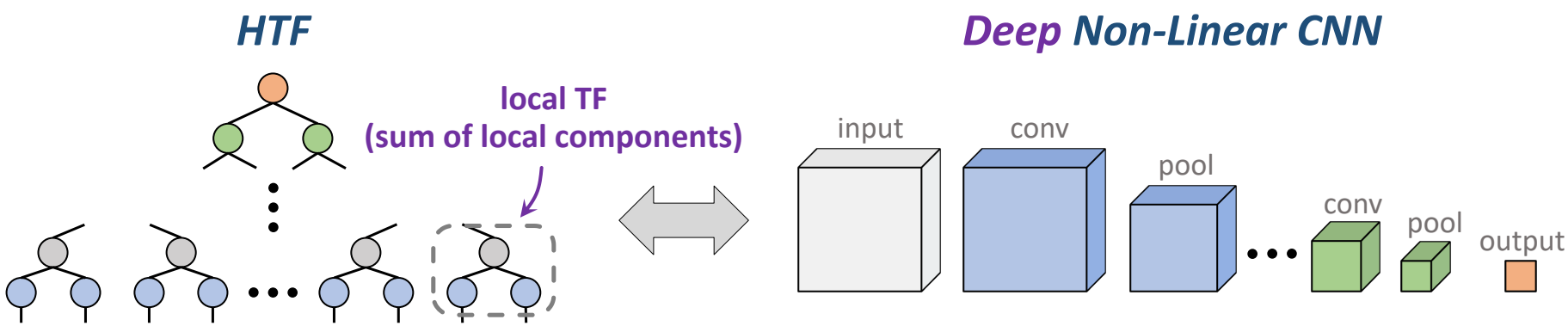

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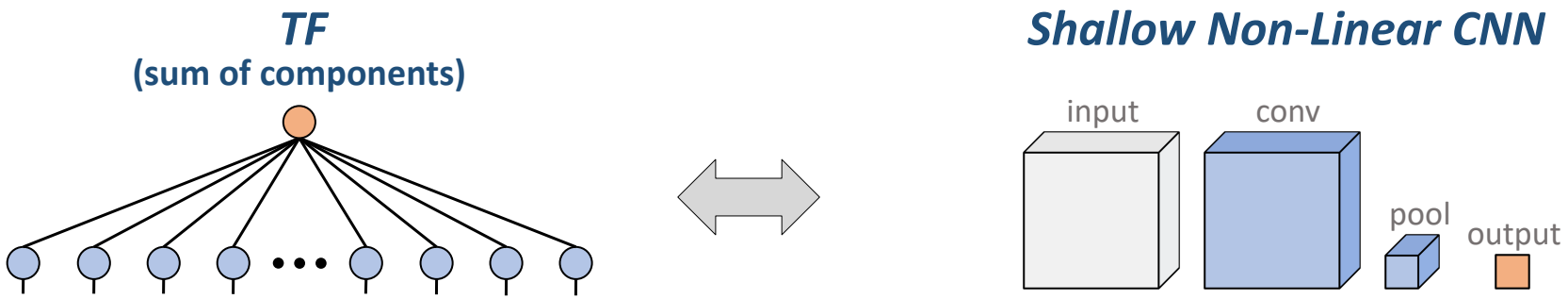

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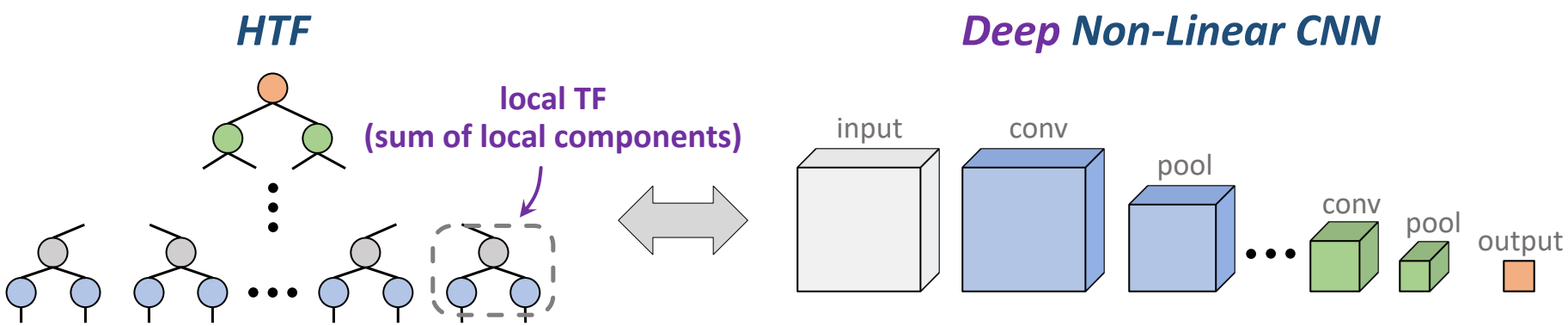

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Representation w/ few local components $\Longrightarrow$ low hierarchical tensor rank

Dynamical Analysis of Implicit Regularization in HTF

$\sigma_H^{(r)}(t)$ — Frobenius norm of r'th local component in a location of HTF

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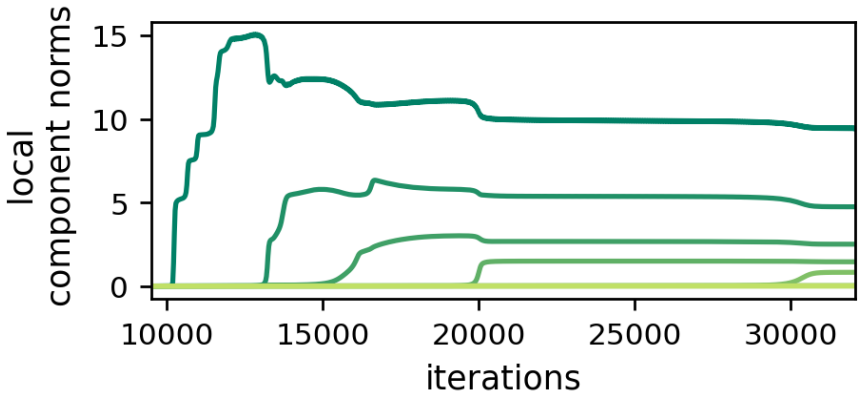

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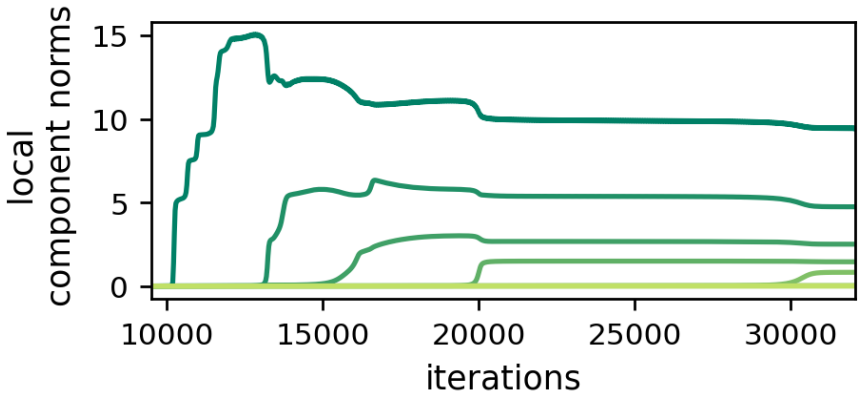

Incremental learning of local components leads to low hierarchical tensor rank!

Analogy Between Implicit Regularizations

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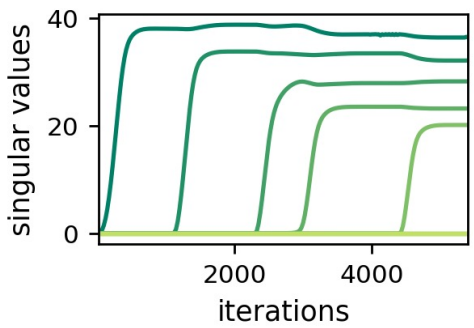
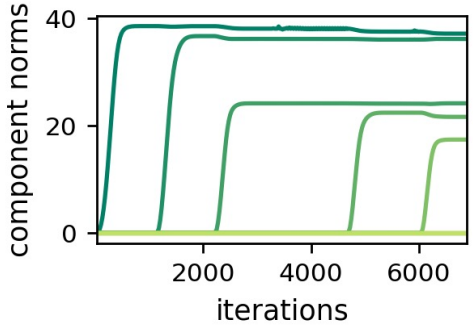
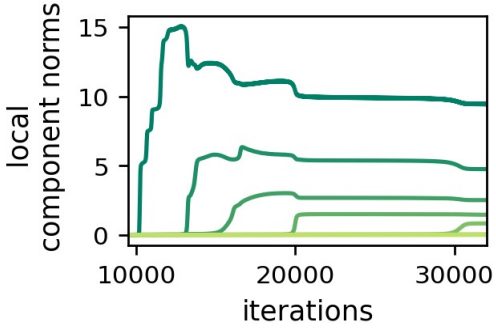
Experiment			
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Quantity	singular values	component norms	local component norms
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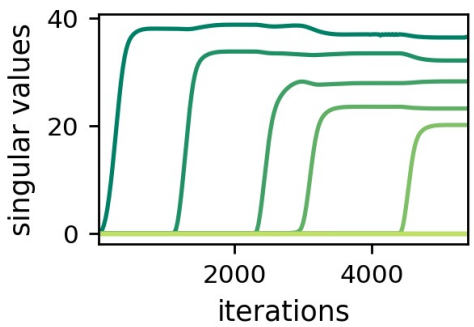
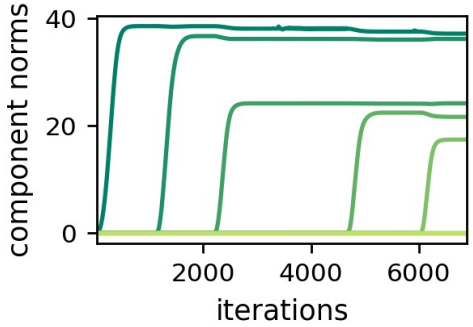
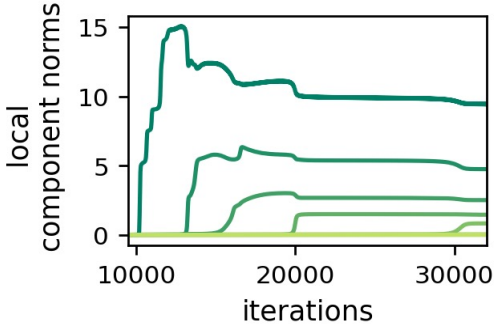
Experiment			
Incremental learning minimizes	**rank**	**tensor rank**	**hierarchical tensor rank**

Implicit regularizations in MF, TF and HTF have identical structure!

Outline

Practical Application: Rank Minimization in NN Layers

Practical Application: Rank Minimization in NN Layers

Parameterize layers of NN as MF / TF / HTF

Practical Application: Rank Minimization in NN Layers

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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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Find complexity measures that:

- Are implicitly minimized by GD over NNs

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

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Implicit minimization of ranks may explain generalization on natural data!

Countering Locality of CNNs via Regularization

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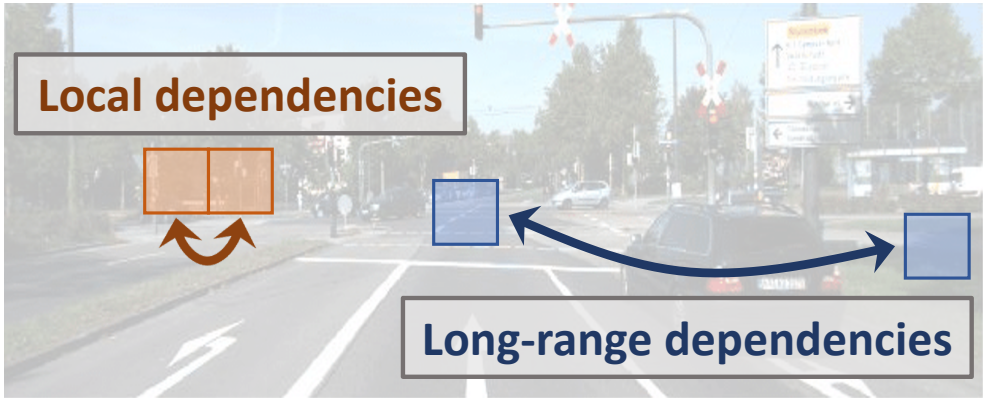
Fact (Cohen & Shashua 2017, Levine et al. 2018)

Hierarchical tensor rank measures long-range dependencies



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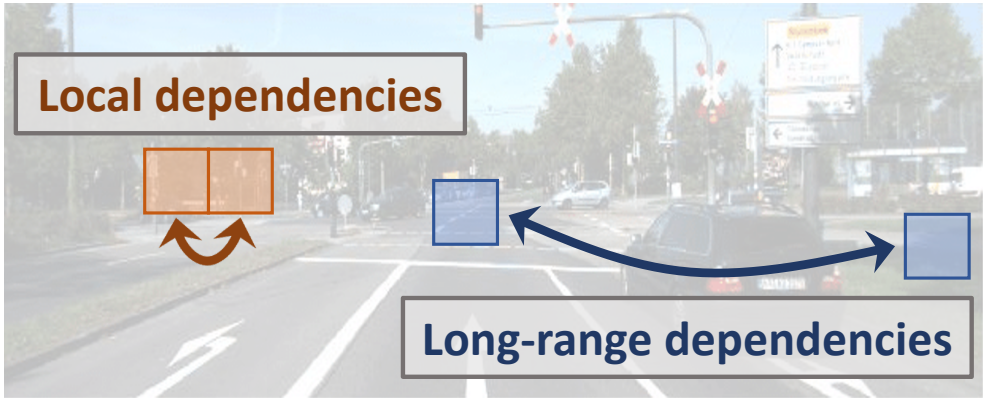

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$\Updownarrow$

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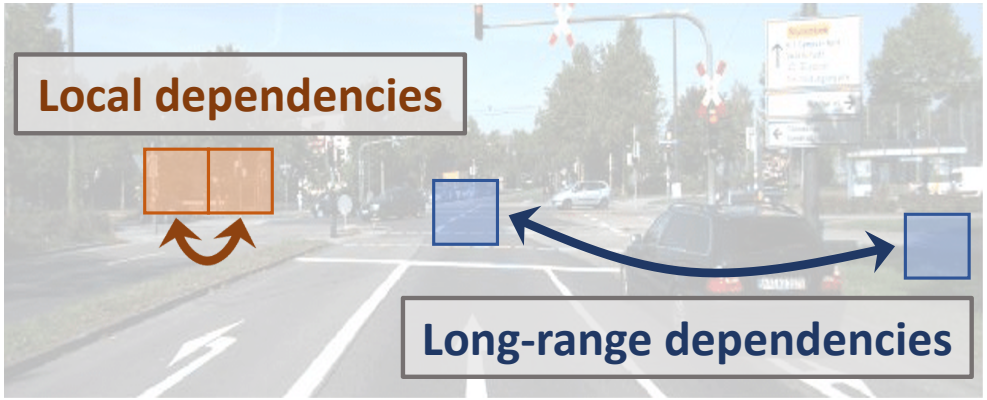

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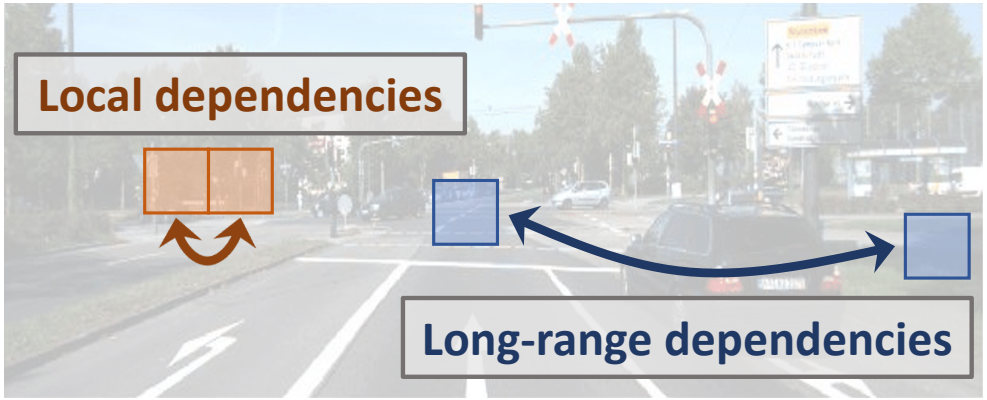

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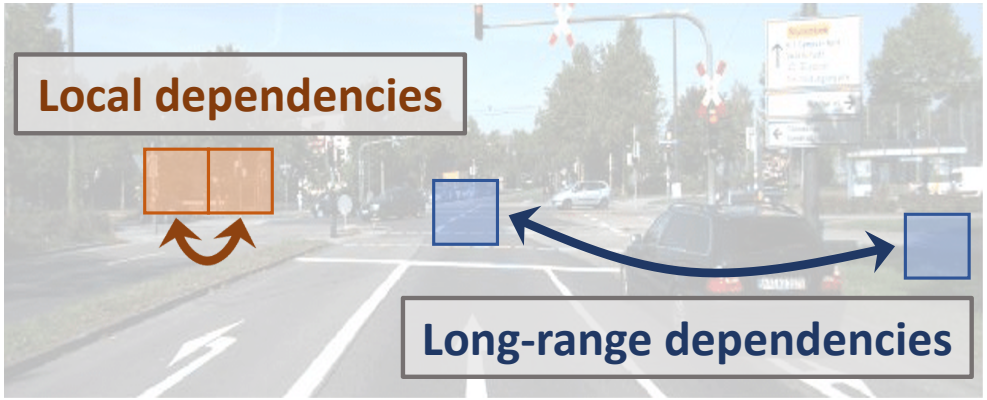

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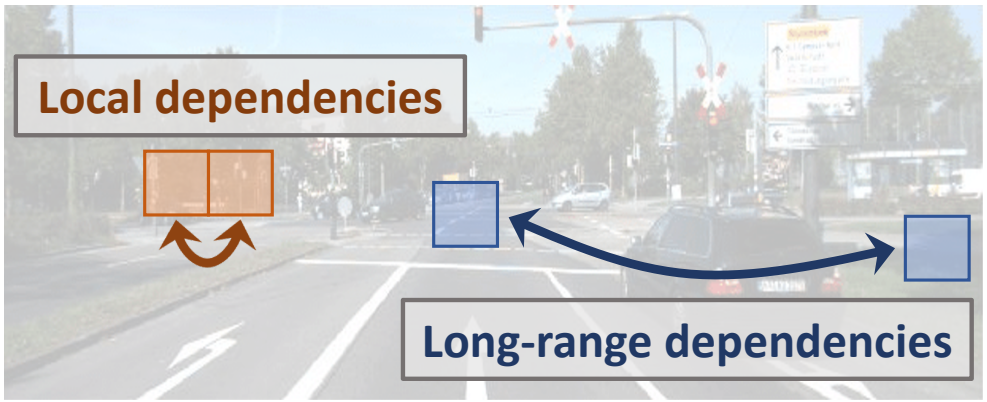

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distance: 0 ✔

distance: 160 ✘

Countering Locality of CNNs via Regularization

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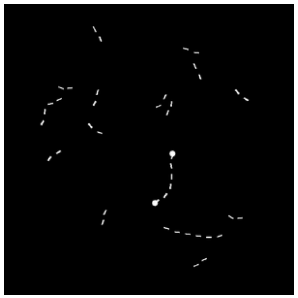
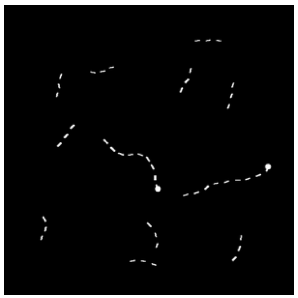
distance: 0 ✔

distance: 160 ✘

length: 6 ✔



length: 9 ✘



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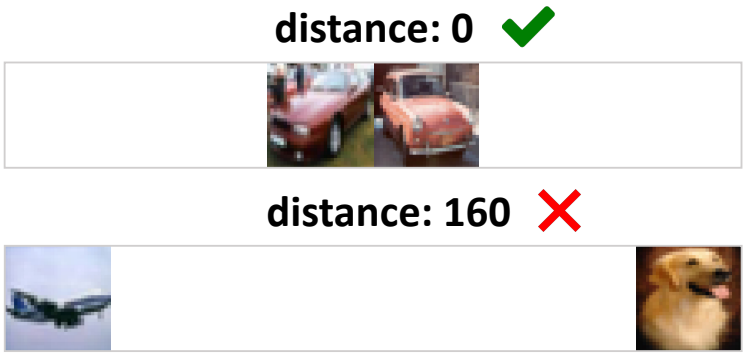

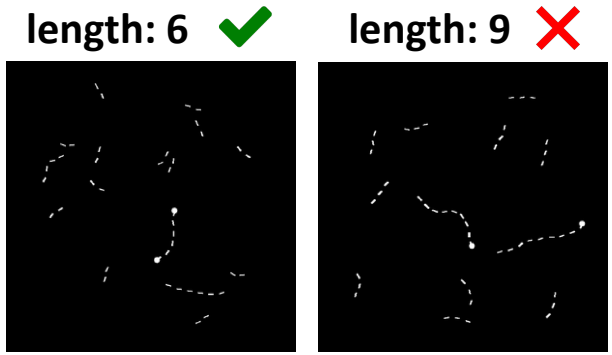

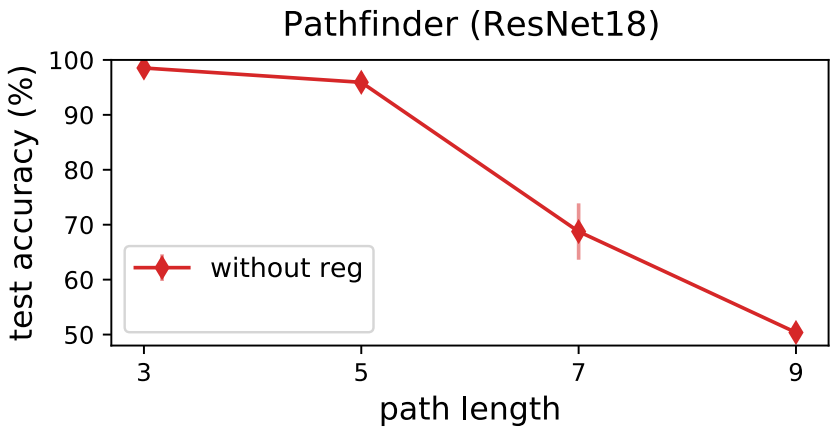

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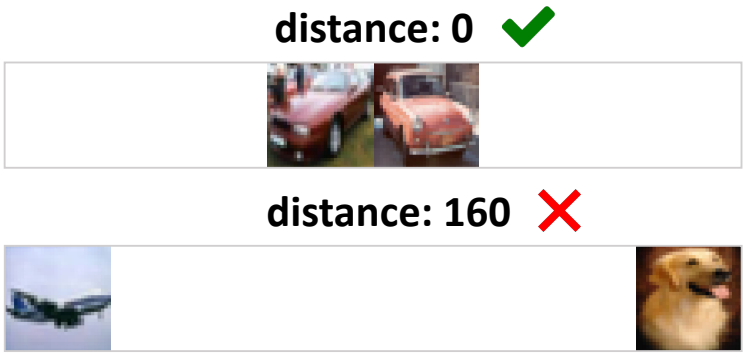
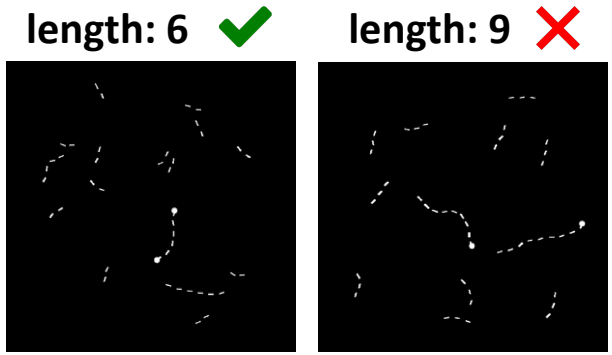
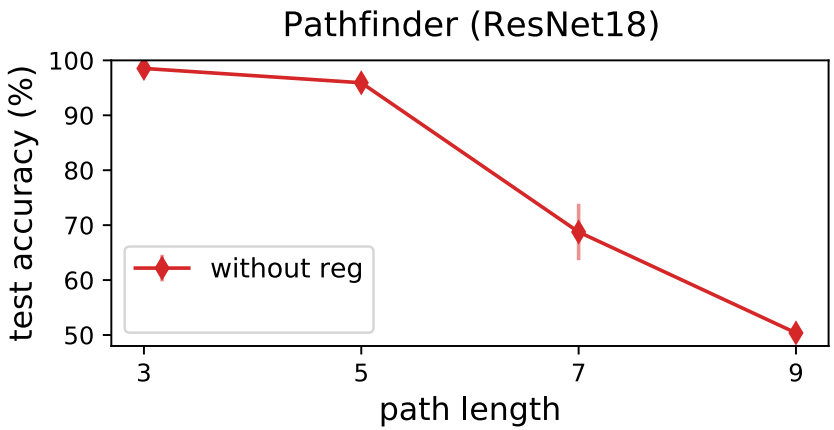




Regularization: promotes high hierarchical tensor rank



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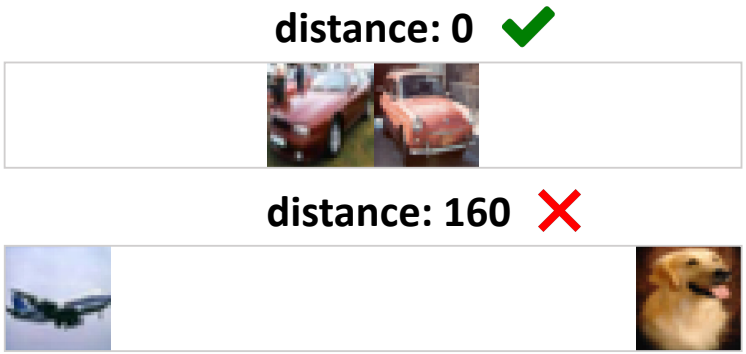

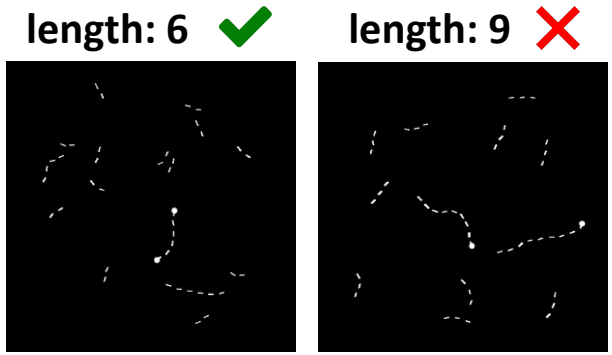

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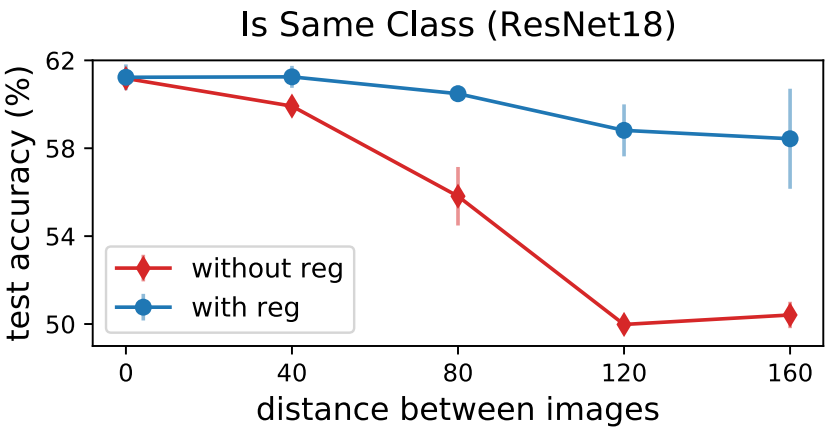

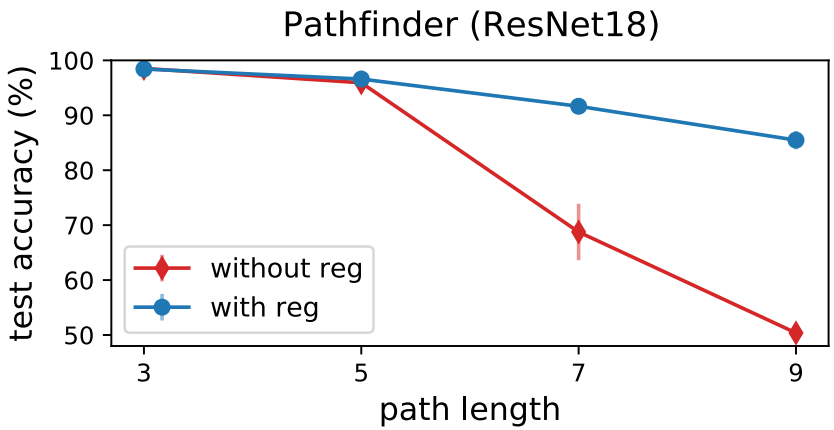

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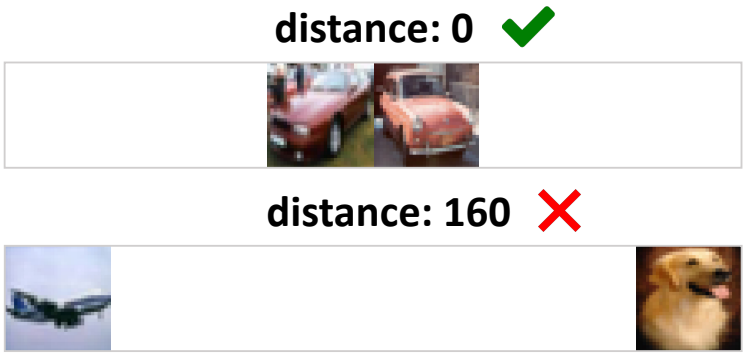

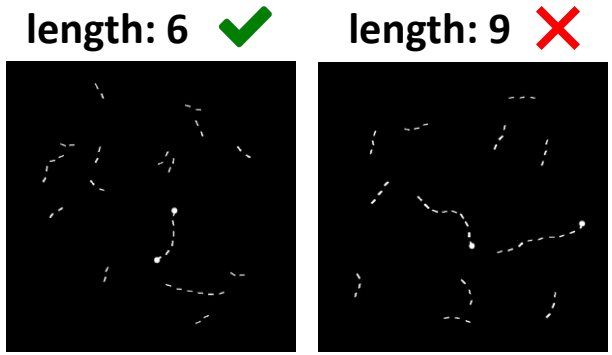

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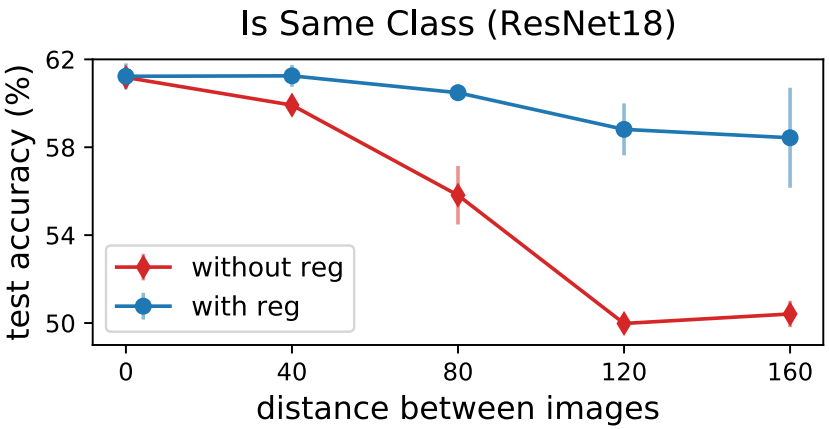

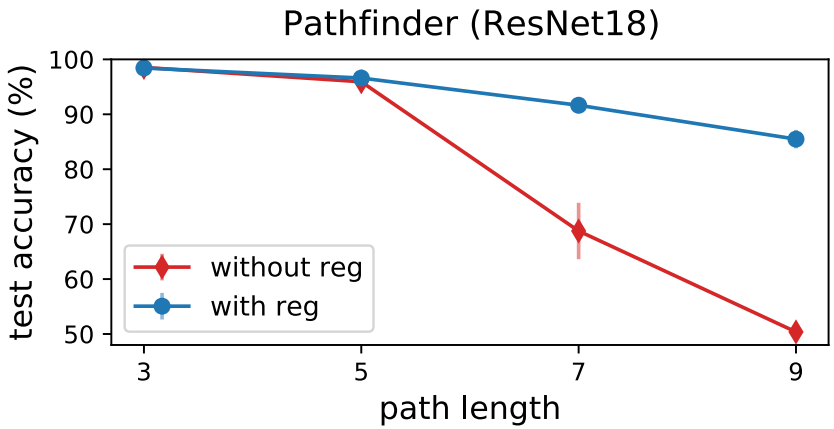

Explicit regularization can improve CNNs on long-range tasks!

Outline

Recap

Goal: understand implicit regularization in deep learning

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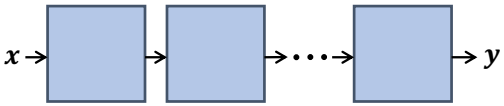
- Rank minimization may explain generalization on natural data
- One may counter locality of CNNs via explicit regularization!

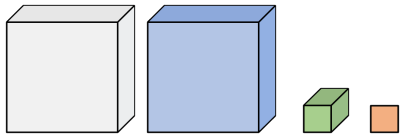
Implicit Rank Minimization in Deep Learning

Linear NN



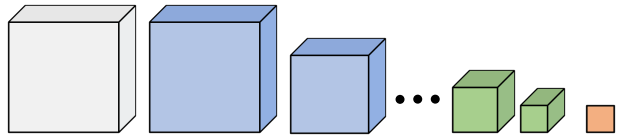
matrix rank minimization

Shallow Non-Linear CNN



tensor rank minimization

Deep Non-Linear CNN



hierarchical tensor rank minimization

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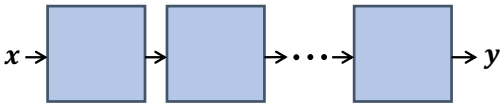

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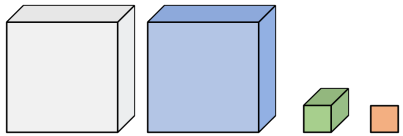

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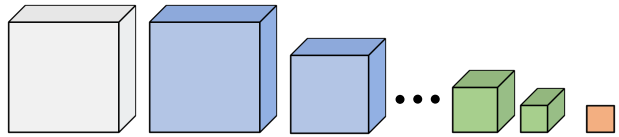
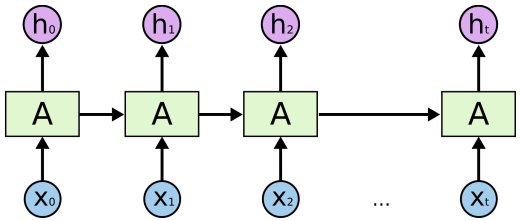
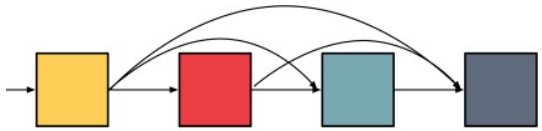


hierarchical tensor rank minimization



??? rank minimization



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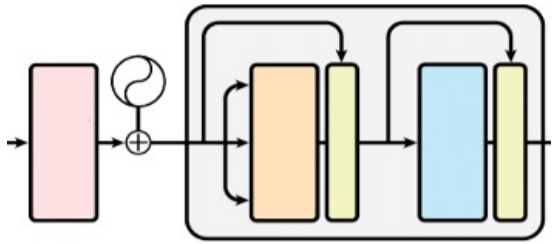
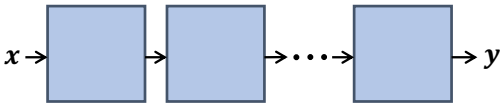


??? rank minimization

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

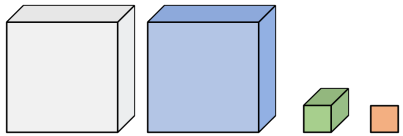
Implicit Rank Minimization in Deep Learning

Linear NN



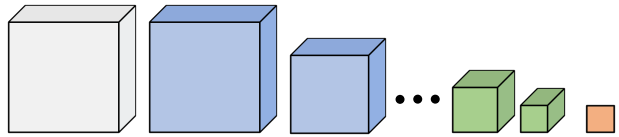
matrix rank minimization

Shallow Non-Linear CNN

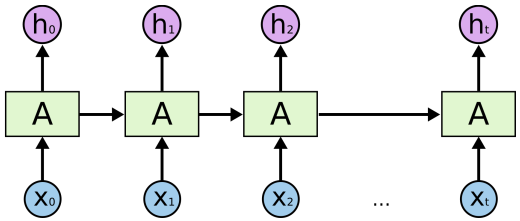


tensor rank minimization

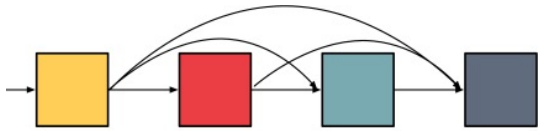
Deep Non-Linear CNN



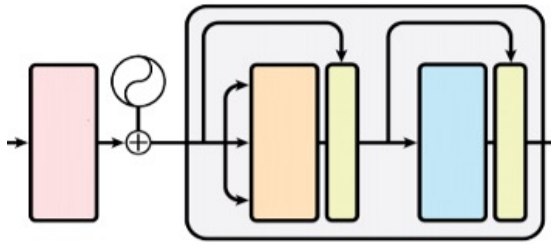
hierarchical tensor rank minimization



??? rank minimization



??? rank minimization



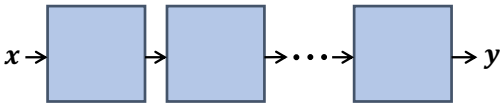
??? rank minimization

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

Discovering minimized notions of rank may pave way to:

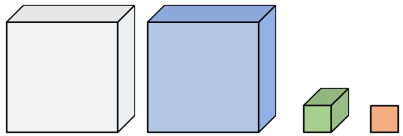
Implicit Rank Minimization in Deep Learning

Linear NN



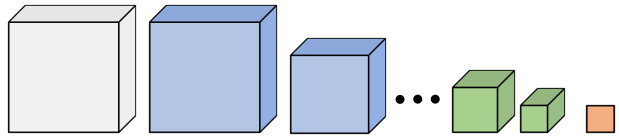
matrix rank minimization

Shallow Non-Linear CNN

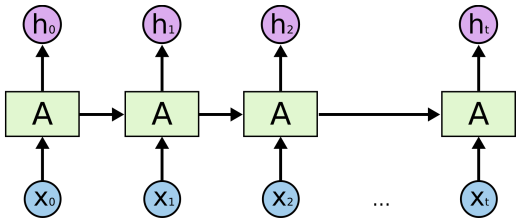


tensor rank minimization

Deep Non-Linear CNN



hierarchical tensor rank minimization



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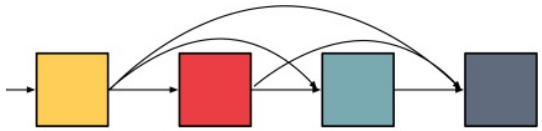

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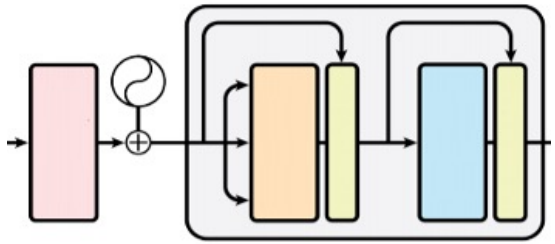

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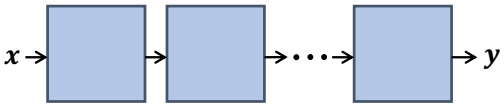
- Explaining generalization

Implicit Rank Minimization in Deep Learning

Linear NN



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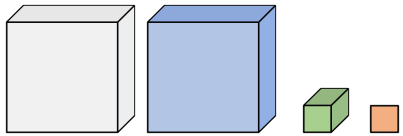
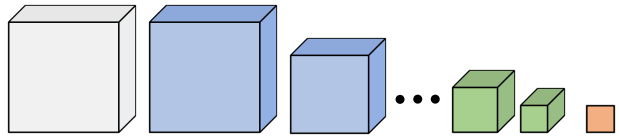
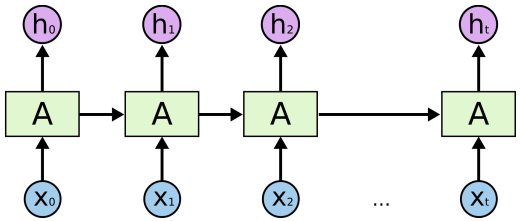


tensor rank minimization

Deep Non-Linear CNN



hierarchical tensor rank minimization



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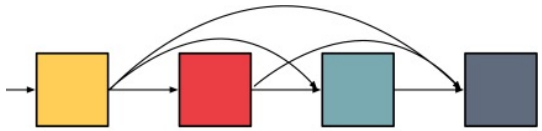

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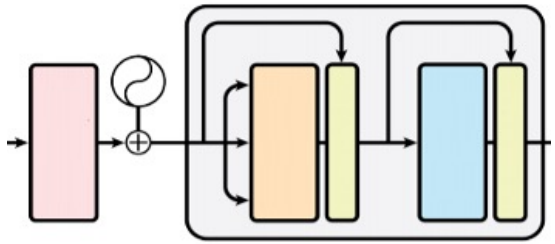

??? rank minimization

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Discovering minimized notions of rank may pave way to:

- Explaining generalization
- Enhancing performance via regularization and architecture design

Thank You!

Work supported by:
Apple Scholars in AI/ML PhD fellowship, Google Research Scholar Award, Google Research Gift, the Yandex Initiative in Machine Learning, the Israel Science Foundation (grant 1780/21), Len Blavatnik and the Blavatnik Family Foundation, Tel Aviv University Center for AI and Data Science, and Amnon and Anat Shashua.