Analyzing Optimization in Deep Learning via Trajectories

Nadav Cohen

Institute for Advanced Study

Institute for Computational and Experimental Research in Mathematics (ICERM)

Workshop on Theory and Practice in Machine Learning and Computer Vision

19 February 2019

EVERY INDUSTRY WANTS DEEP LEARNING

Cloud Service Provider	Medicine	Media & Entertainment	Security & Defense	Autonomous Machines

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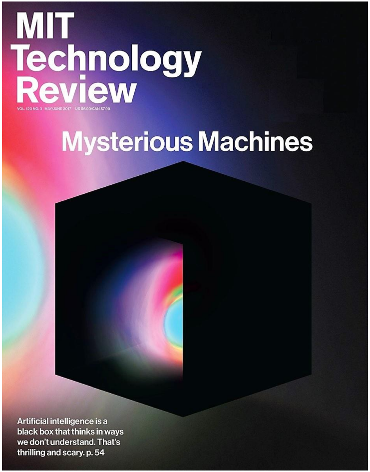
➢ Image/Video classification	➢ Cancer cell detection	➢ Video captioning	➢ Face recognition	➢ Pedestrian detection
➢ Speech recognition	➢ Diabetic grading	➢ Content based search	➢ Video surveillance	➢ Lane tracking
➢ Natural language processing	➢ Drug discovery	➢ Real time translation	➢ Cyber security	➢ Recognize traffic sign

NVIDIA

Source

NVIDIA (www.slideshare.net/openomics/the-revolution-of-deep-learning)

Limited Formal Understanding



Intelligent Machines

The Dark Secret at the Heart of AI

No one really knows how the most advanced algorithms do what they do. That could be a problem.

by Will Knight April 11, 2017

Last year, a strange self-driving car was released onto the quiet roads of Monmouth County, New Jersey. The experimental vehicle, developed by researchers at the chip maker Nvidia, didn't look different from other autonomous cars, but it was unlike anything demonstrated by Google, Tesla, or General Motors, and it showed the rising power of artificial intelligence. The car didn't follow a single instruction provided by an engineer or programmer. Instead, it relied entirely on an algorithm that had taught itself to drive by watching a human do it.

Outline

1. Deep Learning Theory: Expressiveness, Optimization and Generalization

2. Analyzing Optimization via Trajectories

3. Trajectories of Gradient Descent for Deep Linear Neural Networks
    - Convergence to Global Optimum
    - Acceleration by Depth

4. Conclusion

Statistical Learning Setup

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Given training set $S = \{(X_i, y_i)\}_{i=1}^m$ drawn i.i.d. from $\mathcal{D}$, return hypothesis (predictor) $h : \mathcal{X} \to \mathcal{Y}$ that minimizes population loss:

$$L_{\mathcal{D}}(h) := \mathbb{E}_{(X,y)\sim\mathcal{D}}[\ell(y, h(X))]$$

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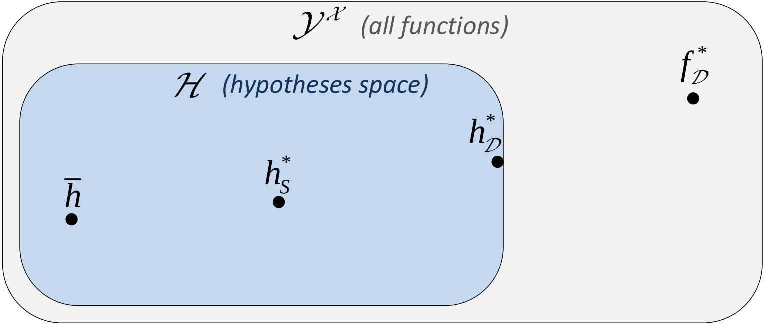
Approach

Predetermine hypotheses space $\mathcal{H}\subset\mathcal{Y}^{\mathcal{X}}$, and return hypothesis $h\in\mathcal{H}$ that minimizes empirical loss:

$$L_S(h):=\frac{1}{m}\sum\nolimits_{i=1}^m\ell(y_i,h(X_i))$$

Three Pillars of Statistical Learning Theory: Expressiveness, Generalization and Optimization



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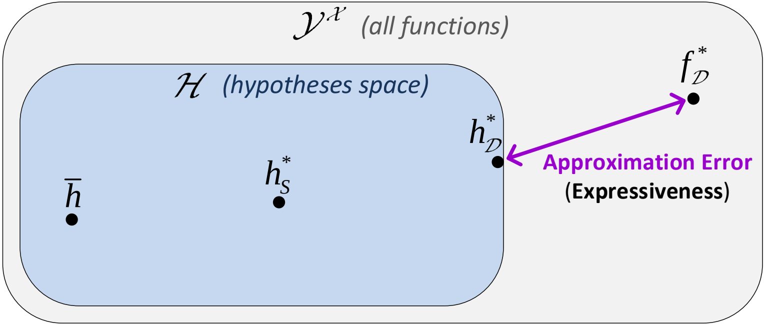

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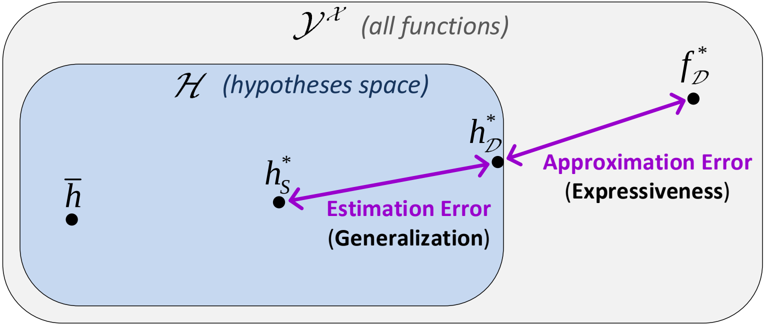

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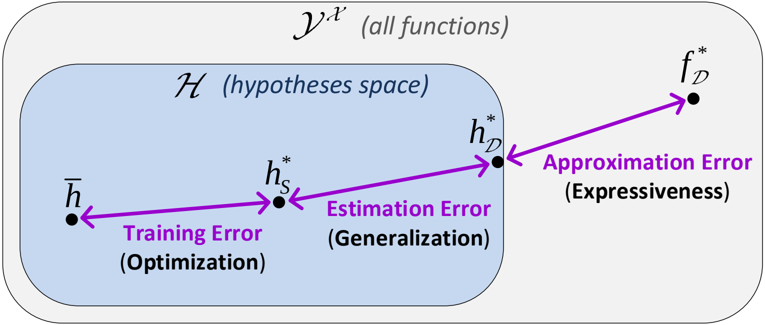

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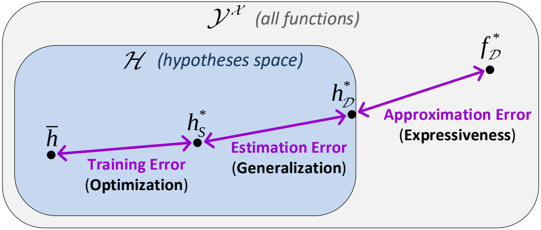

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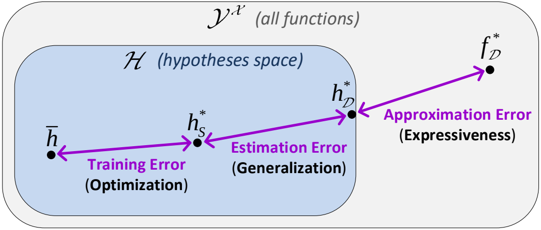

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Empirical loss minimization is a convex program:

$$\bar{h} \approx h^*_S \quad (\text{ training err} \approx 0 \text{ })$$

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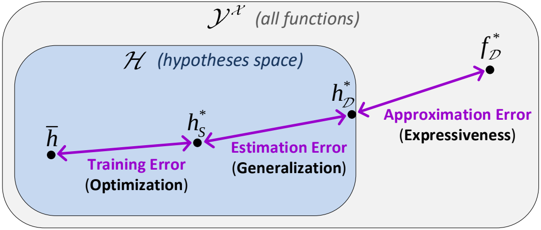

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Bias-variance trade-off:

$\mathcal{H}$	approximation err	estimation err
expands	$\searrow$	$\nearrow$
shrinks	$\nearrow$	$\searrow$

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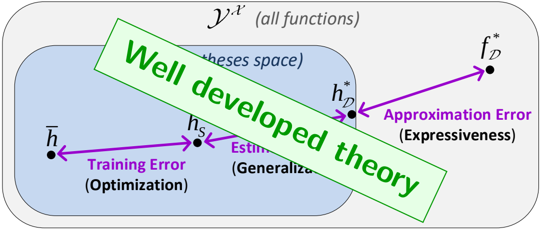

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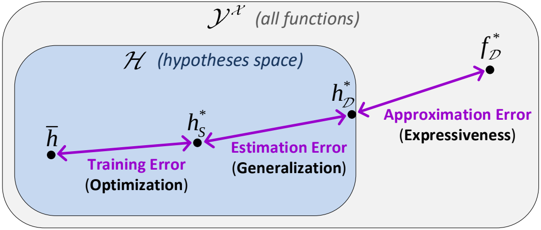

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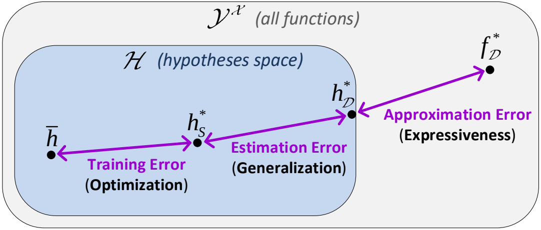

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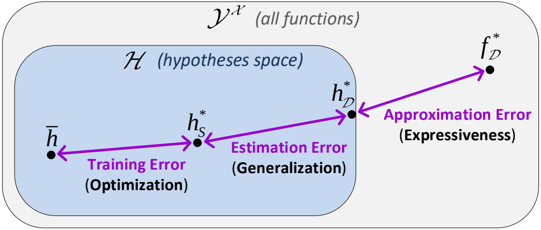

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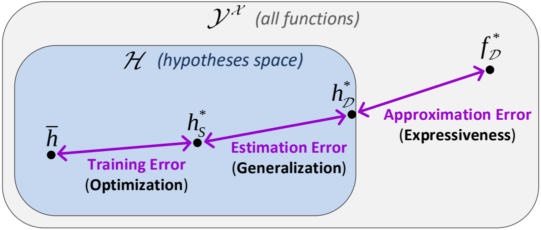

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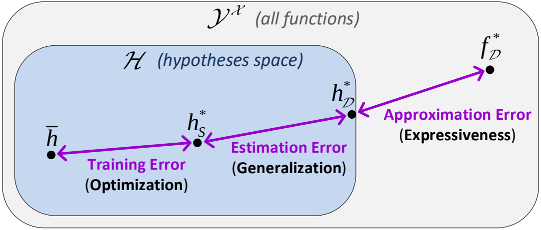

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Vast difference from classical ML:

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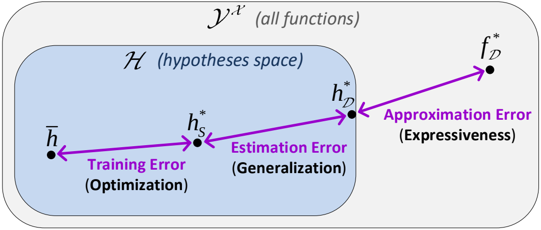

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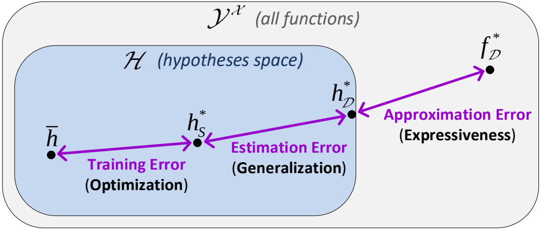

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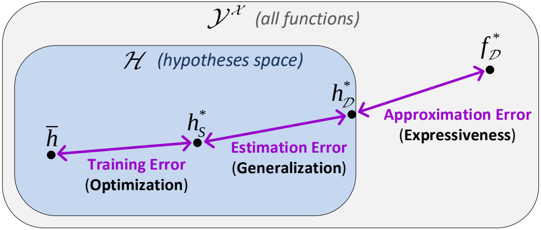

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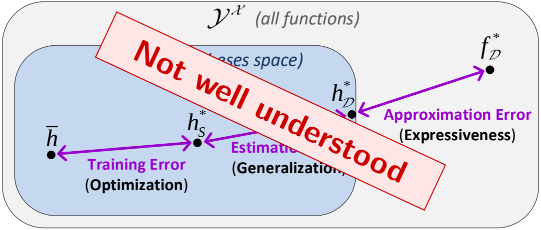

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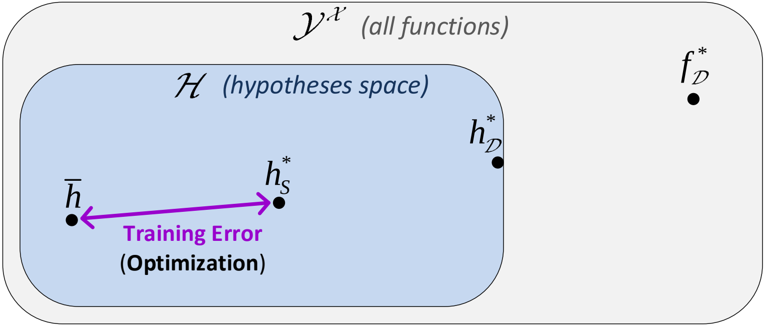

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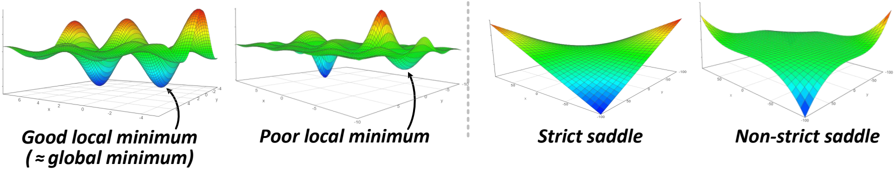
Approach: Convergence via Critical Points

Prominent approach for analyzing optimization in DL is via critical points ($\nabla = 0$) in loss landscape



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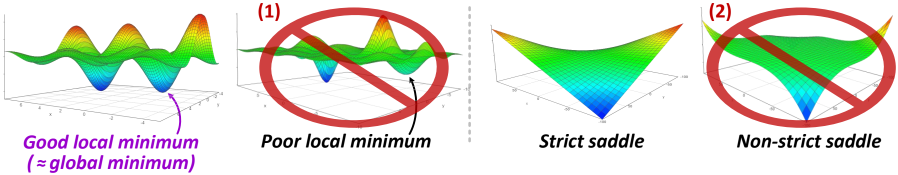

Result *(cf. Ge et al. 2015; Lee et al. 2016)*

If: **(1)** there are no poor local minima; and **(2)** all saddle points are strict, then gradient descent (GD) converges to global minimum

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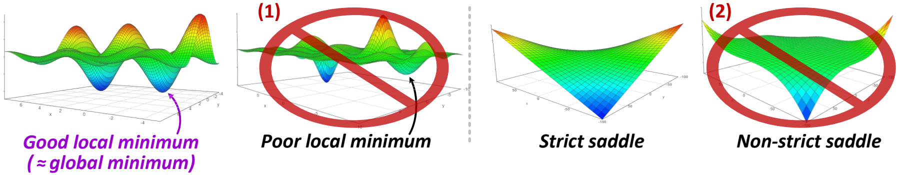

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Motivated by this, many[1] studied the validity of **(1)** and/or **(2)**

[1] e.g. Haeffele & Vidal 2015; Kawaguchi 2016; Soudry & Carmon 2016; Safran & Shamir 2018

Limitations

Convergence of GD to global min was proven via critical points only for problems involving shallow (2 layer) models

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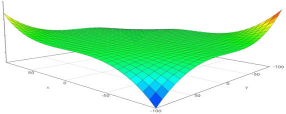

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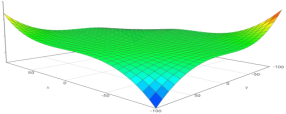
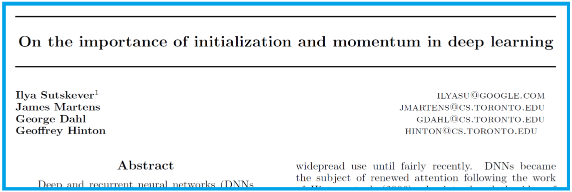


- Algorithmic aspects essential for convergence w/deep models, e.g. proper initialization, are ignored



On the importance of initialization and momentum in deep learning

Ilya Sutskever[1] ILYASU@GOOGLE.COM
James Martens JMARTENS@CS.TORONTO.EDU
George Dahl GDAHL@CS.TORONTO.EDU
Geoffrey Hinton HINTON@CS.TORONTO.EDU

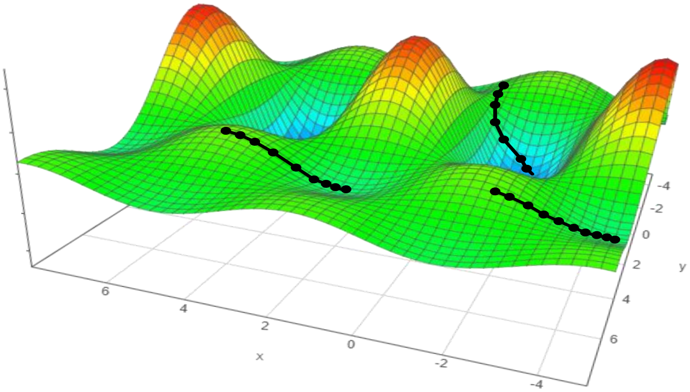
Abstract

Deep and recurrent neural networks (DNNs

widespread use until fairly recently. DNNs became the subject of renewed attention following the work

Optimizer Trajectories Matter

Different optimization trajectories may lead to qualitatively different results



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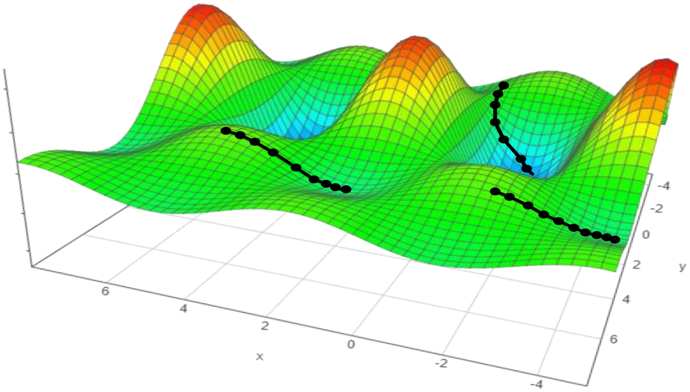

$\Longrightarrow$ details of algorithm and init should be taken into account!

Existing Trajectory Analyses

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Trajectory approach led to successful analyses of shallow models:

- Brutzkus & Globerson 2017
- Li & Yuan 2017
- Zhong et al. 2017
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For deep linear residual networks, trajectories were used to show efficient convergence of GD to global min (Bartlett et al. 2018)

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Sources

On the Optimization of Deep Networks: Implicit Acceleration by Overparameterization

Arora + ***C*** + Hazan (alphabetical order)

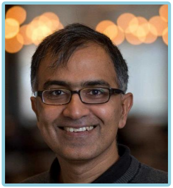
International Conference on Machine Learning (ICML) 2018

A Convergence Analysis of Gradient Descent for Deep Linear Neural Networks

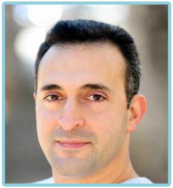
Arora + ***C*** + Golowich + Hu (alphabetical order)

To appear: International Conference on Learning Representations (ICLR) 2019

Collaborators

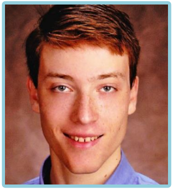


Sanjeev Arora



Elad Hazan

Wei Hu



Noah Golowich

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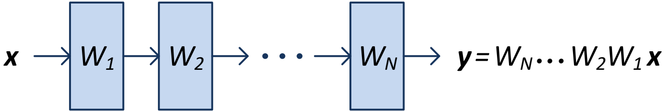
Linear Neural Networks

Linear neural networks (LNN) are fully-connected neural networks w/linear (no) activation



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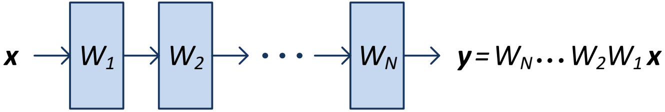

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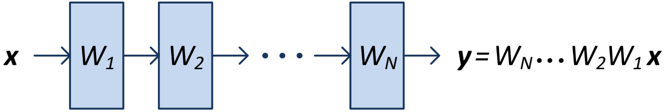

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Existing Result *(Bartlett et al. 2018)*

W/linear residual networks (a special case: W_j are square and init to I_d), for ℓ_2 loss on certain data, GD efficiently converges to global min

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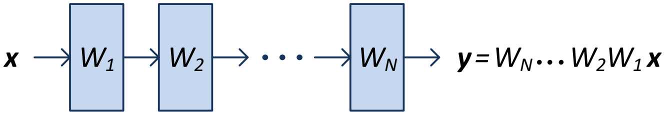

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↑

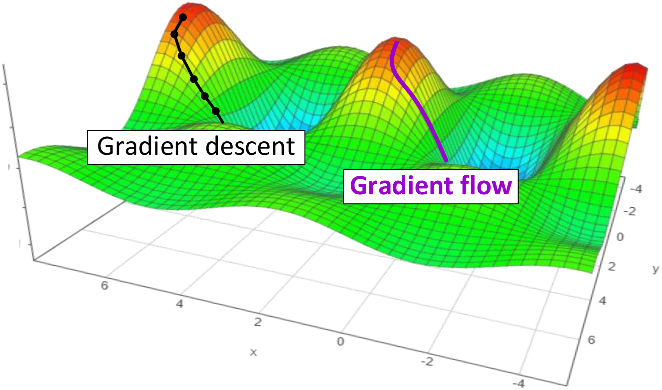
Only existing proof of efficient convergence to global min for GD training deep model

[1] e.g. Saxe et al. 2014; Kawaguchi 2016; Hardt & Ma 2017; Laurent & Brecht 2018

Gradient Flow

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

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



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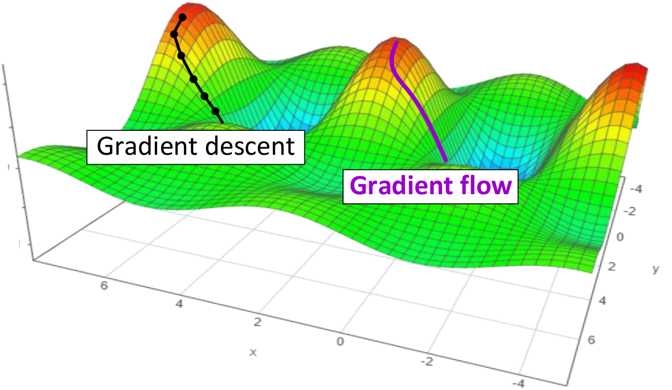
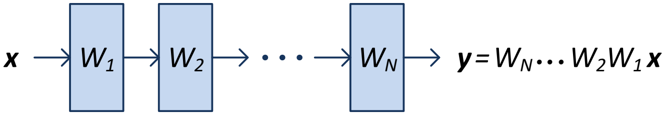


Admits use of theoretical tools from differential geometry/equations

Trajectories of Gradient Flow



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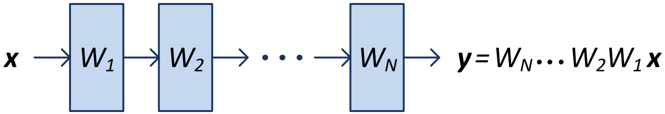

Loss $\ell(\cdot)$ for linear model induces **overparameterized objective** for LNN:

$$\phi(W_1, \ldots, W_N) := \ell(W_N \cdots W_2 W_1)$$

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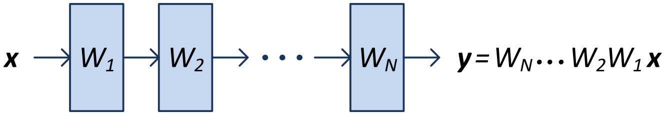

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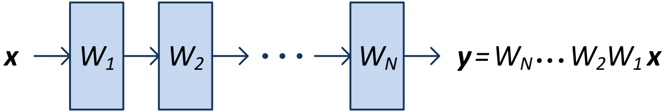

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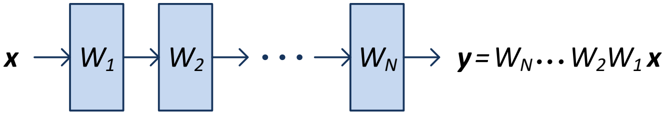

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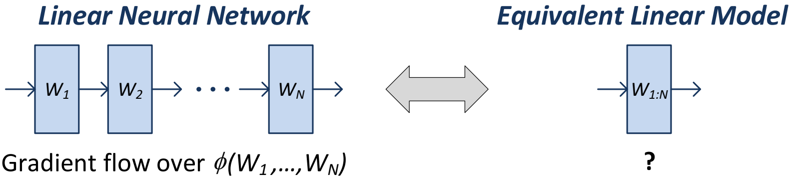
Claim

Trajectories of GF over LNN preserve balancedness: if $W_1 \ldots W_N$ are balanced at init, they remain that way throughout GF optimization

Implicit Preconditioning

Question

How does **end-to-end matrix** $W_{1:N} := W_N \cdots W_1$ move on GF trajectories?



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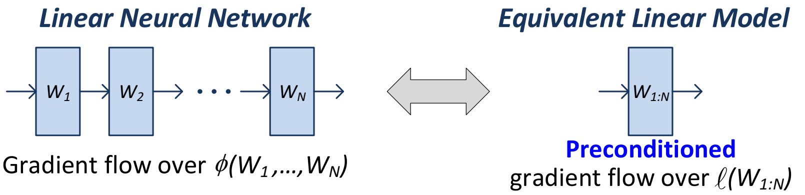

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*If $W_1 \ldots W_N$ are balanced at init, $W_{1:N}$ follows **end-to-end dynamics**:*

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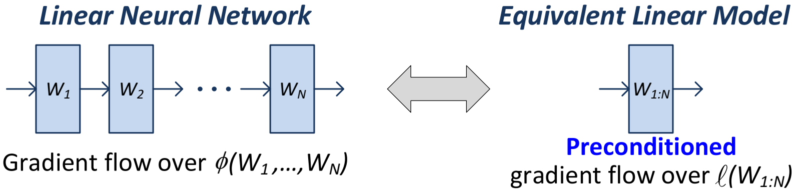

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Adding (redundant) linear layers to classic linear model induces preconditioner promoting movement in directions already taken!

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Corollary

Assume $\ell(\cdot)$ is convex and LNN is init such that:

- $W_1 \ldots W_N$ *are balanced*
- $\ell(W_{1:N}) < \ell(W)$ *for any singular* W

Then, GF converges to global min

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For $\delta \geq 0$, weights $W_1 \ldots W_N$ are **δ-balanced** if:
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Suppose $\ell(\cdot) = \ell_2$ loss $\left(\text{i.e. } \ell(W) = \frac{1}{m}\sum_{i=1}^{m} \|W\mathbf{x}_i - \mathbf{y}_i\|_2^2\right)$

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Assume GD over LNN is init s.t. $W_1 \ldots W_N$ have deficiency margin $c > 0$ and are δ-balanced w/ $\delta \leq \mathcal{O}(c^2)$. Then, for any learning rate $\eta \leq \mathcal{O}(c^4)$:

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Guarantee of efficient (linear rate) convergence to global min!
Most general guarantee to date for GD efficiently training deep net.

Outline

1. Deep Learning Theory: Expressiveness, Optimization and Generalization
2. Analyzing Optimization via Trajectories
3. Trajectories of Gradient Descent for Deep Linear Neural Networks
   - Convergence to Global Optimum
   - Acceleration by Depth
4. Conclusion

The Effect of Depth

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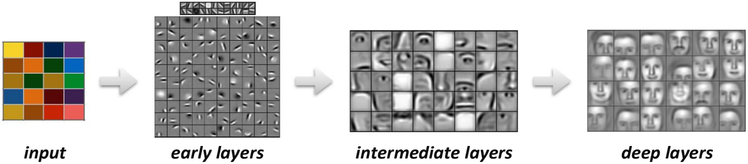
Conventional wisdom:

- Depth boosts expressiveness



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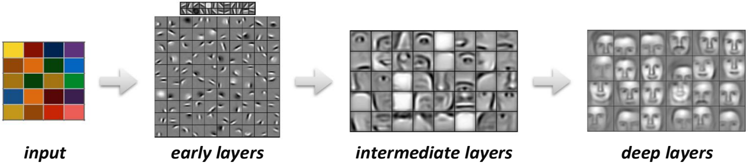

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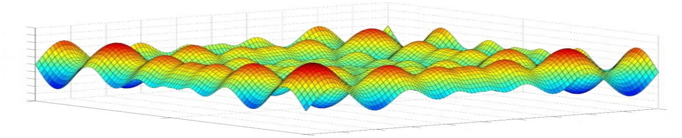

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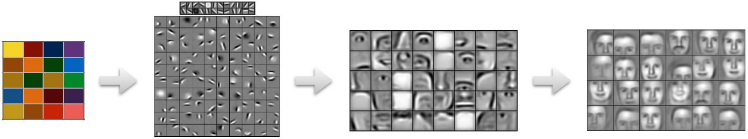

input ***early layers*** ***intermediate layers*** ***deep layers***

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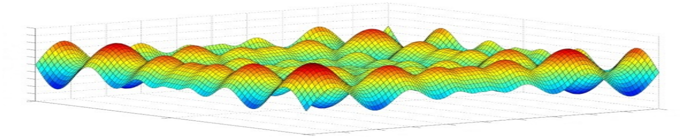

We will see: not always true...

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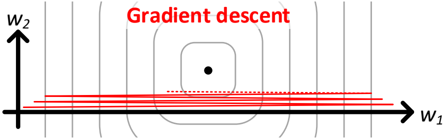

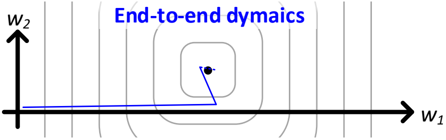

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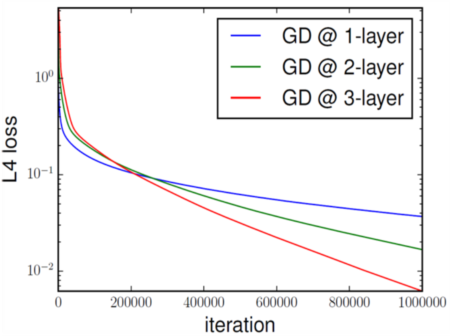

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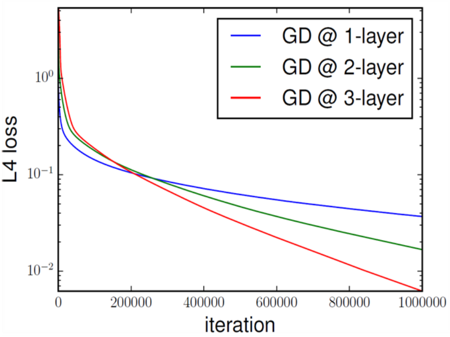

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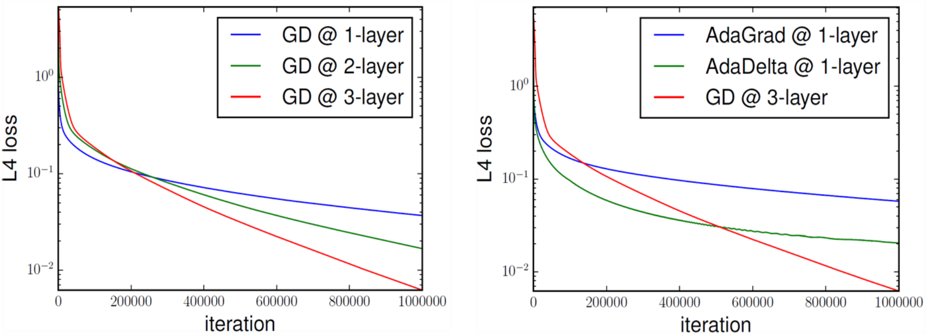

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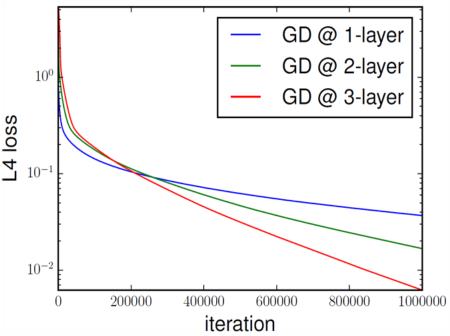

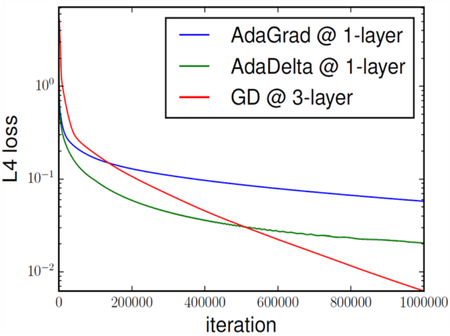

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This speed-up can outperform popular acceleration methods designed for convex problems!

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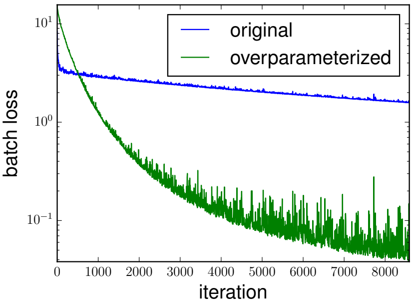


[1] https://github.com/tensorflow/models/tree/master/tutorials/image/mnist

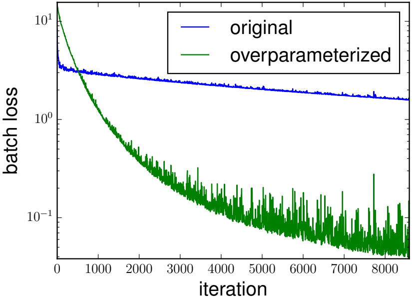
Experiments (cont')

Non-linear neural networks:

TensorFlow convolutional network tutorial for MNIST: [1]

- Arch: (conv → ReLU → max pool) x 2 → dense → ReLU → dense
- Training: stochastic GD w/momentum, dropout

We overparameterized by adding linear layer after each dense layer



Adding depth, w/o any gain in expressiveness, and only $+15\%$ in params, accelerated non-linear net by orders-of-magnitude!

[1] `https://github.com/tensorflow/models/tree/master/tutorials/image/mnist`

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1. Deep Learning Theory: Expressiveness, Optimization and Generalization

2. Analyzing Optimization via Trajectories

3. Trajectories of Gradient Descent for Deep Linear Neural Networks
   - Convergence to Global Optimum
   - Acceleration by Depth

4. Conclusion

Recap

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Understanding DL calls for addressing three fundamental Qs:

Expressiveness Optimization Generalization

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Expressiveness   Optimization   Generalization

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Deep (≥ 3 layer) models can't be treated via geometry alone

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- Derived **guarantee for convergence to global min at linear rate** (most general guarantee to date for GD efficiently training deep model)

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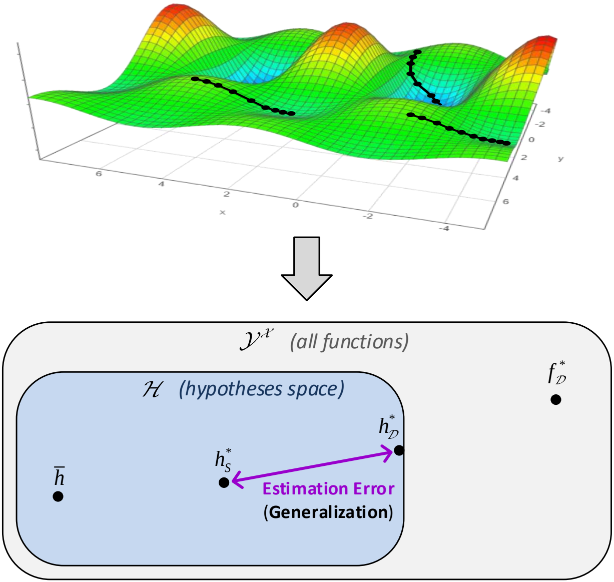
We **analyzed trajectories of GD over deep linear neural nets**:

- Derived **guarantee for convergence to global min at linear rate** (most general guarantee to date for GD efficiently training deep model)
- **Depth induces preconditioner that can accelerate convergence**, w/o any gain in expressiveness, and despite introducing non-convexity

Next Step: Analyzing Generalization via Trajectories



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Thank You