On the Optimization of Deep Networks: Implicit Acceleration by Overparameterization

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Institute for Advanced Study

Symposium on the Mathematical Theory of Deep Neural Networks

Princeton Neuroscience Institute

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Outline

Deep Learning

EVERY INDUSTRY WANTS DEEP LEARNING

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

➢ 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`)

Why Depth?

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Conventional wisdom:

- Depth boosts expressive power

  The Power of Depth for Feedforward Neural Networks (Eldan & Shamir, 2016)

  On the Expressive Power of Deep Neural Networks (Raghu et al., 2017)

  On the Ability of Neural Nets to Express Distributions (Lee et al., 2017)

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  Exploring Strategies for Training Deep Neural Networks (Larochelle et al., 2009)

  Understanding the Difficulty of Training Deep Feedforward Neural Networks (Glorot & Bengio, 2010)

  Training Very Deep Networks (Srivastava et al., 2015)

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This work:

Depth can accelerate optimization!

Common Approach – Landscape Characterization

Optimization in deep learning typically studied via characterization of critical points (local min, saddles) in training objective

Deep Learning Without Poor Local Minima (Kawaguchi, 2016)

Identity Matters in Deep Learning (Hardt & Ma, 2016)

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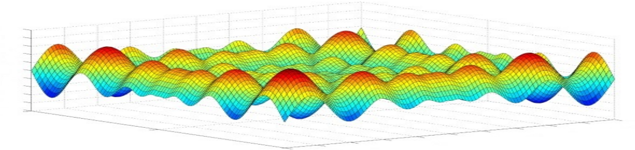

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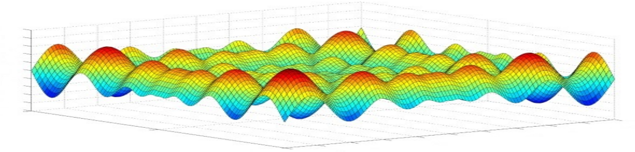

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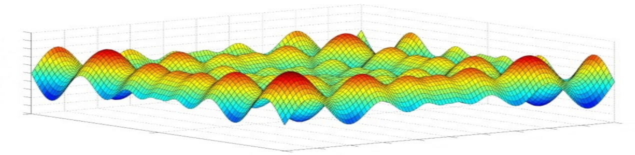

This approach prefers convex objectives – cannot argue in favor of depth

To do so, one must consider dynamics of optimization algorithm

Decoupling Optimization from Expressiveness

Problem:

Expressiveness can interfere with our study – deeper networks may optimize "faster" per being able to reach lower training error

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Resolution:

- We focus on models whose expressiveness is oblivious to depth – **linear neural networks**
- Adding layers amounts to replacing matrix param by product of matrices – **overparameterization**

Warm-Up

Training objective for scalar linear regression with ℓ_p loss:

$$L(\mathbf{w}) = \sum_{(\mathbf{x},y)\in S} \tfrac{1}{p}(\mathbf{x}^\top \mathbf{w} - y)^p$$

Warm-Up

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Gradient descent:

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \eta \nabla_{\mathbf{w}^{(t)}}$$

Warm-Up (cont')

Now overparameterize – replace $\mathbf{w}$ by vector $\mathbf{w}_1$ times scalar ω_2:

$$L(\mathbf{w}_1, \omega_2) = \sum_{(\mathbf{x},y)\in S} \tfrac{1}{p}(\mathbf{x}^\top \mathbf{w}_1 \omega_2 - y)^p$$

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Gradients:

$$\begin{aligned}
\nabla_{\mathbf{w}_1} &= \sum_{(\mathbf{x},y)\in S} (\mathbf{x}^\top \mathbf{w}_1\omega_2 - y)^{p-1}\mathbf{x}\omega_2 \\
\nabla_{\omega_2} &= \sum_{(\mathbf{x},y)\in S} (\mathbf{x}^\top \mathbf{w}_1\omega_2 - y)^{p-1}\mathbf{x}^\top \mathbf{w}_1
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Question:

How does $\mathbf{w} = \mathbf{w}_1 \omega_2$ behave during gradient descent over $\mathbf{w}_1, \omega_2$?

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Assuming small learning rate ($\eta \ll 1$) and near-zero init ($\mathbf{w}_1{}^{(0)}, \omega_2{}^{(0)} \approx 0$):

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for suitable $\rho^{(t)}, \mu^{(t,\tau)} \in \mathbb{R}$

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Overparameterization by single scalar gave certain adaptive learning rate and momentum

Outline

Formal Setup

Depth-N linear neural network:

$$\mathbf{x} \mapsto W_N W_{N-1} \cdots W_1 \mathbf{x} \qquad (W_j \text{ -- weight matrices})$$

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End-to-End Update Rule

Gradient descent over $W_1 \ldots W_N$:

$$W_j^{(t+1)} \leftarrow W_j^{(t)} - \eta \frac{\partial L^N}{\partial W_j}(W_1^{(t)}, \ldots, W_N^{(t)}) \quad \forall j$$

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$$W_e^{(t+1)} \leftarrow W_e^{(t)} - \eta \sum_{j=1}^{N} \left[W_e^{(t)} (W_e^{(t)})^\top \right]^{\frac{j-1}{N}} \frac{dL}{dW}(W_e^{(t)}) \left[(W_e^{(t)})^\top W_e^{(t)} \right]^{\frac{N-j}{N}}$$

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Overparameterization with deep linear net gives closed-form update rule! No dependence on layer widths!

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- Assumption $\eta \ll 1$ implies:

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- Left singular spaces of $W_j^{(t)}$ thus coincide with right ones of $W_{j+1}^{(t)}$
- Products of the form $W_{j+m} \cdots W_{j+1} W_j$ then simplify

  $\implies$ update for end-to-end matrix W_e can be computed explicitly $\square$

End-to-End Update Rule (cont')

Question:

Do our assumptions (small learning rate, near-zero init) hold in practice?

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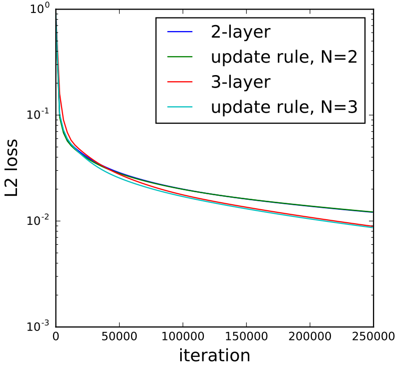
Empirical validation:



Analytical update rule indeed complies with deep network optimization

End-to-End Update Rule – Interpretation

$$\boxed{W_e^{(t+1)} \hookleftarrow W_e^{(t)} - \eta \sum\nolimits_{j=1}^{N} \left[W_e^{(t)} (W_e^{(t)})^\top \right]^{\frac{j-1}{N}} \frac{dL}{dW}(W_e^{(t)}) \left[(W_e^{(t)})^\top W_e^{(t)} \right]^{\frac{N-j}{N}}}$$

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Claim

End-to-end update rule can be written as:

$$vec\left[W_e^{(t+1)}\right] \hookleftarrow vec\left[W_e^{(t)}\right] - \eta \cdot P_{W_e^{(t)}} vec\left[\tfrac{dL}{dW}(W_e^{(t)})\right]$$

where $P_{W_e^{(t)}}$ is a preconditioning (PSD) matrix with:

- *Eigendirections: formed by sing vectors of $W_e^{(t)}$*
- *Eigenvalues: large (small) if sing vectors have high (low) sing values*

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Since we assume near-zero init ($W_e^{(0)} \approx 0$):

Overparameterization induces preconditioning, that promotes movement along directions already taken!

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Claim

In single (scalar) output case, end-to-end update rule can be written as:

$$W_e^{(t+1)} \leftarrow W_e^{(t)} - \eta \|W_e^{(t)}\|_2^{2-\frac{2}{N}} \left(\frac{dL}{dW}(W_e^{(t)}) + (N-1) Pr_{W_e^{(t)}} \left\{ \frac{dL}{dW}(W_e^{(t)}) \right\} \right)$$

where $Pr_{W_e^{(t)}}\{\cdot\}$ *is the projection onto the direction of* $W_e^{(t)}$

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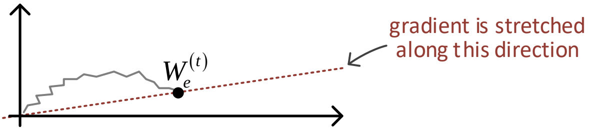
- $\|W_e^{(t)}\|_2^{2-\frac{2}{N}}$ – adaptive learning rate, increases steps away from init
- $(N-1)Pr_{W_e^{(t)}}\{\frac{dL}{dW}(W_e^{(t)})\}$ – "momentum", favors azimuth taken so far



Overparameterization Goes Beyond Regularization

End-to-end update rule (single output case):

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Is this equivalent to gradient descent over some regularized objective?

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Theorem

Assuming $\frac{dL}{dW}(0) \neq 0$, *there exists no func (of* W*) whose gradient is:*

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Effect of overparameterization can't be attained through any modification of the objective!

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Proof sketch:

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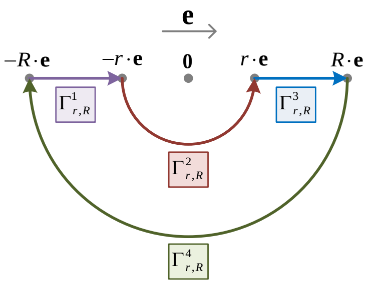
- Let $\mathbf{e} := \frac{dL}{dW}(0) / \left\| \frac{dL}{dW}(0) \right\|$, and $\Gamma_{r,R}$ be a curve as follows:



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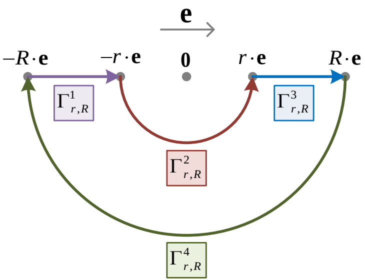

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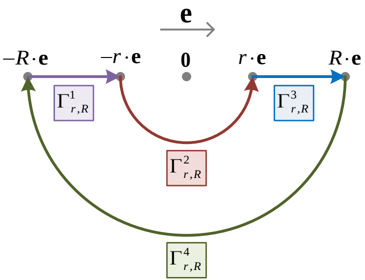

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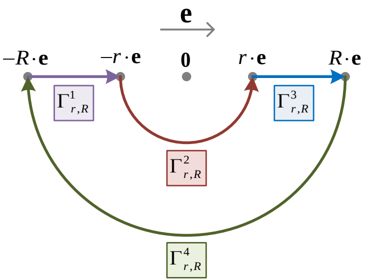

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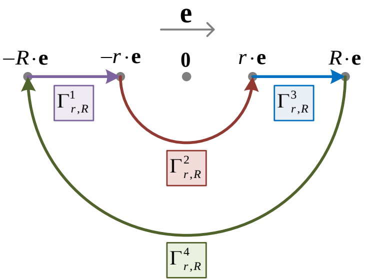

- We compute a lower bound on $\oint_{\Gamma_{r,R}} F = \sum_{i=1}^{4} \int_{\Gamma^i_{r,R}} F$
- Show lower bound is positive for sufficiently small r, R
- $F(\cdot)$ thus contradicts fundamental theorem for line integrals

  $\implies$ cannot be a gradient! $\square$

Illustration of Acceleration

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$$L(w_1, w_2) = \frac{1}{p}(w_1 - y_1)^p + \frac{1}{p}(w_2 - y_2)^p$$

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To prevent divergence, learning rate must satisfy:

$$\eta < \frac{2}{\max\left\{|\Delta_1^{(0)}|, |\Delta_2^{(0)}|\right\}^{p-2}} \underbrace{\approx}_{w_i^{(0)} \approx 0} \frac{2}{\max\left\{|y_1|, |y_2|\right\}^{p-2}}$$

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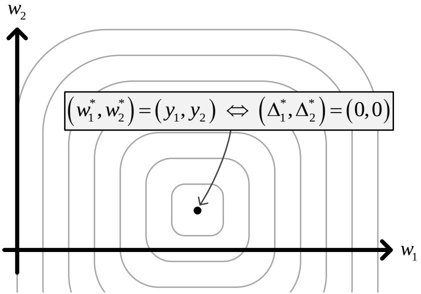

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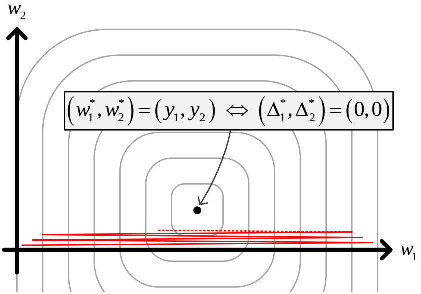
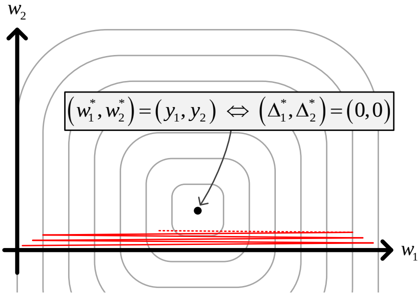


If $p > 2$: $\eta \ll \frac{2}{y_2^{p-2}} \implies$ coordinate 2 will converge slowly

Illustration of Acceleration (cont')



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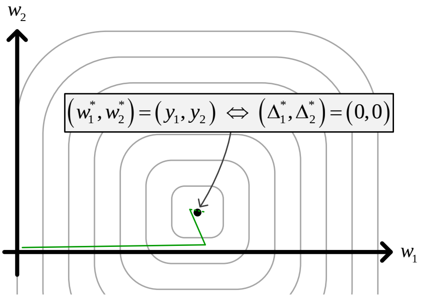

With overparameterization (end-to-end update rule):

- Learning rate effectively multiplied by $(w_1 + w_2)^{2-\frac{2}{N}}$

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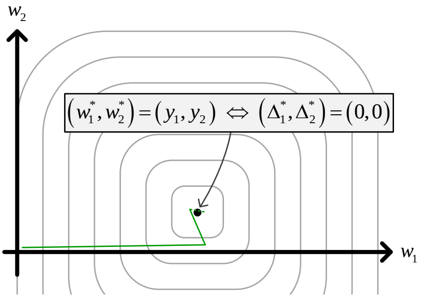

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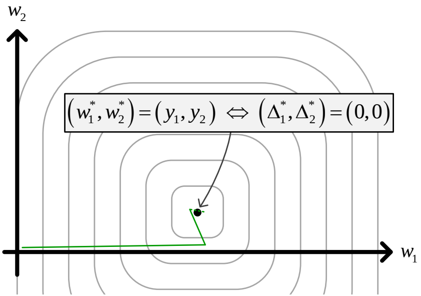

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- Optimization may begin with small steps to avoid divergence, increasing step size as safe grounds are reached

Outline

ℓ_p Regression

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Dataset: Scalar regression problem from UCI ML Repository

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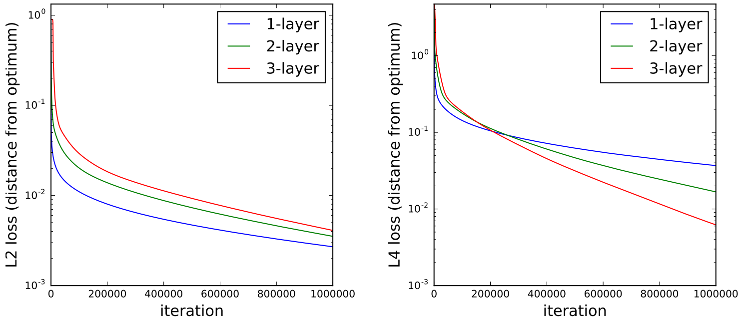

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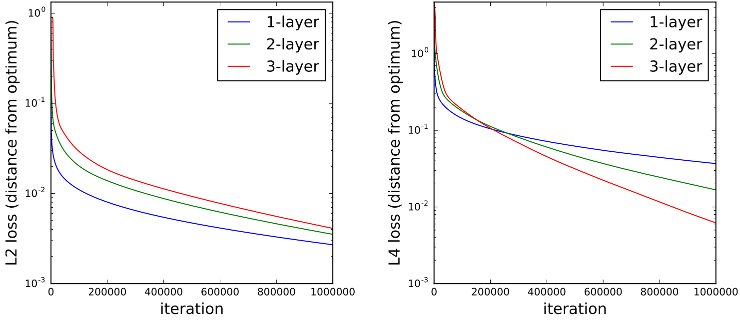
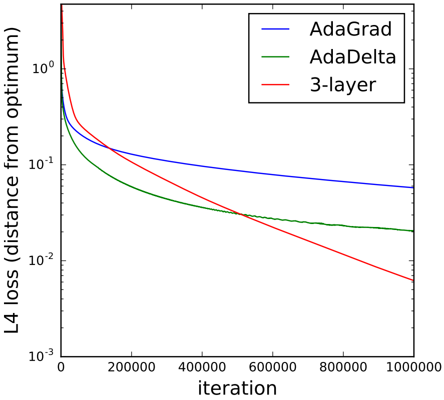


Overparameterization significantly accelerated ℓ_p regression for $p > 2$ (in line with qualitative analysis)!

Overparameterization vs. Explicit Accelerators



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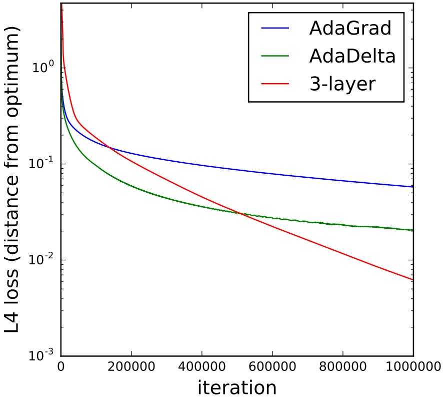
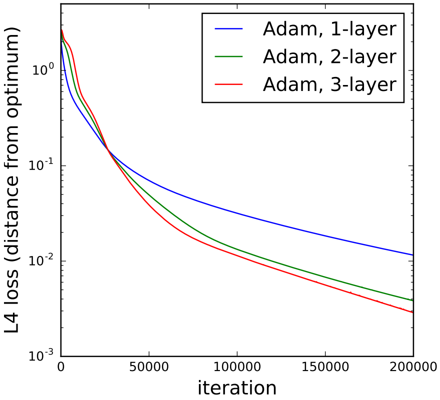


Implicit acceleration of overparameterization was faster than explicit acceleration of AdaGrad and AdaDelta!

Overparameterization vs. Explicit Accelerators (cont')

Overparameterization was slower than Adam, but when applied on top:



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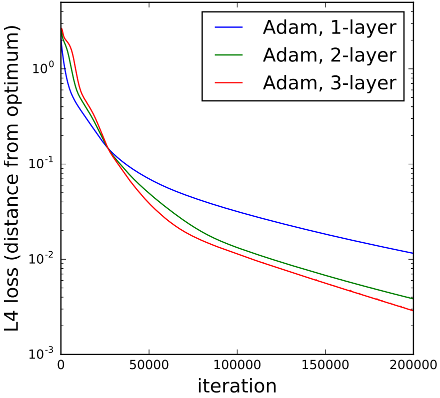

Overparameterization may help not only gradient descent, but also state-of-the-art algorithms

Going Deeper with Residual Networks

Question:

If depth indeed accelerates, why not go deeper and deeper?

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Vanishing gradient problem:

With large N:

small weight init $\implies$ $W_e := W_N \cdots W_1$ starts extremely close to 0

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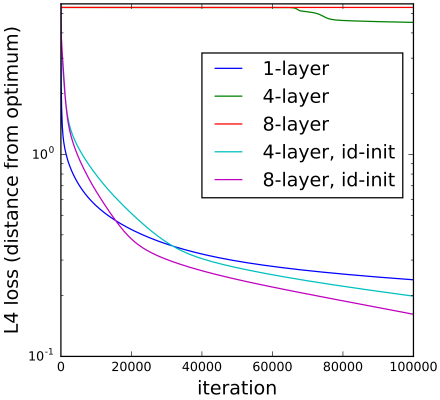
Resolution:

- Larger weight init (still small enough to prevent W_e "explosion")
- Specifically: identity init $\longleftrightarrow$ **linear residual networks**

Going Deeper with Residual Networks (cont')

Deep nets with near-zero vs. identity init:



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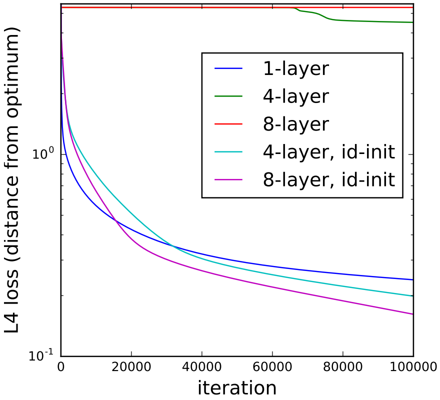

Identity init eliminated vanishing grad problem
$\Longrightarrow$ **linear residual nets can go deeper!**

Non-Linear Convolutional Network

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Non-Linear Convolutional Network

TensorFlow ConvNet tutorial for MNIST:[1]

- Architecture:
  - 5×5 conv, 32 channels, ReLU
  - 2×2 max pooling
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  - $7 \cdot 7 \cdot 64 \rightarrow 512$ dense, ReLU
  - $512 \rightarrow 10$ dense
- Training:
  - SGD+momentum, batch size 64
  - Momentum coeff 0.9, learning rate 0.01 (gradually decays)
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Sanity test:

Overparameterize – add excess matrix to each dense layer

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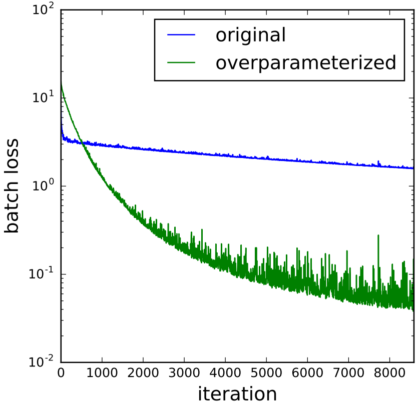
Non-Linear Convolutional Network (cont')

Training convergence:



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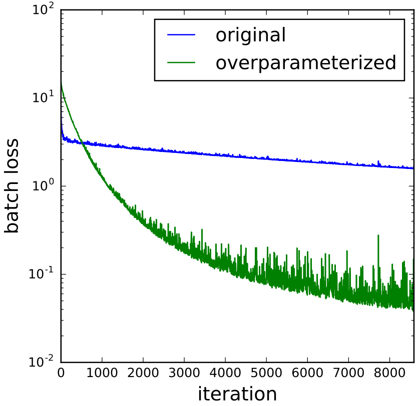

With $+15\%$ in params, overparameterization accelerated non-linear net by orders-of-magnitude!

Outline

1. Prelude
2. Theoretical Analysis
3. Experiments
4. Conclusion

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- **Perspective:**

  Understanding optimization in deep learning likely requires direct analysis of specific problems, models and algorithms

Outline

Thank You