Some Representation and Optimization Properties of Deep Residual Networks

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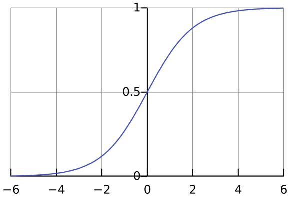
Deep Networks

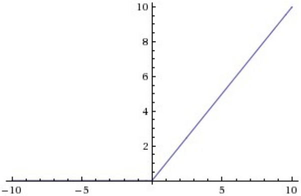
Deep compositions of nonlinear functions

$$h = h_m \circ h_{m-1} \circ \cdots \circ h_1$$

e.g., $h_i : x \mapsto \sigma(W_i x)$ $\qquad$ $h_i : x \mapsto r(W_i x)$

$$\sigma(v)_i = \frac{1}{1 + \exp(-v_i)}, \qquad r(v)_i = \max\{0, v_i\}$$





Deep Networks

Representation learning

Depth provides an effective way of representing useful features.

Rich non-parametric family

Depth provides parsimonious represention*s.

Nonlinear parameterizations provide better rates of approximation. (Birman & Solomjak, 1967), (DeVore et al, 1991)

Some functions require much more complexity for a shallow representation. (Telgarsky, 2015), (Eldan & Shamir, 2015)

But...

- Optimization?
  - Nonlinear parameterization.
  - Apparently worse as the depth increases.

Outline

- Deep residual networks
  - Representing with near-identities
  - Global optimality of stationary points
- Optimization in deep linear residual networks
  - Gradient descent
  - Symmetric maps and positivity
  - Regularized gradient descent and positive maps

Outline

- **Deep residual networks**
  - Representing with near-identities
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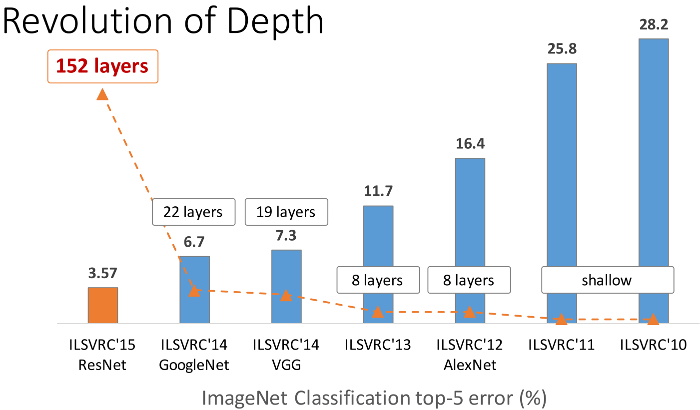
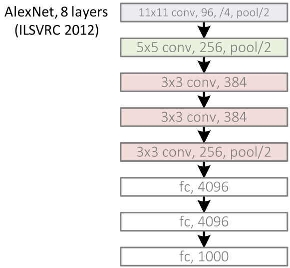
Deeper Networks



(Deep Residual Networks. Kaiming He. 2016)

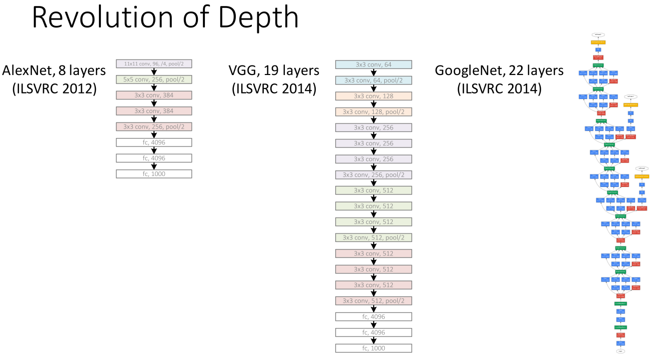
Deeper Networks

Revolution of Depth



(Deep Residual Networks. Kaiming He. 2016)

Deeper Networks



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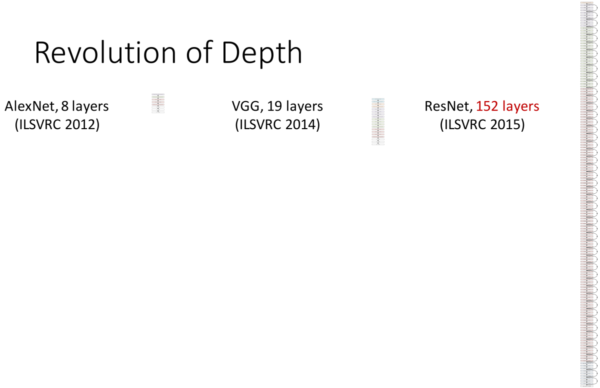
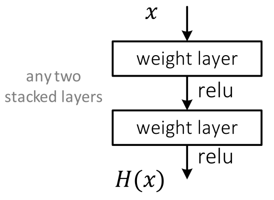
Deeper Networks



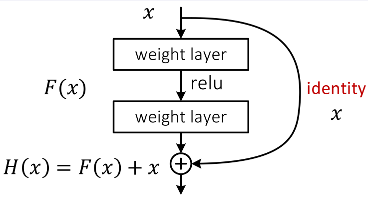
(Deep Residual Networks. Kaiming He. 2016)

Deep Residual Networks

Deep network component



Residual network component



(Deep Residual Networks. Kaiming He. 2016)

Deep Networks

Deep compositions of nonlinear functions

$$h = h_m \circ h_{m-1} \circ \cdots \circ h_1$$

e.g., $h_i \colon x \mapsto x + A_i \sigma(B_i x)$ $\qquad$ $h_i \colon x \mapsto x + A_i r(B_i x)$

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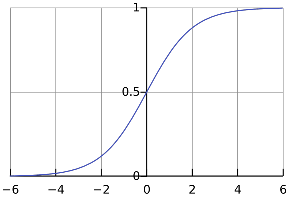
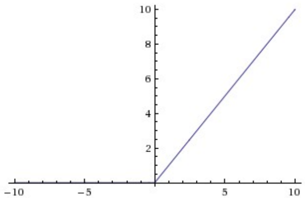
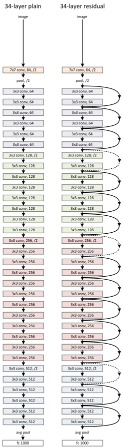




Deep Residual Networks

Advantages

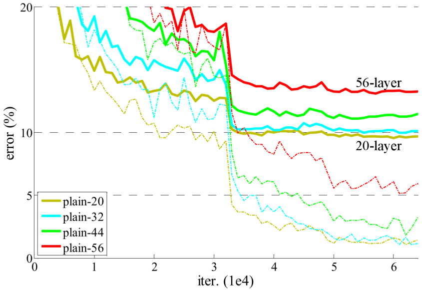
- With zero-valued parameters, the network computes the identity.
- Identity connections provide useful feedback throughout the network.

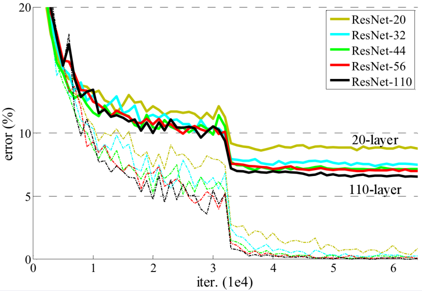


(Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun. 2016)

Deep Residual Networks

Training deep plain nets vs deep residual nets: CIFAR-10





(Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun. 2016)

Large improvements over plain nets (e.g., ImageNet Large Scale Visual Recognition Challenge, Common Objects in Context Detection Challenge).

Related work

- Deep linear compositions: $(I + A_m) \cdots (I + A_1)$. (Hardt & Ma, 2016)
- Residual nets: $a^\top(x + Bf_\theta(x))$. (Shamir, 2018)
- Empirical risk landscape for $n > p$. e.g.,(Soudry and Carmon, 2016), (Kawaguchi, 2016)
- SGD learning linear separators (Brutkus, Globerson, Malach, Shalev-Shwartz, 2017)
- Optimization landscape and gradient descent(Du & Lee, 2018), (Du, Lee, Tian, Poczos, Singh, 2017), (Soltanolkotabi, Javanmard, Lee, 2017)

Some intuition: linear functions

Products of near-identity matrices

1. Every invertible* A can be written as

$$A = (I + A_m) \cdots (I + A_1),$$

where $\|A_i\| = O(1/m)$.

(Hardt and Ma, 2016)

* Provided $\det(A) > 0$.

Some intuition: linear functions

Products of near-identity matrices

2. For a linear Gaussian model,

$$y = Ax + \epsilon, \qquad \epsilon \sim \mathcal{N}(0, \sigma^2 I),$$

consider choosing $A_1, \ldots, A_m$ to minimize quadratic loss:

$$\mathbb{E}\|(I + A_m) \cdots (I + A_1)x - y\|^2.$$

If $\|A_i\| < 1$, every stationary point of the quadratic loss is a global optimum:

$$\forall i,\ \nabla_{A_i} \mathbb{E}\|(I + A_m) \cdots (I + A_1)x - y\|^2 = 0$$
$$\Rightarrow \qquad A = (I + A_m) \cdots (I + A_1).$$

(Hardt and Ma, 2016)

Outline

- Deep residual networks
  - **Representing with near-identities**
  - Global optimality of stationary points
- Optimization in deep linear residual networks

Steve Evans
Berkeley, Stat/Math

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arXiv:1804.05012

Representing with near-identities

Result

The computation of a smooth invertible map h can be spread throughout a deep network,

$$h_m \circ h_{m-1} \circ \cdots \circ h_1 = h,$$

so that all layers compute near-identity functions:

$$\|h_i - \mathrm{Id}\|_L = O\left(\frac{\log m}{m}\right).$$

Definition: the *Lipschitz seminorm* of f satisfies, for all x, y,

$$\|f(x) - f(y)\| \leq \|f\|_L \|x - y\|.$$

Think of the functions h_i as near-identity maps that might be computed as

$$h_i(x) = x + \underbrace{A_i}\sigma(\underbrace{B_i x}).$$

Representing with near-identities

Theorem

Consider a function $h : \mathbb{R}^d \to \mathbb{R}^d$ on a bounded domain $\mathcal{X} \subset \mathbb{R}^d$. Suppose that h is

1. Differentiable,
2. Invertible,
3. Smooth: For some $\alpha > 0$ and all x, y, u, $\|Dh(y) - Dh(x)\| \leq \alpha \|y - x\|$.
4. Lipschitz inverse: For some $M > 0$, $\|h^{-1}\|_L \leq M$.
5. Positive orientation: For some x_0, $\det(Dh(x_0)) > 0$.

Then for all m, there are m functions $h_1, \ldots, h_m : \mathbb{R}^d \to \mathbb{R}^d$ satisfying $\|h_i - \mathrm{Id}\|_L = O(\log m/m)$ and $h_m \circ h_{m-1} \circ \cdots \circ h_1 = h$ on $\mathcal{X}$.

- Dh is the derivative; $\|Dh(y)\|$ is the induced norm:
  $\|f\| := \sup \left\{ \frac{\|f(x)\|}{\|x\|} : \|x\| > 0 \right\}$.

Representing with near-identities

Key ideas

1. Assume $h(0) = 0$ and $Dh(0) = \mathrm{Id}$ (else shift and linearly transform).
2. Construct the h_i so that

$$h_1(x) = \frac{h(a_1 x)}{a_1}$$

$$h_2(h_1(x)) = \frac{h(a_2 x)}{a_2}$$

$$\vdots$$

$$h_m(\cdots(h_1(x))\cdots) = \frac{h(a_m x)}{a_m},$$

3. Pick $a_m = 1$ so $h_m \circ \cdots \circ h_1 = h$.
4. Ensure that a_1 is small enough that $h_1 \approx Dh(0) = \mathrm{Id}$.
5. Ensure that a_i and a_{i+1} are sufficiently close that $h_i \approx \mathrm{Id}$.
6. Show $\|h_i - \mathrm{Id}\|_L$ is small on small and large scales (c.f. $a_i - a_{i-1}$).

Representing with near-identities

Result

The computation of a smooth invertible map h can be spread throughout a deep network,

$$h_m \circ h_{m-1} \circ \cdots \circ h_1 = h,$$

so that all layers compute near-identity functions:

$$\left\| h_i - \mathrm{Id} \right\|_L = O\left(\frac{\log m}{m} \right).$$

- Deeper networks allow flatter nonlinear functions at each layer.

Outline

- Deep residual networks
  - Representing with near-identities
  - **Global optimality of stationary points**
- Optimization in deep linear residual networks

Stationary points

Result

For (X, Y) with an arbitrary joint distribution, define the squared error,

$$Q(h) = \frac{1}{2}\mathbb{E}\left\|h(X) - Y\right\|_2^2,$$

define the minimizer $h^*(x) = \mathbb{E}[Y|X = x]$.
Consider a function $h = h_m \circ \cdots \circ h_1$, where $\left\|h_i - \mathrm{Id}\right\|_L \leq \epsilon < 1$.
Then for all i,

$$\|D_{h_i} Q(h)\| \geq \frac{(1-\epsilon)^{m-1}}{\|h - h^*\|}\left(Q(h) - Q(h^*)\right).$$

- e.g., if (X, Y) is uniform on a training sample,
then Q is empirical risk and h^* an empirical risk minimizer.
- $D_{h_i} Q$ is a Fréchet derivative; $\|h\|$ is the induced norm.

Stationary points

What the theorem says

- If the composition h is sub-optimal and each function h_i is a near-identity, then there is a downhill direction in function space: the functional gradient of Q wrt h_i is non-zero.
- Thus every stationary point is a global optimum.
- There are no local minima and no saddle points.

Stationary points

What the theorem says

- The theorem does not say there are no local minima of a deep residual network of ReLUs or sigmoids with a fixed architecture.
- Except at the global minimum, there is a downhill direction in function space. But this direction might be orthogonal to functions that can be computed with this fixed architecture.
- We should expect suboptimal stationary points in the ReLU or sigmoid parameter space, but these cannot arise because of interactions between parameters in different layers; they arise only within a layer.

Stationary points

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Stationary points

Proof ideas (1)

If $\|f - \mathrm{Id}\|_L \leq \alpha < 1$ then

1. f is invertible.
2. $\|f\|_L \leq 1 + \alpha$ and $\|f^{-1}\|_L \leq 1/(1 - \alpha)$.
3. For $F(g) = f \circ g$, $\|DF(g) - \mathrm{Id}\| \leq \alpha$.
4. For a linear map h (such as $DF(g) - \mathrm{Id}$), $\|h\| = \|h\|_L$.

- $\|f\|$ denotes the induced norm: $\|g\| := \sup \left\{ \frac{\|g(x)\|}{\|x\|} : \|x\| > 0 \right\}$.

Stationary points

Proof ideas (2)

1. Projection theorem implies

$$Q(h) = \frac{1}{2}\mathbb{E}\left\|h(X) - h^*(X)\right\|_2^2 + \text{constant}.$$

2. Then

$$D_{h_i}Q(h) = \mathbb{E}\left[(h(X) - h^*(X)) \cdot \mathrm{ev}_X \circ D_{h_i}h\right].$$

3. It is possible to choose a direction Δ s.t. $\|\Delta\| = 1$ and

$$D_{h_i}Q(h)(\Delta) = c\mathbb{E}\left\|h(X) - h^*(X)\right\|_2^2.$$

4. Because the h_js are near-identities,

$$c \geq \frac{(1-\epsilon)^{m-1}}{\|h - h^*\|}.$$

- ev_x is the evaluation functional, $\mathrm{ev}_x(f) = f(x)$.

Stationary points

Result

For (X, Y) with an arbitrary joint distribution, define the squared error,

$$Q(h) = \frac{1}{2}\mathbb{E}\left\|h(X) - Y\right\|_2^2,$$

define the minimizer $h^*(x) = \mathbb{E}[Y|X = x]$.
Consider a function $h = h_m \circ \cdots \circ h_1$, where $\left\|h_i - \mathrm{Id}\right\|_L \leq \epsilon < 1$.
Then for all i,

$$\left\|D_{h_i} Q(h)\right\| \geq \frac{(1-\epsilon)^{m-1}}{\left\|h - h^*\right\|}\left(Q(h) - Q(h^*)\right).$$

- e.g., if (X, Y) is uniform on a training sample,

then Q is empirical risk and h^* an empirical risk minimizer.
- $D_{h_i} Q$ is a Fréchet derivative; $\|h\|$ is the induced norm.

Deep compositions of near-identities

Questions

- If the mapping is not invertible?
  e.g., $h : \mathbb{R}^d \to \mathbb{R}$?
  If h can be extended to a bi-Lipschitz mapping to $\mathbb{R}^d$, it can be represented with flat functions at each layer.
  What if it cannot?
- Implications for optimization?
  Related to Polyak-Łojasiewicz function classes; proximal algorithms for these classes converge quickly to stationary points.
- Regularized gradient methods for near-identity maps?

Outline

- Deep residual networks
- **Optimization in deep linear residual networks**
  - Gradient descent
  - Symmetric maps and positivity
  - Regularized gradient descent and positive maps

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arXiv:1802.06093

Optimization in deep linear residual networks

Linear networks

- Consider $f_\Theta : \mathbb{R}^d \to \mathbb{R}^d$ defined by $f_\Theta(x) = \Theta_L \cdots \Theta_1 x$.
- Suppose $(x, y) \sim P$, and consider using gradient methods to choose Θ to minimize $\ell(\Theta) = \frac{1}{2}\mathbb{E}\|f_\Theta(x) - y\|^2$.

Assumptions

1. $\mathbb{E}xx^\top = I$
2. $y = \Phi x$ for some matrix Φ (wlog, because of projection theorem)

Optimization in deep linear residual networks

why wlog?

Define Φ as the minimizer of $\mathbb{E}\|\Phi x - y\|^2$ (the *least squares map*).
Then the projection theorem implies

$$\begin{aligned}\mathbb{E}\|\Theta x - y\|^2 &= \mathbb{E}\|\Theta x - \Phi x\|^2 + 2\mathbb{E}(\Theta x - \Phi x)^\top(\Phi x - y) + \mathbb{E}\|\Phi x - y\|^2 \\ &= \mathbb{E}\|\Theta x - \Phi x\|^2 + \mathbb{E}\|\Phi x - y\|^2,\end{aligned}$$

so wlog we can assume $y = \Phi x$ and define, for linear f_Θ,

$$\ell(\Theta) = \frac{1}{2}\mathbb{E}\|f_\Theta(x) - \Phi x\|^2.$$

Optimization in deep linear residual networks

Recall $f_\Theta(x) = \Theta_L \cdots \Theta_1 x = \Theta_{1:L} x$,
where we use the notation $\Theta_{i:j} = \Theta_j \Theta_{j-1} \cdots \Theta_i$.

Gradient descent

$$\Theta^{(0)} = \left(\Theta_1^{(0)}, \Theta_2^{(0)}, \ldots, \Theta_L^{(0)}\right) := (I, I, \ldots, I)$$

$$\Theta_i^{(t+1)} := \Theta_i^{(t)} - \eta(\Theta_{i+1:L})^\top \left(\Theta_{1:L}^{(t)} - \Phi\right) (\Theta_{1:i-1}^{(t)})^\top,$$

where η is a step-size.

Gradient descent in deep linear residual networks

Theorem

There is a positive constant c_0 and polynomials p_1 and p_2 such that if $\ell(\Theta^{(0)}) \leq c_0$ and $\eta \leq 1/p_1(d, L)$, after $p_2(d, L, 1/\eta) \log(1/\epsilon)$ iterations, gradient descent achieves $\ell(\Theta^{(t)}) \leq \epsilon$.

Gradient descent: proof idea

Lemma [Hardt and Ma] (Gradient is big when loss is big)

If, for all layers i, $\sigma_{\min}(\Theta_i) \geq 1 - a$, then $||\nabla_\Theta \ell(\Theta)||^2 \geq 4\ell(\Theta)L(1-a)^{2L}$.

Lemma (Hessian is small for near-identities)

For Θ with $||\Theta_i||_2 \leq 1 + z$ for all i,

$$\|\nabla^2_\Theta \ell(\Theta)\|_F \leq 3Ld^5(1+z)^{2L}.$$

Lemma (Stay close to the identity)

$$\mathcal{R}(t+1) \leq \mathcal{R}(t) + \eta(1+\mathcal{R}(t))^L\sqrt{2\ell(t)},$$

where $\mathcal{R}(t) := \max_i ||\Theta_i^{(t)} - I||_2$ and $\ell(t) := \frac{1}{2}||\Theta_{1:L}^{(t)} - \Phi||_F^2$.

Then for sufficiently small step-size η, the gradient update ensures that $\ell(t)$ decreases exponentially.

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Optimization in deep linear residual networks

Definition (γ-positive matrix)

A matrix A is γ-*positive* for $\gamma > 0$ if, for all unit length u, we have $u^\top Au > \gamma$.

Theorem

Suppose that the least squares map Φ is symmetric.

(a) There is an absolute positive constant c_3 such that if Φ is γ-positive $(0 < \gamma < 1)$, $L \geq c_3 \ln(||\Phi||_2/\gamma)$, and $\eta \leq \frac{1}{L(1+||\Phi||_2^2)}$, after $t = \mathrm{poly}(L, ||\Phi||_2/\gamma, 1/\eta) \log(d/\epsilon)$ iterations, gradient descent achieves $\ell(f_{\Theta^{(t)}}) \leq \epsilon$.

(b) If Φ has a negative eigenvalue $-\lambda$ and L is even, then gradient descent satisfies $\ell(\Theta^{(t)}) \geq \lambda^2/2$ (as does any penalty-regularized version of gradient descent).

Symmetric linear functions

Proof idea

(a) A set of symmetric matrices $\mathcal{A}$ is *commuting normal* if there is a single unitary matrix U such that for all $A \in \mathcal{A}$, $U^\top AU$ is diagonal.
Clearly, $\{\Phi, \Theta_1^{(0)}, \Theta_2^{(0)}, \ldots, \Theta_L^{(0)}\} = \{\Phi, I\}$ is commuting normal.
The gradient update keeps $\bigcup_{i,t}\{\Phi, \Theta_i^{(t)}\}$ commuting normal.
So the dynamics decomposes:

$$\hat{\lambda}^{(t+1)} = \hat{\lambda}^{(t)} + \eta(\hat{\lambda}^{(t)})^{L-1}(\lambda^L - (\hat{\lambda}^{(t)})^L).$$

(b) The eigenvalues stay positive.

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Positive (not necessarily symmetric) linear functions

Theorem

For any γ-positive Φ, there is an algorithm (*power projection*) that, after $t = \mathrm{poly}(d, ||\Phi||_F, \frac{1}{\gamma}) \log(1/\epsilon)$ iterations, produces $\Theta^{(t)}$ with $\ell(\Theta^{(t)}) \leq \epsilon$.

Power projection algorithm idea

1. Take a gradient step for each Θ_i.
2. Project $\Theta_{1:L}$ onto the set of γ-positive linear maps.
3. Set $\Theta_1^{(t+1)}, \ldots, \Theta_L^{(t+1)}$ as the *balanced factorization* of $\Theta_{1:L}$.

Positive (not necessarily symmetric) linear functions

Balanced factorization

We can write any matrix A, with singular values $\sigma_1, \ldots, \sigma_d$, as $A = A_L \cdots A_1$, where the singular values of each A_i are $\sigma_1^{1/L}, \ldots, \sigma_d^{1/L}$.

(Idea: Write the polar decomposition $A = RP$ (i.e., R unitary, P psd); set $A_i = R^{1/L} P_i$, with $P_i = R^{(i-1)/L} P^{1/L} R^{-(i-1)/L}$.)

Optimization in deep linear residual networks

- Gradient descent
  - converges if $\ell(0)$ sufficiently small,
  - converges for a positive symmetric map,
  - cannot converge for a symmetric map with a negative eigenvalue.
- Regularized gradient descent converges for a positive map.
- Convergence is linear in all cases.
- Deep nonlinear residual networks?

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