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., \( h_i : x \mapsto \sigma(W_i x) \) \quad \sigma(v)_i = \frac{1}{1 + \exp(-v_i)},

\( h_i : x \mapsto r(W_i x) \) \quad r(v)_i = \max\{0, v_i\}
Representation learning
Depth provides an effective way of representing useful features.

Rich non-parametric family
Depth provides parsimonious representations.
Nonlinear parameterizations provide better rates of approximation.
Some functions require much more complexity for a shallow representation.

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
  - Global optimality of stationary points
- **Optimization in deep linear residual networks**
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Deeper Networks

Revolution of Depth

![Diagram showing the evolution of depth in ImageNet Classification top-5 error (%)]

ILSVRC'15 ResNet: 3.57
ILSVRC'14 GoogleNet: 6.7
ILSVRC'14 VGG: 7.3
ILSVRC'13: 11.7
ILSVRC'12 AlexNet: 16.4
ILSVRC'11: 25.8
ILSVRC'10: 28.2

152 layers

(ImageNet Classification top-5 error (%))

(Deep Residual Networks. Kaiming He. 2016)
Revolution of Depth

AlexNet, 8 layers (ILSVRC 2012)

11x11 conv, 96, /4, pool/2
5x5 conv, 256, pool/2
3x3 conv, 384
3x3 conv, 384
3x3 conv, 256, pool/2
fc, 4096
fc, 4096
fc, 1000

(Deep Residual Networks. Kaiming He. 2016)
Deeper Networks

Revolution of Depth

AlexNet, 8 layers (ILSVRC 2012)

1x1 conv, 64
5x5 conv, 256, pool/2
3x3 conv, 256
3x3 conv, 256
3x3 conv, 256, pool/2
3x3 conv, 256
3x3 conv, 1024
fc, 1000

VGG, 19 layers (ILSVRC 2014)

3x3 conv, 64
3x3 conv, 64, pool/2
3x3 conv, 128
3x3 conv, 128, pool/2
3x3 conv, 256
3x3 conv, 256
3x3 conv, 256
3x3 conv, 512
3x3 conv, 512
3x3 conv, 512
3x3 conv, 512
3x3 conv, 512
3x3 conv, 512
3x3 conv, 512, pool/2
fc, 1024
fc, 1024
fc, 1000

GoogleNet, 22 layers (ILSVRC 2014)

(Deep Residual Networks. Kaiming He. 2016)
Deeper Networks

Revolution of Depth

- AlexNet, 8 layers (ILSVRC 2012)
- VGG, 19 layers (ILSVRC 2014)
- ResNet, 152 layers (ILSVRC 2015)

(Deep Residual Networks. Kaiming He. 2016)
Deep Residual Networks

Deep network component

\[ H(x) = \text{weight layer} \rightarrow \text{relu} \rightarrow \text{weight layer} \rightarrow \text{relu} \rightarrow x \]

Residual network component

\[ F(x) = \text{weight layer} \rightarrow \text{relu} \rightarrow \text{weight layer} \rightarrow \text{id} \]

\[ H(x) = F(x) + x \]

(Deep Residual Networks. Kaiming He. 2016)
Deep Residual Networks

Advantages

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

(Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun. 2016)
Training deep plain nets vs deep residual nets: CIFAR-10

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

(Kaiming He, Xiangyu Zhang, Shaoqing Ren, Jian Sun. 2016)
Some intuition: linear functions

Products of near-identity matrices

Every invertible* matrix $A$ can be written as

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

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

(Hardt and Ma, 2016)

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

For a linear Gaussian model,

\[ y = Ax + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2 I), \]

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:

\[ \forall i, \nabla_{A_i} \mathbb{E} \| (I + A_m) \cdots (I + A_1)x - y \|^2 = 0 \]

\[ \Rightarrow \quad A = (I + A_m) \cdots (I + A_1). \]

(Hardt and Ma, 2016)
Deep residual networks
  - Representing with near-identities
  - Global optimality of stationary points
Optimization in deep linear residual networks

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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:

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

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

$$h_i(x) = x + A\sigma(Bx).$$
Representing with near-identities

Theorem

Consider a function \( h : \mathbb{R}^d \to \mathbb{R}^d \) on a bounded domain \( X \subset \mathbb{R}^d \).

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
\[
\| h_i - \text{Id} \|_L = O(\log m/m) \quad \text{and} \quad h_m \circ h_{m-1} \circ \cdots \circ h_1 = h \text{ on } X.
\]

\( \bullet \) \( Dh \) 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 \( Dh(0) = \text{Id} \) (else shift and linearly transform).
2. Construct the \( h_i \) so that
   \[
   h_1(x) = \frac{h(a_1x)}{a_1}
   \]
   \[
   h_2(h_1(x)) = \frac{h(a_2x)}{a_2}
   \]
   \[
   \vdots
   \]
   \[
   h_m(\cdots(h_1(x))\cdots) = \frac{h(a_mx)}{a_m},
   \]
3. Pick \( a_m = 1 \) so \( h_m \circ \cdots \circ h_1 = h \).
4. Ensure that \( a_1 \) is small enough that \( h_1 \approx Dh(0) = \text{Id} \).
5. Ensure that \( a_i \) and \( a_{i+1} \) are sufficiently close that \( h_i \approx \text{Id} \).
6. Show \( \|h_i - \text{Id}\|_L \) is small on small and large scales (c.f. \( a_i - a_{i-1} \)).
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:

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

- Deeper networks allow flatter nonlinear functions at each layer.
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,

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

define the minimizer \(h^*(x) = \mathbb{E}[Y|X = x]\).

Consider a function \(h = h_m \circ \cdots \circ h_1\), where \(\| h_i - \text{Id} \|_L \leq \epsilon < 1\).

Then for all \(i\),

\[
\| D_{h_i} Q(h) \| \geq \frac{(1 - \epsilon)^{m-1}}{\| h - h^* \|} (Q(h) - Q(h^*)).
\]

- 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

Result

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

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

define the minimizer \(h^*(x) = \mathbb{E}[Y|X = x]\).

Consider a function \(h = h_m \circ \cdots \circ h_1\), where \(\|h_i - \text{Id}\|_L \leq \epsilon < 1\).

Then for all \(i\),

\[
\| D_{h_i} Q(h) \| \geq \frac{(1 - \epsilon)^{m-1}}{\| h - h^* \|} (Q(h) - Q(h^*)) .
\]

- 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

Proof ideas (1)

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

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

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

Proof ideas (2)

1. Projection theorem implies

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

2. Then

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

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

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

4. Because the \( h_j \)'s are near-identities,

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

- \( \text{ev}_X \) is the evaluation functional, \( \text{ev}_X(f) = f(x) \).
Stationary points

**Result**

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

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

define the minimizer \(h^*(x) = \mathbb{E}[Y|X=x]\).

Consider a function \(h = h_m \circ \cdots \circ h_1\), where \(\|h_i - \text{Id}\|_L \leq \epsilon < 1\).

Then for all \(i\),

\[ \| D_{h_i} Q(h) \| \geq \frac{(1 - \epsilon)^{m-1}}{\| h - h^* \|} (Q(h) - Q(h^*)). \]

- 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., $h : \mathbb{R}^d \rightarrow \mathbb{R}$?
- 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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Consider $f_\Theta : \mathbb{R}^d \rightarrow \mathbb{R}^d$ defined by $f_\Theta(x) = \Theta_L \cdots \Theta_1 x$.

Suppose $(x, y) \sim P$, and consider using gradient methods to choose $\Theta$ 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 $\Phi$ (wlog, because of projection theorem)
Define $\Phi$ as the minimizer of $\mathbb{E}\|\Phi x - y\|^2$ (the least squares map). Then the projection theorem implies

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

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

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

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

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

where \( \eta \) is a step-size.
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 in deep linear residual networks
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 $\Theta$ 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)**

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

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

Then for sufficiently small step-size $\eta$, the gradient update ensures that $\ell(t)$ decreases exponentially.
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  - Regularized gradient descent and positive maps
Definition (positive margin matrix)

A matrix $A$ has margin $\gamma > 0$ if, for all unit length $u$, we have $u^\top Au > \gamma$.

Theorem

Suppose $\Phi$ is symmetric.

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

(b) If $\Phi$ 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).
(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, $\{\Phi, \Theta^{(0)}_1, \Theta^{(0)}_2, \ldots, \Theta^{(0)}_L\} = \{\Phi, I\}$ is commuting normal. The gradient update keeps $\bigcup_{i,t} \{\Phi, \Theta^{(t)}_i\}$ 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.
Outline

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Positive (not necessarily symmetric) linear functions

**Theorem**

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

**Power projection algorithm idea**

1. Take a gradient step for each $\Theta_i$.
2. Project $\Theta_{1:L}$ onto the set of linear maps with margin $\gamma$.
3. Set $\Theta_1^{(t+1)}, \ldots, \Theta_L^{(t+1)}$ as the *balanced factorization* of $\Theta_{1:L}$.
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 $\sigma_i^{1/L}, \ldots, \sigma_d^{1/L}$.

(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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