Optimization in 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., \[ h_i : x \mapsto \sigma(W_i x) \]

\[ \sigma(v)_i = \frac{1}{1 + \exp(-v_i)}, \]

\[ r(v)_i = \max\{0, v_i\} \]
Deep Networks

Representation learning
Depth provides an effective way of representing useful features.

Rich non-parametric family
Depth provides parsimonious 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
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
Deeper Networks

Revolution of Depth

152 layers

ILSVRC'15 ResNet 3.57
ILSVRC'14 GoogleNet 6.7
ILSVRC'14 VGG 7.3
ILSVRC'13 8 layers 11.7
ILSVRC'12 AlexNet 8 layers 16.4
ILSVRC'11 shallow 25.8
ILSVRC'10 shallow 28.2

ImageNet Classification top-5 error (%)

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

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)

VGG, 19 layers (ILSVRC 2014)

GoogleNet, 22 layers (ILSVRC 2014)

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

<table>
<thead>
<tr>
<th>Network</th>
<th>Layers</th>
<th>Year (ILSVRC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlexNet</td>
<td>8</td>
<td>2012</td>
</tr>
<tr>
<td>VGG</td>
<td>19</td>
<td>2014</td>
</tr>
<tr>
<td>ResNet</td>
<td>152</td>
<td>2015</td>
</tr>
</tbody>
</table>

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

Deep network component

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

Residual network component

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

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

(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.,

\[ h_i: x \mapsto x + A_i \sigma(B_i x) \]
\[ h_i: x \mapsto x + A_i r(B_i x) \]

\[ \sigma(v)_i = \frac{1}{1 + \exp(-v_i)} \]
\[ r(v)_i = \max\{0, v_i\} \]
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)
Large improvements over plain nets (e.g., ImageNet Large Scale Visual Recognition Challenge, Common Objects in Context Detection Challenge).
Products of near-identity matrices

1. Every invertible\(^*\) \( A \) can be written as

\[
A = (I + A_m) \cdots (I + A_1),
\]

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

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\(^*\) Provided \( \det(A) > 0 \).
Some intuition: linear functions

Products of near-identity matrices

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)
Outline

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

Steve Evans
Berkeley, Stat/Math

Phil Long
Google

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

$$h_i(x) = x + A\sigma(Bx).$$
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
\[ \| h_i - \text{Id} \|_L = O(\log m / m) \] 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 $Dh(0) = \text{Id}$ (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 $h_1 \approx Dh(0) = \text{Id}$.
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.
Outline

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

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

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 \(i\),

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- 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, \( \text{ev}_X(f) = f(x) \).
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?  
es.e., $h : \mathbb{R}^d \rightarrow \mathbb{R}$? 
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?
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 $f_\Theta : \mathbb{R}^d \to \mathbb{R}^d$ defined by $f_\Theta(x) = \Theta_L \cdots \Theta_1 x$.

Suppose $(x, y) \sim P$, and consider using gradient methods to choose $\Theta$ 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)
Optimization in deep linear residual networks

why wlog?

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 $f_\Theta$,

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

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

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

where $\eta$ 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 $\Theta$ 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 $\ell(t) := \frac{1}{2} \|\Theta^{(t)}_{1:L} - \Phi\|_F^2$.

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

Optimization in deep linear residual networks
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Optimization in deep linear residual networks

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).

(Shamir, 2018) gives a stronger negative result in dimension 1.
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.
Outline

- Deep residual networks
- Optimization in deep linear residual networks
  - Gradient descent
  - Symmetric maps and positivity
  - Regularized gradient descent and positive maps
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 $\Theta_{1:L}$.
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?
Deep residual networks
  - Representing with near-identities
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 Optimization in deep linear residual networks
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