# Introduction to Neural Networks and Deep Learning Deep Forward Neural Networks

Andres Mendez-Vazquez

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- Limitations of Shallow Architectures
- Highly-varying functions
- Local vs Non-Local Generalization
- From Simpler Features to More Complex Features
- Deep Forward Architectures
- Introduction
- Convolutional Neural Networks
  - Image Processing
- Auto Encoders
- Boltzmann Machines
- Generative Adversarial Networks
- There Are Many More

#### 3 The Vanishing and Exploding Gradients

- Introduction
- Reasoning Iteratively
- Fixed Points
- Stabilizing the Network
  - Gradient Clipping
  - Normalizing your Data
  - Normalization Layer AKA Batch Normalization

#### Problems with Deeper Architectures

- The Degradation Problem
- The Residual Networks
- Conclusions

# Outline

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# For this initial analysis

### We will look at the paper by Bengio

• "Learning deep architectures for AI", Foundations and trends in Machine Learning 2, 1 (2009), pp. 1--127.

#### And for this, we will look at Boolean functions

 After Shanon pointed out the fact they are useful to represent complex problems [1].

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## Architecture

# A two-layer circuit of logic gates can represent any boolean function [2]

- Any boolean function can be written as a sum of products, disjunctive normal form:
  - AND gates on the first layer with optional negation of inputs,
  - And OR gate on the second layer

#### Example

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### Example



# The Exponential Width

### Here, we have a small problem

- There are functions computable with a polynomial-size logic gates circuit of depth k that require **exponential size** when restricted to depth k 1[3]
  - ► For Example

$$parity: (b_1, ..., b_d) \in \{0, 1\}^d \mapsto \begin{cases} 1 & \text{if } \sum_{i=1}^d b_i \\ -1 & \text{otherwise} \end{cases} \text{ is even}$$

#### How this impact shallow learning in Machine Learning?

 Many of the results for boolean circuits can be generalized to architectures whose computational elements are linear threshold units

$$f\left(x\right) = 1_{wx+b>0}$$

The fan-in of a circuit is the maximum number of inputs of a particular element.

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# Therefore

### How this impact shallow learning in Machine Learning?

• First, we define the concept of  $f_k$  function

#### Definition

The function f<sub>k</sub> is a function of N<sup>2k-2</sup> variables. It is defined by a depth k circuit that is a tree. At the leaves of the tree there are unnegated variable, The i<sup>th</sup> level from the bottom consists of ∧-gates if i is even and otherwise it consists of ∨-gates.

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# An Important Theorem

### Of particular interest is the following theorem

• Monotone weighted threshold circuits (i.e. multi-layer neural networks with linear threshold units and positive weights)

#### Theorem [4]

 A monotone weighted threshold circuit of depth k - 1 computing a function f<sub>k</sub> has size at least 2<sup>cN</sup> for some constant c > 0 and N > N<sub>0</sub>.

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# Meaning

### This theorem does not fail any type of architecture

• But the question arises, Are the depth 1, 2 and 3 architectures (many Machine Learning algorithms) too shallow to represent efficiently more complicated functions?

#### What happens in Deep Architectures

Bengio et al. argues that they can represent highly-varying functions
[5]

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- Introduction
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# Highly-varying functions

### Meaning

• We say that a function is highly-varying when a piecewise approximation of that function would require a large number of pieces.

#### Clearly

 Deeper Architectures can handle such functions in a easier way than shallow ones.

#### For Example

The polynomial ∏<sup>n</sup><sub>i=1</sub> ∑<sup>m</sup><sub>j=1</sub> a<sub>ij</sub>x<sub>j</sub> can be represented as a product of sums with only O (nm) elements

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# Basically

We have a Perceptron Layer and a Product Second Layer



#### What if I do a product of sums

What will happen?

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# Ok, we have a problem

### Because for our case

$$\prod_{i=1}^{3} \sum_{j=1}^{6} a_{ij} x_j = \sum_{j=1}^{6} \prod_{i=1}^{3} a_{ij} x_j$$

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# Actually

### You could claim

• Machine Learning shallow learning depends on complex computational units to handle complex functions

#### Deep Learning

 Proposes simpler units but deeper structures to handle complex functions

#### What about both ideas together

- Complex adaptive units
- Deeper architectures to helps such units
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# Local vs Non-Local Generalization

### Something Notable

• A local estimator partitions the input space in regions

#### Thus, local estimators are based on matching local templates

• It can be thought of as having two levels...

#### The first level

It is made of a set of templates which can be matched to the input.

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# Then

A template unit will output a value that indicates the degree of matching

# $K\left( x|\Theta \right)$

#### The second level combines these values

Typically a simple linear combination or product combination

$$L\left(x\right) = \sum_{i=1}^{k} K\left(x|\Theta_{i}\right)$$

#### Classic Example, the kernel machine

$$f(x) = b + \sum_{i=1}^{k} \alpha_i K(x, x_i)$$

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### As you can see

### The Kernel has a local influence based on the support vectors

• For example the Gaussian Kernel

$$K(x, x_i) = \exp\left\{-\frac{\|x - x_i\|^2}{\sigma^2}\right\}$$

#### The Problem of Kernel

 The assumption that the target function is smooth or can be well approximated with a smooth function.

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They have motivated a lot of research in designing kernels [6, 7]

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## For Example, in supervised learning

### If we have the training example $(x_i, y_i)$

• We want to build predictor that output something near  $y_i$  when any other sample is near  $x_i$ 

#### Basically the situation when regularizing

• Bengio and Le Cun claim this is not enough [8, 9]

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 That such highly varying space is due to a lack of the correct feature selection process.

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 Let f (x) = b + ∑<sub>i=1</sub><sup>2<sup>a</sup></sup> α<sub>i</sub>K (x<sub>i</sub>, x) be an affine combination of Gaussian with the same width σ centered on points x<sub>i</sub> ∈ {-1,1}<sup>d</sup>. If f solve the parity problem, then there are at least 2<sup>d-1</sup> non-zero support vectors.

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## For example

Tensors have been used to add memory to SVM

$$\min_{\boldsymbol{U}_{i}^{(m)},\boldsymbol{K}^{(m)},\boldsymbol{\beta},\boldsymbol{b}} \gamma \sum_{i=1}^{N} \left\| \boldsymbol{\mathcal{X}}_{i} - \left[ \left[ \boldsymbol{K}^{(1)} \boldsymbol{U}_{i}^{(1)}, \cdots, \boldsymbol{K}^{(M)} \boldsymbol{U}_{i}^{(M)} \right] \right] \right\|_{F}^{2} + \cdots \\ \lambda \boldsymbol{\beta}^{T} \widehat{\boldsymbol{K}} \boldsymbol{\beta} + \sum_{i=1}^{N} \left[ 1 - y_{i} \left( \widehat{\boldsymbol{k}}_{i}^{T} \boldsymbol{\beta} + b \right) \right]_{+}$$

•  $\mathbf{K}^{(m)}$  are kernel matrices defined on each mode to capture the nonlinear part.

• 
$$oldsymbol{U}^{(m)} = \left[oldsymbol{u}_1^{(m)}, \dots, oldsymbol{u}_R^{(m)}
ight]$$
 are factor matrices of size  $I_m imes R_m$ 

### A Problem

- You are limiting the Machine Learning operations to matrix additions and products and non-linear operations.
  - In a shallow way...

#### We need to add more complex functions

 After all deeper architectures construct complex functions layer by layer

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- Introduction
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## By Using Weights in Certain Deep Learners



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#### Introduction

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- Introduction
- Reasoning Iteratively
- Fixed Points
- Stabilizing the Network
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## Some of the Models to be Reviewed of Models

### Convolutional Neural Networks

• The classic model that started the phenomena of Neural Networks.

#### Auto Encoder

How to generate novel features by funneling.

### Boltzmann Machine

• Energy Based Models.

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### We will see that there are many possible architectures

And more with the different layers
 [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20] :



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Introduction

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- Introduction
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Introduction

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- Introduction
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## Digital Images as pixels in a digitized matrix



Scene element

## Further

### Pixel values typically represent

• Gray levels, colours, heights, opacities etc

### Something Notable

 Remember digitization implies that a digital image is an approximation of a real scene

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## Therefore, we have the following process

### Low Level Process

Input	Processes	Output
	Noise	
Image	Removal	Improved
	Image	Image
	Sharpening	

#### Example, Edge Detection

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### Example, Edge Detection



## Then

## Mid Level Process

Input	Processes	Output
Image	Object Recognition Segmentation	Attributes

### Object Recognition

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## Mid Level Process

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## Therefore

### It would be nice to automatize all these processes

• We would solve a lot of headaches when setting up such process

#### Why not to use the data set:

By using a Neural Networks that replicates the process.

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## Convolutional Neural Networks History

### Work by Hubel and Wiesel in the 1950s and 1960s

• They showed that cat and monkey visual cortexes contain neurons that individually respond to small regions of the visual field.

#### After all more studies about the visual cortex happened

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### Kunihiko Fukushima [21]

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• Proposed the use of Maxpooling to recognize 3D objects in 2D images

The Beginning of the Dream!!!

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• Proposed the use of Maxpooling to recognize 3D objects in 2D images

### Yan LeCunn finally proposed the use of backpropagation [24]

• The Beginning of the Dream!!!
## Convolutional Neural Networks

### Basically they are deep learners based in convolutions or its variants

$$(f * g)(i, j) = \sum_{k=n}^{-n} \sum_{l=-n}^{n} f(k, l) \times g(i - k, j - l)$$
(1)

**Basically Filters** 

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# Example of CNN

### A Basic Convolutional Network



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# We have several techniques for that

### Principal Component Analysis

$$L\left(\boldsymbol{u}_{1}\right) = \boldsymbol{u}_{1}^{T} S \boldsymbol{u}_{1} + \lambda_{1} \left(1 - \boldsymbol{u}_{1}^{T} \boldsymbol{u}_{1}\right)$$

#### Linear Locally Embeddings

$$\Phi\left(Y\right) = \sum_{i} \left|Y_{i} - \sum_{j} W_{ij}Y_{j}\right|^{2}$$

#### And recently

 Uniform Manifold Approximation and Projection for Dimension Reduction [25]

# We have several techniques for that

#### Principal Component Analysis

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# Therefore

### We have the need to codify the original feature into better ones

• This can be done by a series of mappings that act as funnels, How?



#### Basically, we have a series of mappings

### $x \in \mathbb{R}^{n_1} \to f_1(x) \in \mathbb{R}^{n_2} \to f_2(x_1) \in \mathbb{R}^{n_3} \dots \longrightarrow f_m(x_{m-1}) \in \mathbb{R}^{n_{m+1}}$

#### Where

 $n_1 < n_2 < \cdots < n_m < n_{m+1}$ 

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## Then, we can use linear mappings for this

### With the following matrix functions

$$\sigma\left[f_{A_{i+1}}\left(x_{i}\right)\right] = \sigma\left(A_{i+1}x\right)$$

#### Therefore

• Therefore, we have the following architecture.

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• Therefore, we have the following architecture.

# The Basic Auto Encoder Architecture



# Taxonomy

### Most popular Auto Encoders



# Outline

#### Introduction

- Limitations of Shallow Architectures
- Highly-varying functions
- Local vs Non-Local Generalization
- From Simpler Features to More Complex Features

#### Deep Forward Architectures

- Introduction
- Convolutional Neural Networks
  - Image Processing
- Auto Encoders

#### Boltzmann Machines

- Generative Adversarial Networks
- There Are Many More

#### 3 The Vanishing and Exploding Gradients

- Introduction
- Reasoning Iteratively
- Fixed Points
- Stabilizing the Network
  - Gradient Clipping
  - Normalizing your Data
  - Normalization Layer AKA Batch Normalization

#### Problems with Deeper Architectures

- The Degradation Problem
- The Residual Networks
- Conclusions

# The Basic Energy Models

### We have that the Boltzmann Machines

• A Boltzmann machine is a network of units that are connected to each other

#### Here, we have N be the number of units

• Each unit takes a binary value in  $\{0,1\}$ 

• Represented by a random variable  $X_i$ , i = 1, ..., N.

#### Additionally, it has parameters

• Bias  $b_i$ 

• Weight  $w_{ij}$  between unit i and unit j,  $(i,j) \in [1,N-1] \times [i+1,N]$ 

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## The Energy Based Structure

### The energy of the Boltzmann machine is defined by

$$E_{W,\boldsymbol{b}}[\boldsymbol{x}] = -\sum_{i=1}^{N} b_i x_i - \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} w_{ij} x_i x_j = -\boldsymbol{b}^T \boldsymbol{x} - \boldsymbol{x}^T W \boldsymbol{x}$$

I his allows to define a probability distribution

$$\mathbb{P}_{W,b}\left(\boldsymbol{x}\right) = \frac{\exp\left(-E_{W,b}\left[\boldsymbol{x}\right]\right)}{\sum_{\widetilde{\boldsymbol{x}}}\exp\left(-E_{W,b}\left[\widetilde{\boldsymbol{x}}\right]\right)}$$

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# Example



## Thus, using it as a basic model



# Outline

#### Introductio

- Limitations of Shallow Architectures
- Highly-varying functions
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#### Deep Forward Architectures

- Introduction
- Convolutional Neural Networks
  - Image Processing
- Auto Encoders
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#### 3 The Vanishing and Exploding Gradients

- Introduction
- Reasoning Iteratively
- Fixed Points
- Stabilizing the Network
  - Gradient Clipping
  - Normalizing your Data
  - Normalization Layer AKA Batch Normalization

#### Problems with Deeper Architectures

- The Degradation Problem
- The Residual Networks
- Conclusions

## Generative Adversarial Networks

### They can be seen as an Accept-Reject MCMC Model

- However, they do not require Markov Chains with the classic problem:
  - The independence between the samples to generate ergodic probabilities (The real one)

#### As in the Accept-Reject

- The generator network tries to produce realistic-looking samples
- The discriminator network tries to figure out whether an image came from the training set or the generator network

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### As in the Accept-Reject

- The generator network tries to produce realistic-looking samples
- The **discriminator network** tries to figure out whether an image came from the training set or the generator network

# Graphically

### We have the following Basic Model



## Here

### There is a need to join both functions

• So, we can use the idea of Backpropagation to obtain the desired minimization.

#### How can we do this?

 We can define a sensible learning criterion when the dataset is not linearly separable

For this, we can use the **logistic cross-entropy loss** (We will explain more about this later)

### $\mathcal{L}_{LCE}(z,t) = L_{CE}(\sigma(z),t) = t \log(1+e^{-z}) + (1-t)\log(1+e^{z})$

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# Therefore, we have



## In this basic Generator

### $\boldsymbol{D}$ denote the discriminator's predicted probability of being data

 $\mathcal{J}_{D} = E_{\boldsymbol{x} \sim \mathcal{D}} \left[ -\log D\left(\boldsymbol{x}\right) \right] + E_{\boldsymbol{z}} \left[ -\log \left(1 - D\left(G\left(\boldsymbol{z}\right)\right) \right) \right]$ 

#### One possible cost function for the generator

$$\mathcal{J}_{G} = -\mathcal{J}_{D} = const + E_{z} \left[ \log \left( 1 - D \left( G \left( z \right) \right) \right) \right]$$

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# Then using both functions

### The minimax formulation

• Since the generator and discriminator are playing a zero-sum game against each other.

#### Basically

 $\max_{G} \min_{D} \mathcal{J}_{D}$ 

#### There are other examples using the LSE [26

$$\mathcal{J}_{G}=rac{1}{N}\sum_{i=1}^{N}\left[G\left(oldsymbol{z}
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## Now



## Outline

#### Introduction

- Limitations of Shallow Architectures
- Highly-varying functions
- Local vs Non-Local Generalization
- From Simpler Features to More Complex Features

#### Deep Forward Architectures

- Introduction
- Convolutional Neural Networks
  - Image Processing
- Auto Encoders
- Boltzmann Machines
- Generative Adversarial Networks
- There Are Many More

#### 3 The Vanishing and Exploding Gradients

- Introduction
- Reasoning Iteratively
- Fixed Points
- Stabilizing the Network
  - Gradient Clipping
  - Normalizing your Data
  - Normalization Layer AKA Batch Normalization

#### Problems with Deeper Architectures

- The Degradation Problem
- The Residual Networks
- Conclusions

## There Are Many More!!! Here a few more...



Deep Belief Network



**Convolutional Network** 



## Furthermore

**Deconvolutional Network** 



Autoencoder



Generative Adversarial Network



Deep Residual Network



## Outline

#### Introduction

- Limitations of Shallow Architectures
- Highly-varying functions
- Local vs Non-Local Generalization
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#### Deep Forward Architectures

- Introduction
- Convolutional Neural Networks
  - Image Processing
- Auto Encoders
- Boltzmann Machines
- Generative Adversarial Networks
- There Are Many More

#### 3 The Vanishing and Exploding Gradients

#### Introduction

- Reasoning Iteratively
- Fixed Points
- Stabilizing the Network
  - Gradient Clipping
  - Normalizing your Data
  - Normalization Layer AKA Batch Normalization

#### Problems with Deeper Architectures

- The Degradation Problem
- The Residual Networks
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## As We know

### In Recurrent Neural Networks, we have the problem

### • Vanishing and Exploding Gradients

#### In the Deeper Architectures as encoder-decoder we have such phenomena

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In Recurrent Neural Networks, we have the problem

• Vanishing and Exploding Gradients

# In the Deeper Architectures as encoder-decoder we have such phenomena



## Consider a simple encoder encoder network



We have the following structure

$$h_t = w_t x_t + z_{t-1}$$
$$z_t = s_t h_t$$

## Consider a simple encoder encoder network



### We have the following structure

$$h_t = w_t x_t + z_{t-1}$$
$$z_t = s_t h_t$$

## Backpropagation Rules

### Then, we get the following backpropagation rules

$$\begin{aligned} \frac{\partial h_t}{\partial w_i} &= \frac{\partial h_t}{\partial h_{t-1}} \times \frac{\partial h_{t-1}}{\partial h_{t-2}} \times \ldots \times \frac{\partial h_i}{\partial w_i} \\ \frac{\partial h_t}{\partial s_i} &= \frac{\partial h_t}{\partial h_{t-1}} \times \frac{\partial h_{t-1}}{\partial h_{t-2}} \times \ldots \times \frac{\partial h_{i+1}}{\partial s_i} \end{aligned}$$

## Then, we have

### By Using Our simplifying assumption that

$$\frac{\partial h_t}{\partial h_{t-1}} = \frac{\partial \left(w_t x_t + s_{t-1} h_{t-1}\right)}{\partial h_{t-1}} = s_{t-1}$$



#### Finally, we have that

$$\frac{\partial h_t}{\partial w_i} = x_t \left[ \prod_{k=t-1}^{i-1} s_k \right]$$

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And for  $\frac{\partial h_i}{\partial w_i}$ 

$$\frac{\partial h_i}{\partial w_i} = x_i$$

### Finally, we have that

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## It is clear that

#### Unless the $s_k$ 's are near to 1

- You have the vanishing gradient if  $s_k \in [0, 1)$  for all k.
- You have the exploding gradient if  $s_k \in (1, +\infty]$  for all k.

#### Even with activation functions

 These terms tend to appear in the Deep Learners when Backpropagation is done

#### In the case of Forward

• We have many activation function that squash the signal...

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## Outline

#### Introduction

- Limitations of Shallow Architectures
- Highly-varying functions
- Local vs Non-Local Generalization
- From Simpler Features to More Complex Features

#### Deep Forward Architectures

- Introduction
- Convolutional Neural Networks
  - Image Processing
- Auto Encoders
- Boltzmann Machines
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- There Are Many More

#### 3 The Vanishing and Exploding Gradients

Introduction

#### Reasoning Iteratively

- Fixed Points
- Stabilizing the Network
  - Gradient Clipping
  - Normalizing your Data
  - Normalization Layer AKA Batch Normalization

#### Problems with Deeper Architectures

- The Degradation Problem
- The Residual Networks
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## Instead of doing this

### Let us to do the following

$$f\left(x\right) = 3.5x\left(1-x\right)$$

In the first composition, we get

## Instead of doing this

### Let us to do the following

$$f\left(x\right) = 3.5x\left(1-x\right)$$

### In the first composition, we get



## Now, as we compound the function

Second one,  $y = f \circ f(x)$ 



## Now, as we increment iterations

### Third one, $y = f \circ f \circ f(x)$



## Finally

### We see the increment in the gradient part negative or positive



## Actually, we have

### A Frontier defining the Vanishing and Exploding Gradient [27]



## Outline

#### Introduction

- Limitations of Shallow Architectures
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#### Deep Forward Architectures

- Introduction
- Convolutional Neural Networks
  - Image Processing
- Auto Encoders
- Boltzmann Machines
- Generative Adversarial Networks
- There Are Many More

#### 3 The Vanishing and Exploding Gradients

- Introduction
- Reasoning Iteratively

#### Fixed Points

- Stabilizing the Network
  - Gradient Clipping
  - Normalizing your Data
  - Normalization Layer AKA Batch Normalization

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77 / 132

#### Problems with Deeper Architectures

- The Degradation Problem
- The Residual Networks
- Conclusions



### Eventually, the iterates go to infinity or zero OR

• They wind up at a fixed point...

#### A Fixed Point?

## $x = f\left(x\right)$

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### Eventually, the iterates go to infinity or zero OR

• They wind up at a fixed point...

### A Fixed Point?

$$x = f\left(x\right)$$

## Basically

### The fixed points can be thought

- Some fixed points repel the iterates; these are called sources.
- Other fixed points attract the iterates; these are called sinks.

#### Basically f'(x) < 1 are sinks and f'(x) > 1 are sources

## Basically

### The fixed points can be thought

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## Areas of attraction

# Basically, we have that there are areas the pull in the iterations of the function



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## These fixed points

### In Deep Structures as RNN without sigmoid functions

$$h_t = W_{sd} x_t + U_{ss} h_{t-1}$$
$$y_t = V_{os} h_t$$

#### We have

### $oldsymbol{x}_t = V_{os}\left[W_{sd}oldsymbol{x}_t + U_{ss}oldsymbol{h}_{t-1} ight]$

#### For the tensor of $m{b} = V_{os} U_{ss} m{h}_{t-1}$

Then, we have that

 $\boldsymbol{x}_t = V_{os} W_{sd} \boldsymbol{x}_t + V_{os} U_{ss} \boldsymbol{h}_{t-1} = I \boldsymbol{x}_t + 0$ 

## These fixed points

### In Deep Structures as RNN without sigmoid functions

$$egin{aligned} m{h}_t &= W_{sd} m{x}_t + U_{ss} m{h}_{t-1} \ m{y}_t &= V_{os} m{h}_t \end{aligned}$$

### We have

$$\boldsymbol{x}_t = V_{os} \left[ W_{sd} \boldsymbol{x}_t + U_{ss} \boldsymbol{h}_{t-1} \right]$$

#### Therefore if $b=V_{os}U_{ss}h_{t-}$

Then, we have that

 $\boldsymbol{x}_t = V_{os} W_{sd} \boldsymbol{x}_t + V_{os} U_{ss} \boldsymbol{h}_{t-1} = I \boldsymbol{x}_t + 0$ 

## These fixed points

### In Deep Structures as RNN without sigmoid functions

$$egin{aligned} m{h}_t &= W_{sd} m{x}_t + U_{ss} m{h}_{t-1} \ m{y}_t &= V_{os} m{h}_t \end{aligned}$$

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## They define an area

### Where $V_{os}$ and $W_{sd}$

### • They are the inverse of each other

#### And the hidden state is almost zero

 Basically they fixed point converts a RNN without activation functions in a linear model
# They define an area

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- Highly-varying functions
- Local vs Non-Local Generalization
- From Simpler Features to More Complex Features

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  - Image Processing
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- Introduction
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### Stabilizing the Network

- Gradient Clipping
- Normalizing your Data
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85 / 132

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# Gradient Clipping

We prevent gradient from blowing up by rescaling to a certain value

$$\|\nabla_{\theta}L\| > \eta \Longrightarrow \nabla_{\theta}L = \frac{\eta \nabla_{\theta}L}{\|\nabla_{\theta}L\|}$$

### We have a series of nice analysis [28]

 $\min_{x \in \mathbb{R}^d} f\left(x\right)$ 

Furthermore, we define a space

 $S = \{x| \exists y ext{ such that } f\left(y
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## We have then for ${\cal S}$

In  $\mathbb{R}^2$  the following example

## Assumptions

## Assumption 1

 $\bullet$  Function f is lower bounded by  $f^{\ast}$ 

#### Assumption

Function f is twice differentiable

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## Assumption 2

• Function f is twice differentiable

Then, there are the following proposals

## The ordinary gradient descent

$$x_{k+1} = x_k - \eta \nabla f\left(x_k\right)$$

### The Clipped Gradient Descent (CGD)

$$x_{k+1} = x_k - h_c \nabla f(x_k)$$
, where  $h_c = \min\left\{\eta_c, \frac{\gamma \eta_c}{\|\nabla f(x)\|}
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## Remark

## Clipped GD and NGD are almost equivalent

• If we set 
$$\gamma\eta_c=\eta_n$$
 and  $\eta_c=\frac{\eta_n}{\beta}$  then 
$$\frac{1}{2}h_c\leq h_n\leq 2h_c$$

## A Natural Question

## Definition

• The objective f is called L-smooth if  $\left\|\nabla f\left(x\right)-\nabla f\left(y\right)\right\|\leq L\left\|x-y\right\|$  for all  $x,y\in\mathbb{R}^{d}$ 

### This is equivalent under a twice differentiable .

 $\left\|\nabla^2 f\left(x\right)\right\| \le L$ 

Then, you get the following upper-bound

$$f(y) \approx f(x) + \nabla^{T} f(x) (y - x) + \frac{1}{2} (y - x)^{T} \nabla^{2} f(x) (y - x)$$

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Then, it is possible to use the 3 Assumption

## We have that

$$f(y) \le f(x) + \nabla^T f(x) (y - x) + \frac{1}{2}L ||y - x||^2$$

### Then fixing all the other variables and assuming $y = x - h \nabla f(x)$ .

$$h^* = \arg\min_{h} \left[ f(x) - h \|\nabla f(x)\|^2 + \frac{1}{2}Lh^2 \|\nabla f(x)\|^2 \right] = \frac{1}{L}$$

### Basically

• This choice of h leads to GD with a fixed step,

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## Question

• "Is clipped gradient descent optimized for a different smoothness condition?"

### Inspired in the equation

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## Assume that such value optimize the equation

$$f(x) - h \|\nabla f(x)\|^{2} + \frac{1}{2}Lh^{2} \|\nabla f(x)\|^{2}$$

#### Then, we have

 $L(x) = \frac{\left\|\nabla f(x)\right\| + \beta}{\eta}$ 

### Assumption 3 by using $|\nabla^2 f(x)| \leq L$

(L<sub>0</sub>, L<sub>1</sub>)-smoothness. f is (L<sub>0</sub>, L<sub>1</sub>)-smooth, if there exist positive L<sub>0</sub> and L<sub>1</sub> such that ||∇<sup>2</sup>f(x)|| ≤ L<sub>0</sub> + L<sub>1</sub> ||∇f(x)||
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  - $\nabla^{2}f(x)$  is the Hessian

# The final Theorem

## Theorem (CGD) [28]

• Assume that Assumptions 1, 2, and 3 hold in set S. With parameters

$$\eta_c = rac{1}{10L_o} ext{ and } \gamma = \min\left\{rac{1}{\eta_c}, rac{1}{10L_o\eta_c}
ight\},$$

Then Clipped GD terminates in

$$\frac{20L_0\left(f\left(x_0\right) - f^*\right)}{\epsilon^2} + \frac{20\max\left\{1, L_1^2\right\}\left(f\left(x_0\right) - f^*\right)}{L_0} \text{ iterations }$$

## Remarks

## The paper

• It points out to a high correlation between the Jacobian and the Hessian

There are more work to be done

Please read the paper...

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97 / 132

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- Conclusions

## Another way to stabilize the network

## Data Normalization

### • Standardization is the most popular form of preprocessing

Normally mean subtraction and subsequent scaling by the standard deviation.

#### Mean subtraction

$$\mu = rac{1}{N}\sum_{i=1}^N oldsymbol{x}_i$$
 then  $oldsymbol{x}_i^c = oldsymbol{x}_i - \mu$ 

### Finally

 Standardization refers to altering the data dimensions such that they are of approximately the same scale.

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$$x_i^s = \frac{x_i - \mu}{\sigma}$$

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- a ascender curve height relative to baseline
- b baseline absolute vertical position
- c core line position
- d descenders curve position
- $\kappa$  curvature
- s angle

# Softmax Scaling

### Thus

• All new features have zero mean and unit variance.

#### Further

 Other linear techniques limit the feature values in the range of [0,1] or [-1,1] by proper scaling.

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We can non-linear mapping. For example the softmax scaling.

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# Steps of Softmax Scaling

### Softmax Scaling

• It consists of two steps

#### First one



#### Second one

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They are squashed by the exponential part of the function.

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103 / 132

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# Here, the people at Google [17] around 2015

### They commented in the "Internal Covariate Shift Phenomena"

• Due to the change in the distribution of each layer's input

#### They claim

 The min-batch forces to have those changes which impact on the learning capabilities of the network.

#### In Neural Networks, they define this

 Internal Covariate Shift as the change in the distribution of network activations due to the change in network parameters during training. Here, the people at Google [17] around 2015

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# They gave the following reasons

### Consider a layer with the input u that adds the learned bias b

• Then, it normalizes the result by subtracting the mean of the activation over the training data:

$$\widehat{\boldsymbol{x}} = \boldsymbol{x} - E\left[\boldsymbol{x}
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▶  $\mathcal{X} = \{ m{x}, ..., m{x}_N \}$  the data samples and  $E\left[m{x}
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## Now, if the gradient ignores the dependence of $E\left| x ight|$ on b

ullet Then  $b=b+\Delta b$  where  $\Delta b\propto -rac{\partial l}{\partial x}$ 

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# Normalization via Mini-Batch Statistic

It is possible to describe the normalization as a transformation layer

$$\widehat{\boldsymbol{x}} = Norm\left(\boldsymbol{x}, \mathcal{X}\right)$$

 $\bullet$  Which depends on all the training samples  ${\mathcal X}$  which also depends on the layer parameters

For back-propagation, we will need to generate the following terms  $\frac{\partial Norm(x, X)}{\partial x}$  and  $\frac{\partial Norm(x, X)}{\partial X}$ 

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# Normalization via Mini-Batch Statistic

### Problem!!!

• whitening the layer inputs is expensive, as it requires computing the covariance matrix

$$Cov\left[ oldsymbol{x} 
ight] = E_{oldsymbol{x} \in \mathcal{X}} \left[ oldsymbol{x} oldsymbol{x}^T 
ight]$$
 and  $E\left[ oldsymbol{x} 
ight] E\left[ oldsymbol{x} 
ight]^T$ 

To produce the whitened activations

# Therefore

### A Better Options, we can normalize each dimension

$$\widehat{\bm{x}}^{(k)} = \frac{\bm{x}^{(k)} - \mu}{\sigma}$$
• with  $\mu = E\left[\bm{x}^{(k)}\right]$  and  $\sigma^2 = Var\left[\bm{x}^{(k)}\right]$ 

#### This allows to speed up convergence

 Simply normalizing each input of a layer may change what the layer can represent.

#### So, we need to insert a transformation in the network

Which can represent the identity transform

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(1)

### So, we need to insert a transformation in the network

• Which can represent the identity transform

# The Transformation

### The Linear transformation

$$\boldsymbol{y}^{(k)} = \gamma^{(k)} \widehat{\boldsymbol{x}}^{(k)} + \beta^{(k)}$$

#### The parameters $\gamma$

• This allow to recover the identity by setting  $\gamma^{(k)} = \sqrt{Var[x^{(k)}]}$  and  $\beta^{(k)} = E[x^{(k)}]$  if necessary.

# The Transformation

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### Batch Normalizing Transform

Input: Values of x over a mini-batch:  $\mathcal{B} = \{x_{1...m}\}$ , Parameters to be learned:  $\gamma, \beta$ Output:  $\{y_i = BN_{\gamma,\beta}(x_i)\}$ 

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Input: Values of x over a mini-batch:  $\mathcal{B} = \{x_{1...m}\}$ , Parameters to be learned:  $\gamma, \beta$ Output:  $\{y_i = BN_{\gamma,\beta}(x_i)\}$  $\mathfrak{P}_{\mathcal{B}} = \frac{1}{m} \sum_{i=1}^m x_i$  $\sigma_{\mathcal{B}}^2 = \frac{1}{m} \sum_{i=1}^m (x_i - \mu)^2$ 

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## We have the following equations by using the loss function l

 $\frac{\partial l}{\partial \mu_{B}} = \left(\sum_{i=1}^{m} \frac{\partial l}{\partial x_{i}} \times \frac{-1}{\sqrt{\sigma_{B}^{2} + \epsilon}}\right) + \frac{\partial l}{\partial \sigma_{B}^{2}} \times \frac{\sum_{i=1}^{-2 \times (x_{i} - \mu_{B})}}{m}$   $\frac{\partial l}{\partial x_{i}} = \frac{\partial l}{\partial x_{i}} \times \frac{1}{\sqrt{\sigma_{B}^{2} + \epsilon}} + \frac{\partial l}{\partial \sigma_{B}^{2}} \times \frac{2 \times (x_{i} - \mu_{B})}{m} + \frac{\partial l}{\partial \mu_{B}} \times \frac{1}{m}$   $\frac{\partial l}{\partial \gamma} = \sum_{i=1}^{m} \frac{\partial l}{\partial y_{i}} \times \hat{x}_{i}$   $\frac{\partial l}{\partial \beta} = \sum_{i=1}^{m} \frac{\partial l}{\partial y_{i}}$ 

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We have the following equations by using the loss function  $\boldsymbol{l}$ 

• 
$$\frac{\partial l}{\partial \hat{x}_i} = \frac{\partial l}{\partial y_i} \times \gamma$$
  
•  $\frac{\partial l}{\partial \sigma_B^2} = \sum_{i=1}^m \frac{\partial l}{\partial \hat{x}_i} \times (x_i - \mu_B) \times (-\frac{1}{2}) \times (\sigma_B^2 + \epsilon)^{-\frac{3}{2}}$ 

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$$\frac{\partial l}{\partial \mu_{\mathcal{B}}} = \left(\sum_{i=1}^{m} \frac{\partial l}{\partial \hat{x}_{i}} \times \frac{-1}{\sqrt{\sigma_{\mathcal{B}}^{2} + \epsilon}}\right) + \frac{\partial l}{\partial \sigma_{\mathcal{B}}^{2}} \times \frac{\sum_{i=1}^{m} -2 \times (x_{i} - \mu_{\mathcal{B}})}{m}$$

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Input: Network N with trainable parameters  $\Theta$ ; subset of activations  $\{x^{(k)}\}_{k=1}^{K}$ Output: Batch-normalized network for inference  $N_{BN}^{inf}$ 

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Process multiple training mini-batches  $\mathcal{B}$ , each of size m, and average over them

 $E[x] = E_{B}[\mu_{B}] \text{ and } Var[x] = \frac{m}{m-1} \frac{m}{B} \left[\sigma_{B}^{2}\right]$ In  $N_{BN}^{inf}$ , replace the transform  $y = BN_{\gamma,\beta}(x)$  with  $y = \frac{\gamma}{\sqrt{Var[x]}} \times x + \left[\beta - \frac{\gamma B[x]}{\sqrt{Var[x]}}\right]$ 

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$$\text{ for } k = 1...K \text{ do}$$

Modify each layer in  $N_{BN}^{tr}$  with input  $x^{(k)}$  to take  $y^{(k)}$  instead

$$N_{BN}^{inf} = N_{BN}^{tr} / \text{ Inference BN network with frozen parameters}$$

Process multiple training mini-batches  $B_i$  each of size  $m_i$  and average over them

$$E[x] = E_{B}[\mu_{B}] \text{ and } Var[x] = \frac{m}{m-1} \frac{m}{B} \left[\sigma_{B}^{2}\right]$$
  
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 Add transformation 
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 to  $N^{tr}_{BN}$ 
 Modify each layer in  $M^{tr}_{BN}$  with input of the take prime test
 for k = 1...K de
 Process multiple training mini-batches B, each of size m, and
 average over them
 E [x] = Ba [xa] and for [x] =  $\frac{1}{2}$  [xa]
 [x] =  $\frac{1}{2}$  [xa] =  $\frac{1}{2}$  [xa]
 [x] =  $\frac{1}{2}$  [xa] =  $\frac{1}{2}$  [xa]
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Input: Network N with trainable parameters  $\Theta$ ; subset of activations  $\left\{ {{m{x}^{\left( k 
ight)}}} 
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Output: Batch-normalized network for inference  $N_{BN}^{inf}$ 

9 
$$N_{BN}^{tr} = N //$$
 Training BN network
9 for  $k = 1...K$  do
9 Add transformation  $y^{(k)} = BN_{\gamma^{(k)},\beta^{(k)}} \left(x^{(k)}\right)$  to  $N_{BN}^{tr}$ 
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average over them

$$\begin{aligned} E[x] &= E_B[\mu_B] \text{ and } Var[x] = \frac{m}{m-1}_B \left[ \sigma_B^2 \right] \\ & \text{In } N_{BN}^{inf}, \text{ replace the transform } y = BN_{\gamma,\beta}(x) \text{ with} \\ & y = \frac{\gamma}{\sqrt{Var[x] + \epsilon}} \times x + \left[ \beta - \frac{\gamma E[x]}{\sqrt{Var[x] + \epsilon}} \right] \end{aligned}$$

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## However

## Santurkar et al. [18]

• They found thats is not the covariance shift the one affected by it!!!

### Santurkar et al. recognize that

 Batch normalization has been arguably one of the most successful architectural innovations in deep learning.

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## They found something quite interesting



## Actually Batch Normalization

## It does not do anything to the Internal Covariate Shift

- Actually smooth the optimization manifold
  - It is not the only way to achieve it!!!

#### They suggest that

 "This suggests that the positive impact of BatchNorm on training might be somewhat serendipitous."

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 "This suggests that the positive impact of BatchNorm on training might be somewhat serendipitous."

## They actually have a connected result

## To the analysis of gradient clipping!!!

• They are the same group

## Theorem (The effect of BatchNorm on the Lipschitzness of the loss)

For a BatchNorm network with loss L
 and an identical non-BN network with (identical) loss L,

$$\left\|\nabla_{y_j}\widehat{\mathcal{L}}\right\|^2 \leq \frac{\gamma^2}{\sigma_j^2} \left[ \left\|\nabla_{y_j}\mathcal{L}\right\|^2 - \frac{1}{m}\left\langle \mathbf{1}, \nabla_{y_j}\mathcal{L}\right\rangle^2 - \frac{1}{\sqrt{m}}\left\langle \nabla_{y_j}\mathcal{L}, \widehat{y}_j\right\rangle^2 \right]$$

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## Theorem (The effect of BatchNorm on the Lipschitzness of the loss)

• For a BatchNorm network with loss  $\widehat{\mathcal{L}}$  and an identical non-BN network with (identical) loss  $\mathcal{L}$ ,

$$\left\|\nabla_{\boldsymbol{y}_{j}}\widehat{\mathcal{L}}\right\|^{2} \leq \frac{\gamma^{2}}{\sigma_{j}^{2}}\left[\left\|\nabla_{y_{j}}\mathcal{L}\right\|^{2} - \frac{1}{m}\left\langle\mathbf{1}, \nabla_{y_{j}}\mathcal{L}\right\rangle^{2} - \frac{1}{\sqrt{m}}\left\langle\nabla_{y_{j}}\mathcal{L}, \widehat{\boldsymbol{y}}_{j}\right\rangle^{2}\right]$$

## Outline

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- Limitations of Shallow Architectures
- Highly-varying functions
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- From Simpler Features to More Complex Features

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#### 3 The Vanishing and Exploding Gradients

- Introduction
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118 / 132

#### Problems with Deeper Architectures

#### The Degradation Problem

- The Residual Networks
- Conclusions

## Definition

## Degradation Problem

• With the network depth increasing, accuracy gets saturated (which might be unsurprising) and then degrades rapidly.

### Something Notable

Unexpectedly, such degradation is not caused by overfitting,

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120 / 132

#### Problems with Deeper Architectures

• The Degradation Problem

#### The Residual Networks

Conclusions

Therefore, we need to deal with such problems

## The Residual Network [16]

• He, Kaiming et al. - "Deep Residual Learning for Image Recognition"

### Basically they got two layers doing something to an input

 $\mathcal{F}\left(\boldsymbol{x}\right) = A_2 A_1 \boldsymbol{x}$ 

### Fhen imagine you have an ideal mapping $\mathcal{H}\left(x ight)$

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## Blocks of the Original RNN



123 / 132

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## A Winner

### Something Notable

 Winner of ILSVRC 2015 in image classification, detection, and localization, as well as Winner of MS COCO 2015 detection, and segmentation.

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