ECE 1508S2: Applied Deep Learning

Chapter 5: Advancing Our Bag of Tools II

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A Bit of History: *LeNet*

CNNs was first trained via gradient-based algorithms by *Yan LeCun* and his team: *they could develop backpropagation through CNNs and hence they were able to efficiently implement it*[1]

[1] Check out their paper at this link! The diagram is taken from the the paper

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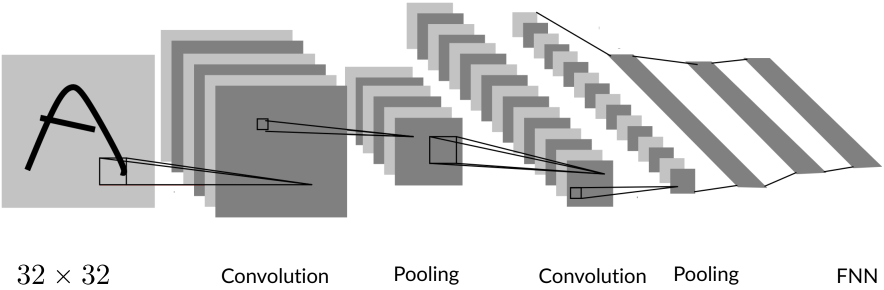

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- *2010: Team NEC-UIUC*
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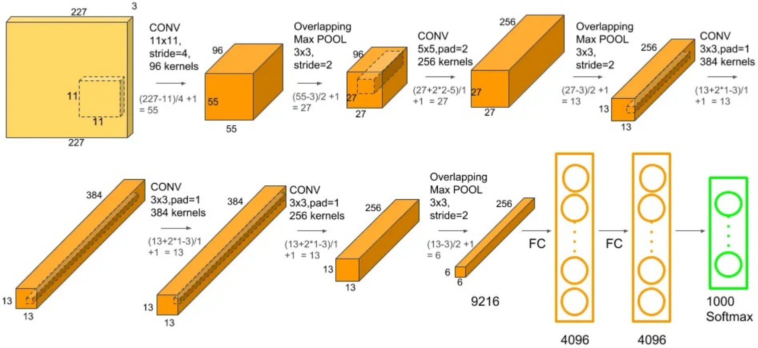
In 2012, Supervision from U of T trained a deep CNN and won ILSVRC

First Deep Winner: *AlexNet*

Alex Krizhevsky, Ilya Sutskever and Geoffrey E. Hinton proposed AlexNet *which could greatly reduce the classification error*[2]



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AlexNet to ZFNet

AlexNet was a deep CNN with 8 learnable layers

- *5 convolutional layers*
- *3 fully-connected layers*

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At this point, going deeper considered as the key to success

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VGG Architectures

Visual Geometry Group at Oxford University developed deeper CNNs: *a class of architectures*[4]

- *VGG-11*
- *VGG-13*
- *VGG-16*
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They could won ILSVRC localization task and took second place in classification: their results also showed an interesting finding

> *As we go deeper, the accuracy gets higher notably up to VGG-16; however, VGG-19 can only give marginal improvements!*

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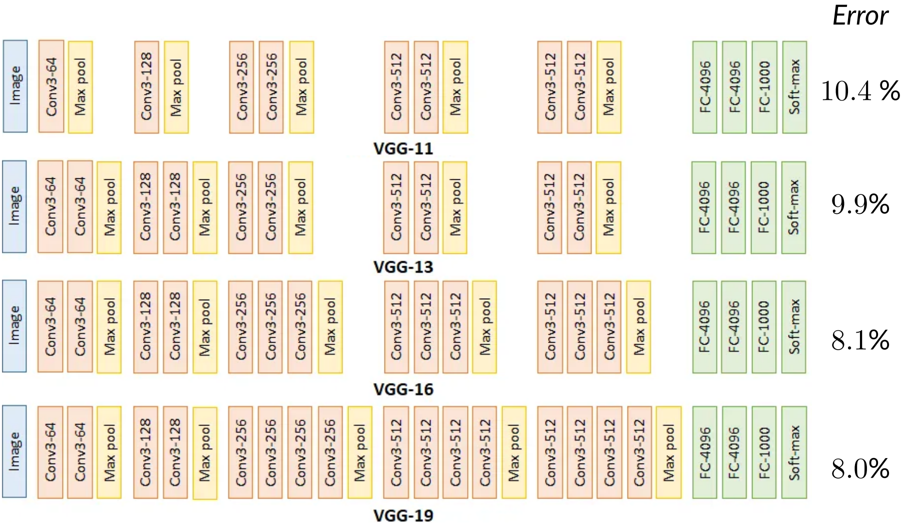
VGG Architectures



GoogLeNet: *2014 Classification Winner*

In 2014, Google introduced GoogLeNet: *a deep CNN which uses fully-connected layer only at the output and is purely based on CNN*[5]

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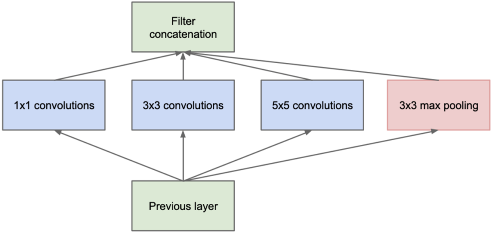
- *They introduced a new module called "inception module"*
  ↳ *It's a collection of parallel convolutions and poolings*



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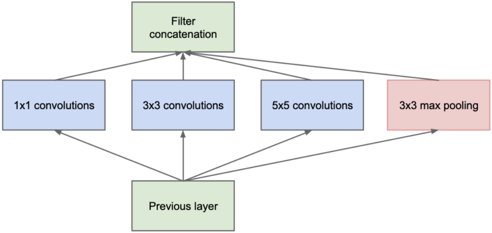

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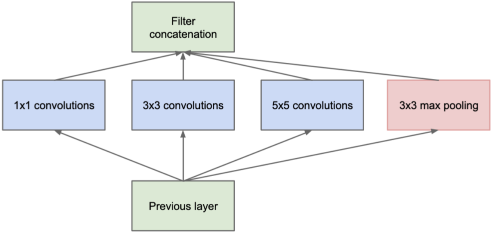

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A Hurdle in Going Deeper

Though deep CNNs were doing good job, *as people kept going deeper they realized that the performance is getting saturated*. Later studies showed that *much deeper CNNs start to perform worse!*

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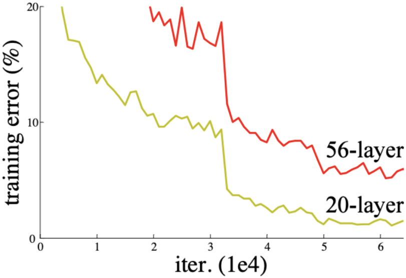

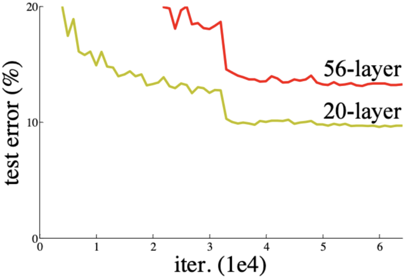

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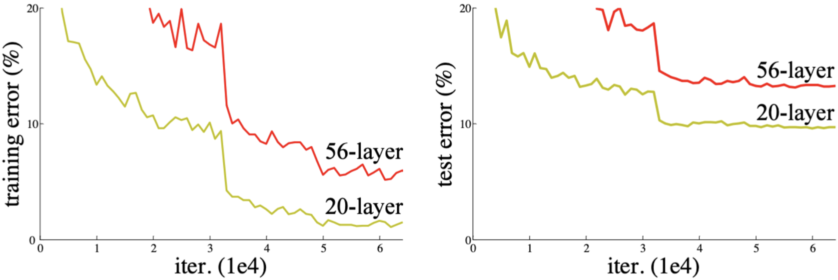

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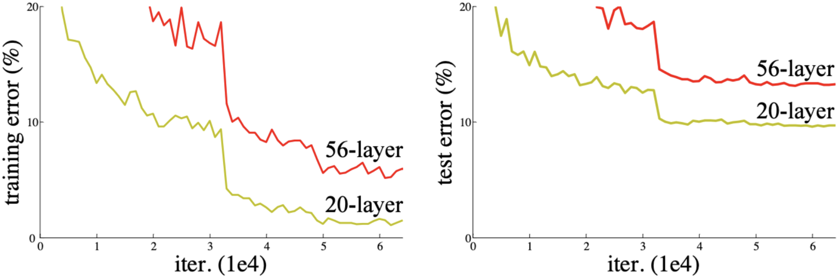

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– Well! *If it's coming from overfitting we should see better training and worst test risk. This is however not the case here!*

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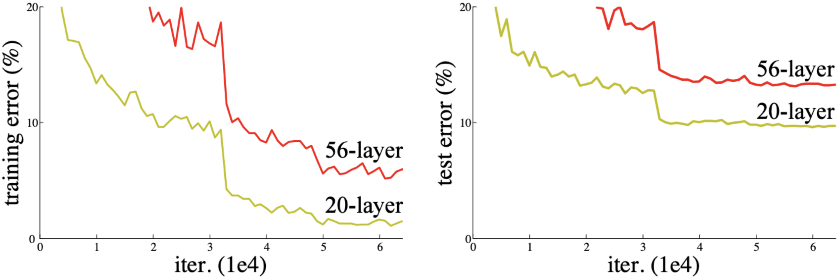

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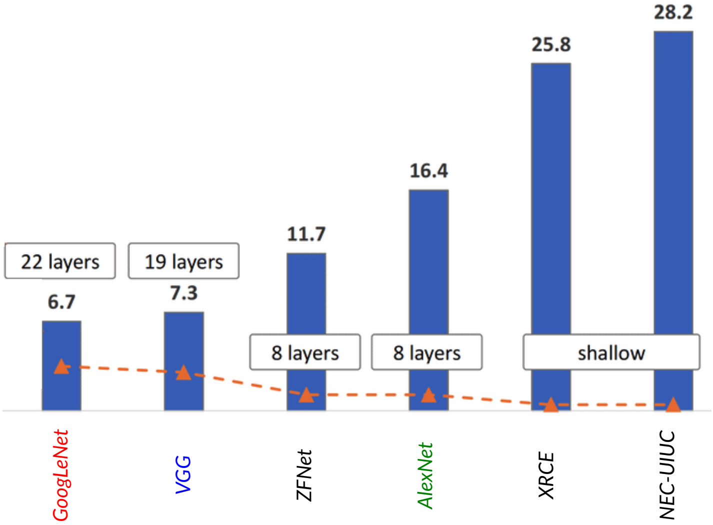
> *People started to blame the vanishing gradient behavior of deep NNs*

Depth vs Accuracy: *ILSVRC Winners till 2014*



Problem of Depth

+ *But, what is the problem of vanishing gradient?*
- This is a general behavior in deep NNs: *as we go deeper, the gradients determined by backpropagation at initial layers get smaller and smaller, such that at some point they stop getting updated anymore, even though they should*
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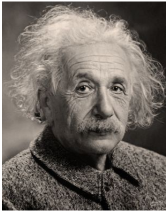
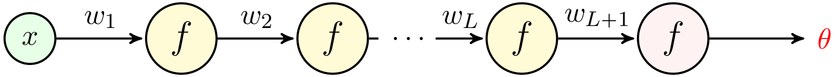
– This is a general behavior in deep NNs: *as we go deeper, the gradients determined by backpropagation at initial layers get smaller and smaller, such that at some point they stop getting updated anymore, even though they should*
+ *How does it come?*
– Let's see it! But we follow Albert Einstein advice!



"Everything should be made as simple as possible, but not simpler!"

Vanishing Gradients: *Simple Example*

Consider the following dummy FNN: *an FNN has a single scalar input*, L *hidden layers and a single scalar output. All neurons are activated by function* $f(\cdot)$ *and have no bias*



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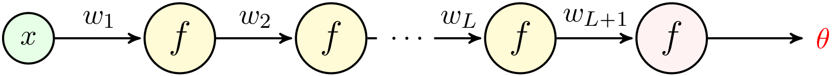

Let's write forward pass

- $y_1 = f(w_1 x)$
- $y_2 = f(w_2 y_1)$

  $\cdots$
- $y_L = f(w_L y_{L-1})$
- $\theta = f(w_{L+1} y_L)$

Vanishing Gradients: *Simple Example*

$$x \xrightarrow{w_1} f \xrightarrow{w_2} f \cdots \xrightarrow{w_L} f \xrightarrow{w_{L+1}} f \longrightarrow \theta$$

Now, we go for backward *pass: we start with* $\overleftarrow{\theta} = \mathrm{d}\hat{R}/\mathrm{d}\theta$ *and go backward*

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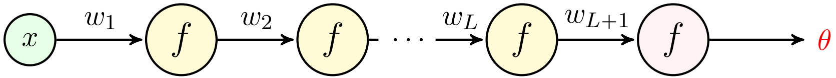

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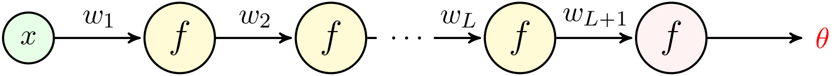

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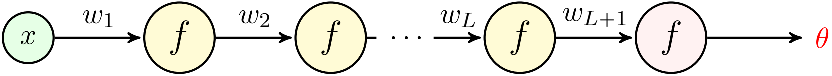

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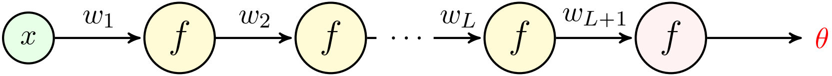

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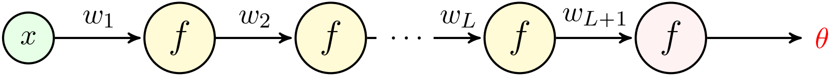

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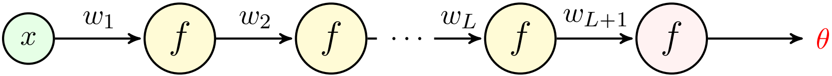

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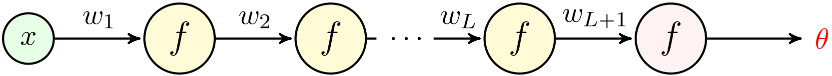

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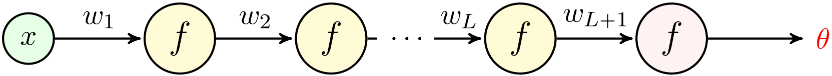

Now, let's compute derivative of loss with respect to the first weight w_1

- $y_1 = f(w_1 x)$

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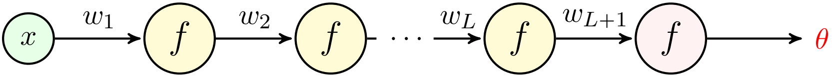

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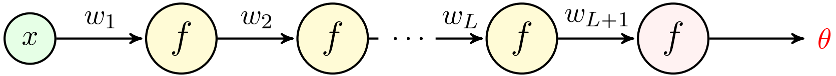

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$$\lim_{L\uparrow\infty} \frac{\mathrm{d}\hat{R}}{\mathrm{d}w_1} = 0$$

↳ *Backpropagation accumulation concentrates at zero!*

Gradient with respect to first layer vanishes as the network gets too deep

Exploding Gradients: *Simple Example*

$$\frac{\mathrm{d}\hat{R}}{\mathrm{d}w_1} = \overleftarrow{\theta} \underbrace{x\dot{f}\left(w_1 x\right) \prod_{\ell=2}^{L+1} w_\ell \dot{f}\left(w_\ell y_{\ell-1}\right)}_{\text{accumulated in backpropagation}}$$

Now, consider the following cases

- ***Case II:*** *We have a ReLU activation and all weight are larger than 1*
  - ↳ *Assume $x > 0$; then, $\dot{f}\left(w_\ell y_{\ell-1}\right) = 1$ since all the sequence is positive*

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Vanishing Gradients: *Simple Example*

$$\frac{\mathrm{d}\hat{R}}{\mathrm{d}w_1} = \overleftarrow{\theta} \underbrace{x\dot{f}\left(w_1 x\right)\prod_{\ell=2}^{L+1} w_\ell \dot{f}\left(w_\ell y_{\ell-1}\right)}_{\text{accumulated in Backpropagation}}$$

Now, consider the following cases

- ***Case I:*** *We have a ReLU activation and all weight are larger than 1*

$$\lim_{L\uparrow\infty} \frac{\mathrm{d}\hat{R}}{\mathrm{d}w_1} \to \infty$$

↳ *Backpropagation accumulation explodes!*

Gradient with respect to first layer explodes as the network gets too deep

Exploding-Vanishing Gradients: *Summary*

Moral of Story

As the network gets very deep, the gradients of initial layers can get extremely small or large

- *The vanishing occurs more frequently*
  - ↳ *Weights are often adjusted by optimizer to get small*
  - ↳ *Once they all get small, the gradient starts to vanish*
- *Weights and derivative of activation function are key deciders*
  - ↳ *We need them to mostly around 1*

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- *Weights and derivative of activation function are key deciders*
  - ↳ *We need them to mostly around 1*

The above observation also explains *why we had some specific preferences*

- We preferred ReLU activation in hidden layers
  - ↳ $\dot{\mathrm{ReLU}}(x) = 1$ *when* $x > 0$
- We preferred normalized features
  - ↳ *this can keep weights normalized*

Exploding-Vanishing Gradients: *Solution*

+ *But, is there any solution for that?*
– Yes! Actually, we already had some one them!

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In practice, we can use different approaches to control this behavior

- We use better activations in deep NNs
  ↳ *this is why in deep CNNs we use mostly ReLU*
- We apply batch-normalization
  ↳ *we already have discussed it!*
- We use skip connection
  ↳ *this helps us go even deeper!*

Let's understand what skip connection is!

Skip Connection: *Residual Learning*

The root idea of skip connection is as follows: *instead of learning a function*

we can learn its residual and add it up with the input

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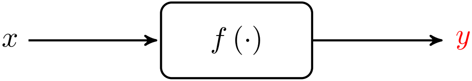
we can learn its residual and add it up with the input

Let's say we have input x and label y

With plain NNs we learn a function $f(\cdot)$ that relates x to y

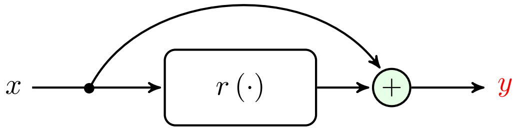


The NN approximates $f(\cdot)$ as best as it could

Skip Connection: *Residual Learning*

Let's say we have input x and label y

But, we can also learn a function $r(\cdot)$ that relates x to $y - x$: the end-to-end function is then given by



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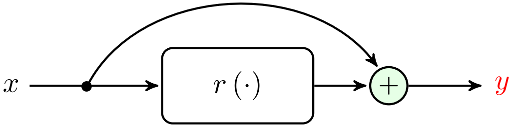
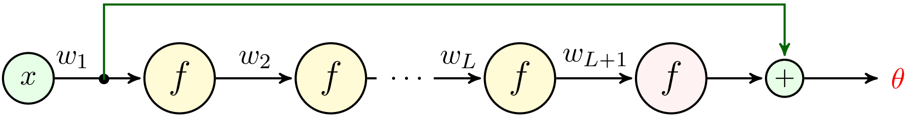


The NN now approximates the residual $r(\cdot)$ as best as it could

+ *But, why should it be any different this time?*
– Let's get back to our simple example

Skip Connection: *Simple Example*

Let's get back to our simple example: *this time we consider skip connection*



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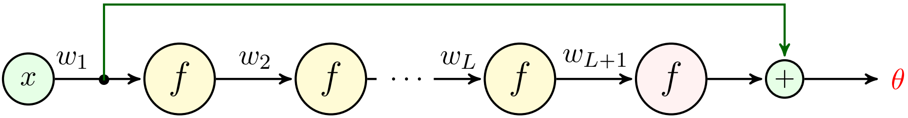
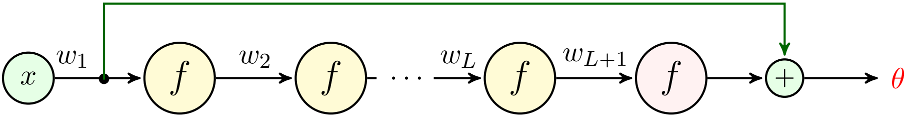


Let's see forward pass

- $y_1 = f(w_1 x)$
- $y_2 = f(w_2 y_1)$

  $\cdots$
- $y_L = f(w_L y_{L-1})$
- $y_{L+1} = f(w_{L+1} y_L)$
- $\theta = y_{L+1} + w_1 x$

Skip Connection: *Simple Example*



What happens backward pass? We start with $\overleftarrow{\theta} = \mathrm{d}\hat{R}/\mathrm{d}\theta$ *again*

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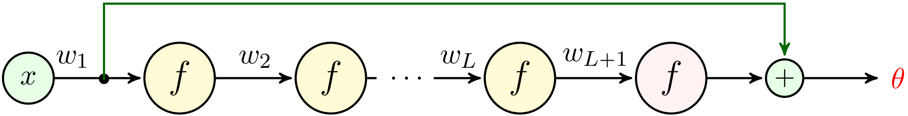

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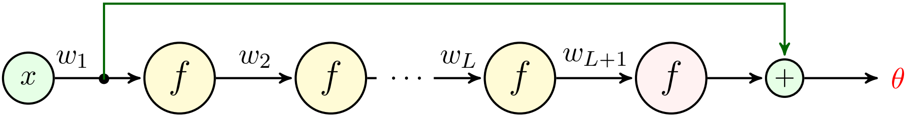

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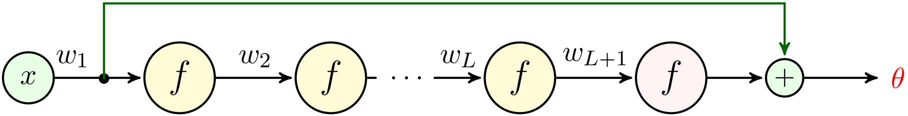
- $y_{L+1} = f\left(w_{L+1} y_L\right)$

$$\overleftarrow{y}_L = \frac{\mathrm{d}\hat{R}}{\mathrm{d}y_L} = \frac{\mathrm{d}\hat{R}}{\mathrm{d}y_{L+1}}\frac{\mathrm{d}y_{L+1}}{\mathrm{d}y_L} = \overleftarrow{y}_{L+1} w_{L+1} \dot{f}\left(w_{L+1} y_L\right)$$

$$= \overleftarrow{\theta}\, w_{L+1} \dot{f}\left(w_{L+1} y_L\right)$$

Skip Connection: *Simple Example*



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- $y_L = f(w_L y_{L-1})$

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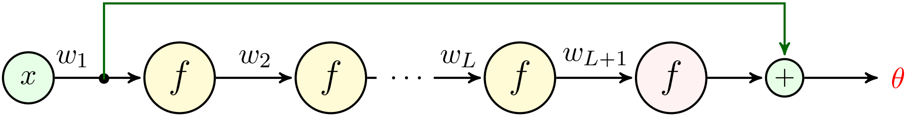
- $\ldots$

Skip Connection: *Simple Example*



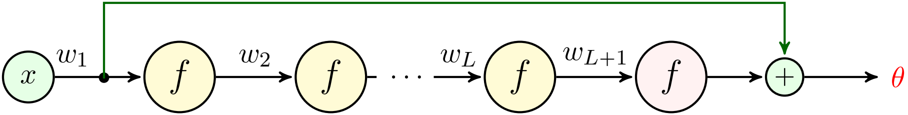
The backward pass looks the same up to the skip connection

- $y_2 = f\left(w_2 y_1\right)$

$$\overleftarrow{y}_1 = \frac{\mathrm{d}\hat{R}}{\mathrm{d}y_1} = \frac{\mathrm{d}\hat{R}}{\mathrm{d}y_2}\frac{\mathrm{d}y_2}{\mathrm{d}y_1} = \overleftarrow{y_2} w_2 \dot{f}\left(w_2 y_1\right)$$

$$= \overleftarrow{\theta} \prod_{\ell=2}^{L+1} w_\ell \dot{f}\left(w_\ell y_{\ell-1}\right)$$

Skip Connection: *Simple Example*



Now, let's compute derivative of loss with respect to the first weight w_1

- *Here, we have two links connected to* w_1 *in the network*
  - ↳ $y_1 = f(w_1 x)$
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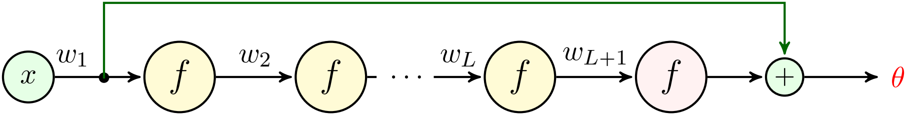
$$\frac{\mathrm{d}\hat{R}}{\mathrm{d}w_1}$$

Skip Connection: *Simple Example*



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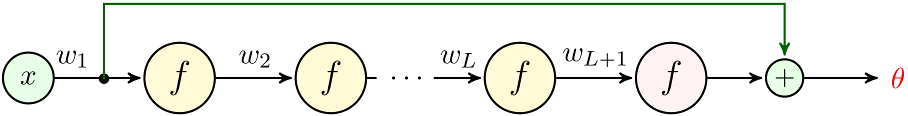
Skip Connection: *Simple Example*



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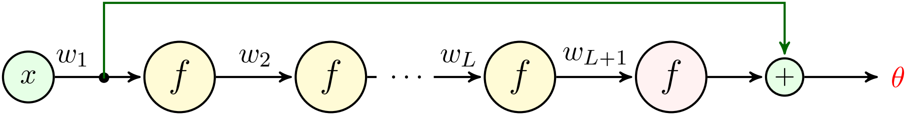

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$$= \overleftarrow{y_1} x \dot{f}(w_1 x) + \overleftarrow{\theta}\, x = \overleftarrow{\theta}\, x \left(\dot{f}(w_1 x) \prod_{\ell=2}^{L+1} w_\ell \dot{f}(w_\ell y_{\ell-1}) + 1 \right)$$

Skip Connection: *Simple Example*

With skip connection, the derivative of loss with respect to the first weight w_1 does not vanish

$$\frac{\mathrm{d}\hat{R}}{\mathrm{d}w_1} = \overleftarrow{\theta}\, x \left(\underbrace{\dot{f}\left(w_1 x\right) \prod_{\ell=2}^{L+1} w_\ell \dot{f}\left(w_\ell y_{\ell-1}\right)}_{\text{accumulated in backpropagation}} + 1 \rightarrow \text{skip connection} \right)$$

Even if all weights and derivatives are smaller than one, as we get very deep $\overleftarrow{\theta}$ is still backpropagating

Skip Connection: *General Form*

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Let $\mathbf{Z}_\ell$ and $\mathbf{Y}_\ell = f(\mathbf{Z}_\ell)$ be outputs of layer ℓ before and after activation

- *This layer can be a convolution or fully-connected layer*
  - ↳ *If convolution, $\mathbf{Z}_\ell$ and $\mathbf{Y}_\ell$ are tensors*
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With a skip connection of depth s, the output of layer ℓ is

$$\mathbf{Y}_\ell = f(\mathbf{Z}_\ell + \mathbf{W} \circ \mathbf{Y}_{\ell-s})$$

↳ $\mathbf{W}$ *is a linear transform that can be potentially learned*

↳ $\circ$ *is a kind of product that matches the dimensions*

Skip Connection: *General Form*

+ *What is exactly $\mathbf{W}$?*
– It is a set of weights, like other weighted components. But, *we don't really need it. We could set it to some fixed values and don't learn it at all*
+ *Why should we connect activated output to linear output?*
– There is actually no should here also!

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– There is actually no should here also!

In original proposal it was suggested to connect *activated output of a layer to the linear output of some next layers, i.e., add* $\mathbf{Y}_{\ell-s}$ to $\mathbf{Z}_{\ell}$

↳ *This combination is only a suggestion!*

↳ *Later suggestions proposed to connect linear output* $\mathbf{Z}_{\ell-s}$

↳ *Similar to batch normalization, best combination is found by experiment*

Residual Unit: *New Building Block via Skip Connection*

Skip connection allowed for training deeper NNs: *experiments showed that*

- *Using skip connection with batch normalization make results sensible*
  ↳ *Deeper networks show better training performance*
- *Skip connection seems to be a crucial component for going deep*

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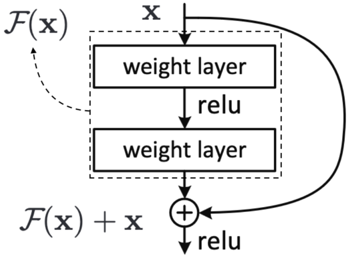
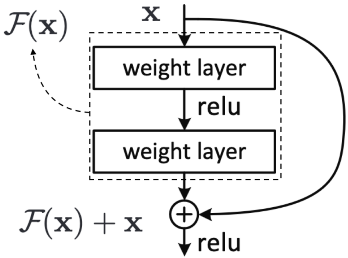
These results led to introduction of a new building block called *residual unit*



Residual Unit



Residual Unit consists of

- *multiple (typically 2) weighted layers, e.g.,*
  - ↳ *convolutional layer*
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The idea was proposed by Microsoft to win ILSVRC in this paper and then expanded in this paper

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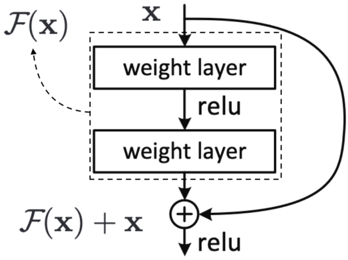

Residual Unit consists of

- *multiple (typically 2) weighted layers, e.g.,*
  - ↳ *convolutional layer*
  - ↳ *standard fully-connected layer*
- *a skip connection that adds input of the unit to the output*
  - ↳ *generally a weighted connection*

$$\text{output} = \mathrm{ReLU}(\mathcal{F}(\mathbf{x}) + \mathbf{W}_{\mathrm{s}}\mathbf{x})$$

  - ↳ *experiments show that when* $\mathcal{F}(\mathbf{x})$ *and* $\mathbf{x}$ *are of same dimension* $\mathbf{W}_{\mathrm{s}} = \mathbf{I}$ *is a good choice*

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Forward Propagation through Residual Units

In original proposal, Residual Units are implemented by convolutional layers

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5. *Output* $\mathbf{Y}$ *is constructed by activating* $\mathbf{Z}_2$ *after skip connection*

$$\mathbf{Y} = f\left(\mathbf{Z}_2 + \mathbf{X}\right)$$

Backpropagation through Residual Units

Assume we have $\nabla_{\mathbf{Y}} \hat{R}$

1. $\nabla_{\mathbf{Z}_2} \hat{R}$ *is computed by entry-wise production with* $\dot{f}(\mathbf{Z}_2 + \mathbf{X})$

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$$\nabla_{\mathbf{Y}_1} \hat{R} = \operatorname{Conv}\left(\nabla_{\mathbf{Z}_2} \hat{R} | \mathbf{W}_1^{2\dagger}, \ldots, \mathbf{W}_C^{2\dagger}\right)$$

3. $\nabla_{\mathbf{Z}_1} \hat{R}$ *is computed by entry-wise production with* $\dot{f}\left(\mathbf{Z}_1\right)$
4. $\nabla_{\mathbf{X}} \hat{R}$ *is given by a new chain rule*

$$\begin{aligned}\nabla_{\mathbf{X}} \hat{R} &= \underbrace{\nabla_{\mathbf{Z}_1} \hat{R} \circ \nabla_{\mathbf{X}} \mathbf{Z}_1}_{\text{Backward convolution}} + \nabla_{\mathbf{Y}} \hat{R} \underbrace{\circ}_{\odot} \underbrace{\nabla_{\mathbf{X}} \mathbf{Y}}_{\dot{f}(\mathbf{Z}_2 + \mathbf{X})} \\ &= \operatorname{Conv}\left(\nabla_{\mathbf{Z}_1} \hat{R} | \mathbf{W}_1^{1\dagger}, \ldots, \mathbf{W}_C^{1\dagger}\right) \underbrace{+ \nabla_{\mathbf{Y}} \hat{R} \odot \dot{f}\left(\mathbf{Z}_2 + \mathbf{X}\right)}_{\text{avoids vanishing gradients}}\end{aligned}$$

Residual Networks

We can now look at *Residual Unit* as a single block in a deep NN

- *We build an architecture by cascading them*
  - ↳ *Intuitively we can go deeper now, since we use skip connection*
- *We also add other kinds of layers that we know, e.g.,*
  - ↳ *convolutional layers, pooling layers, fully-connected layers*
- *We can do whatever we have done before to train them efficiently, e.g.,*
  - ↳ *dropout or other regularization techniques*
  - ↳ *input and batch normalization*
  - ↳ *more advanced optimizers*

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These kinds of NNs are called Residual Networks or shortly ResNet

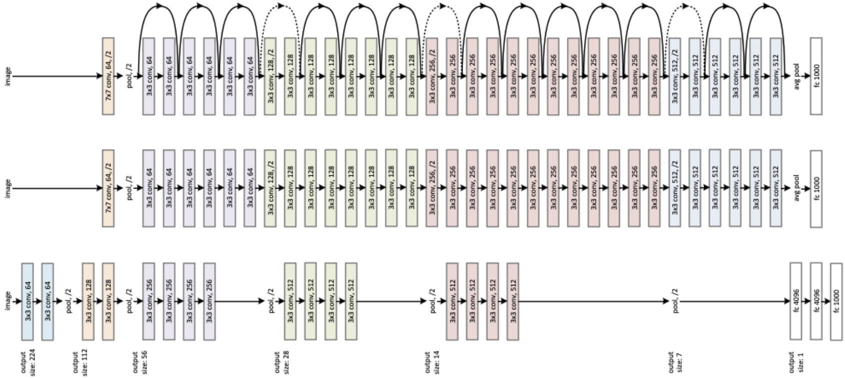
↳ *they were proposed in the original paper introduced Residual Unit*

↳ *they are nowadays a kind of benchmark in many applications*

Residual Networks: *A Nice Experiment*

ResNet inventors did a nice experiment to show the impact of skip connection[7]

- *They investigated 3 architectures: 34-layer ResNet, 34-layer Plain CNN (no skip connection) and benchmark VGG architectures*



[7] Find the details in their paper

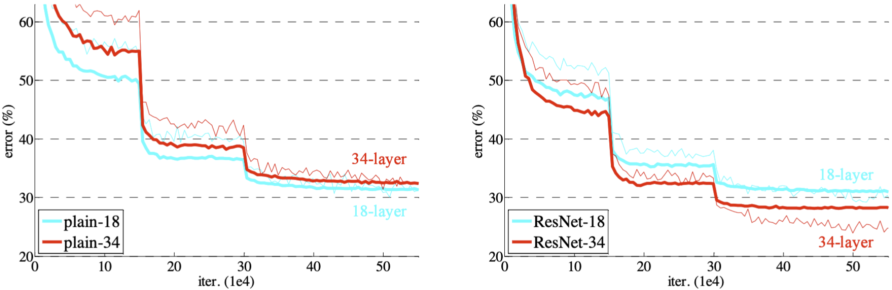
Residual Networks: *A Nice Experiment*

The results was interesting: *the depth challenge is now efficiently addressed, i.e., by going deep we always get better in performance*

model	top-1 err.	top-5 err.
VGG-16 [41]	28.07	9.33
plain-34	28.54	10.02
ResNet-34 A	25.03	7.76
ResNet-34 B	24.52	7.46
ResNet-34 C	24.19	7.40

Residual Networks: *A Nice Experiment*

Recall that *the depth challenge was different from overfitting! With deeper architectures, plain CNNs are showing worse "training" performance. With ResNet, this is not the case anymore*



> *The above figures show training error meaning that*
>
> *the left figure cannot simply show overfitting!*

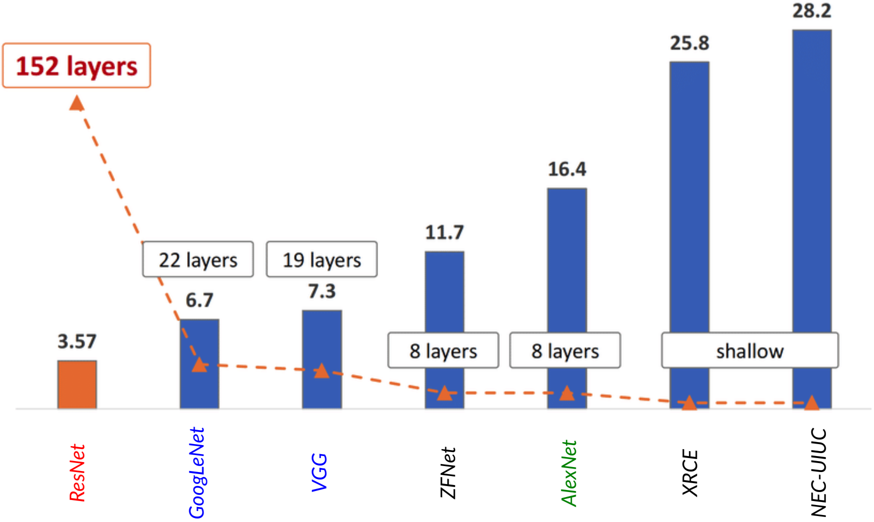
Residual Networks: *ILSVRC*

Getting rid of this undesired behavior *made it easy to go as deep as we want*

method	top-1 err.	top-5 err.
VGG [41] (ILSVRC'14)	-	8.43†
GoogLeNet [44] (ILSVRC'14)	-	7.89
VGG [41] (v5)	24.4	7.1
ResNet-34 B	21.84	5.71
ResNet-34 C	21.53	5.60
ResNet-50	20.74	5.25
ResNet-101	19.87	4.60
ResNet-152	**19.38**	**4.49**

This way ResNet won ILSVRC in 2015!

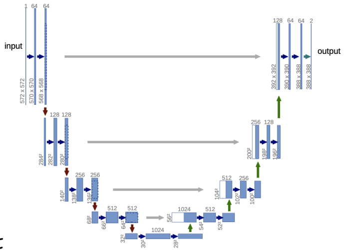
Depth vs Accuracy: *ILSVRC Winners till 2015*



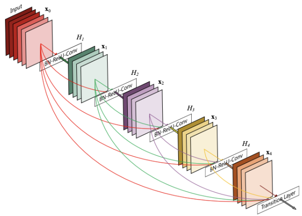
Other Architectures with Skip Connection

ResNet is not the only architecture with skip connection

- *ResNet made a breakthrough by using short skip connection*
- *U-Net uses long and short skip connections*[8]
- *DenseNet uses long and short skip connections densely to go even deeper*[9]



U-Net



DenseNet

[8] Check the original proposal of U-Net here

[9] Check the original proposal of DenseNet here

Notes on Implementation

Many architectures have been already implemented and pre-trained in PyTorch

- *They are implemented using basic blocks in PyTorch*
- *They are pre-trained for ImageNet classification*
  - ↳ *They get 3-channel 224×224 tensor as input*
  - ↳ *They return 1000-dimensional output vector*

We can access them either through `torchvision.models`

```
import torchvision.models as Models
model = Models.
```

```
resnet
ResNet
resnet101
ResNet101_Weights
resnet152
ResNet152_Weights
resnet18
ResNet18_Weights
resnet34
ResNet34_Weights
```

Notes on Implementation

For instance, we could load ResNet-50 with its pre-trained weights

```
from torchvision.models import resnet50, ResNet50_Weights

# Old weights with accuracy 76.130%
resnet50(weights=ResNet50_Weights.IMAGENET1K_V1)

# New weights with accuracy 80.858%
resnet50(weights=ResNet50_Weights.IMAGENET1K_V2)

# Best available weights (currently alias for IMAGENET1K_V2)
# Note that these weights may change across versions
resnet50(weights=ResNet50_Weights.DEFAULT)

# Strings are also supported
resnet50(weights="IMAGENET1K_V2")

# No weights - random initialization
resnet50(weights=None)
```

We could alternatively use `torch.hub` module to load pre-trained models

Notes on Implementation

+ *What is we are using it for other applications with different data size?*
– We could add or modify layer to it; *for instance,*

> *Say we want to use a pre-trained* ResNet *to classify MNIST: we could replace the first convolutional layer with single-channel 28×28 input and the same number of output channels. We further replace the output layer with a fully-connected layer with 10 classes*

+ *But it does not perform well! Does it?!*
– Of course not! It has been trained for ImageNet and there is no reason to work with MNIST! But, *we can start from those weights and do normal training for several epochs*
  ↳ *It probably gets trained much faster as compared to random initialization*
  ↳ *This idea is studied in a much broader sense in Transfer Learning*