Applied Deep Learning

Chapter 5: Skip Connection and Residual Networks

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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

Let's say we have input x and label y

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

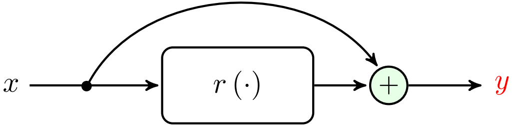
$$x \longrightarrow \boxed{f(\cdot)} \longrightarrow y$$

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

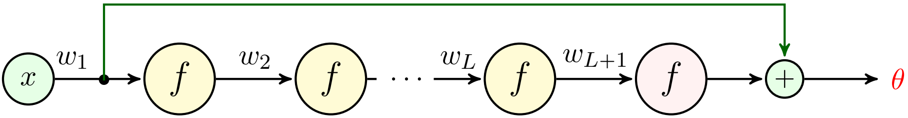


The NN now approximates the residual $r(\cdot)$ as best as it could

+ *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*



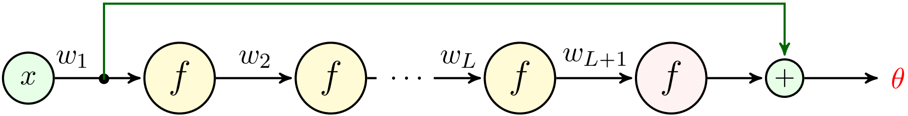
Let's see forward pass

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

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

$\rightarrow$ $\theta = y_{L+1} + w_1 x$

Skip Connection: *Simple Example*



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

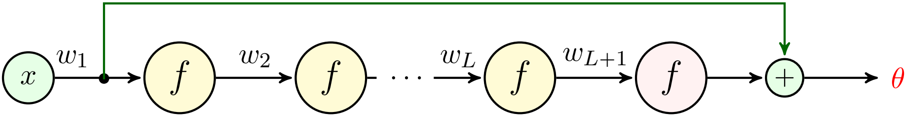
- $\theta = y_{L+1} + w_1 x$

$$\overleftarrow{y}_{L+1} = \frac{\mathrm{d}\hat{R}}{\mathrm{d}y_{L+1}} = \frac{\mathrm{d}\hat{R}}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}y_{L+1}} = \overleftarrow{\theta}$$

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

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

Skip Connection: *Simple Example*



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

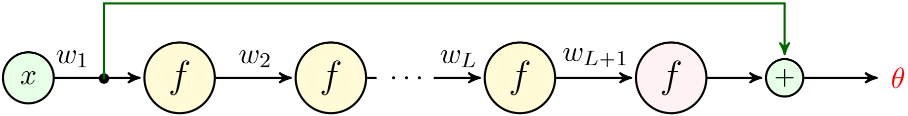
- $y_L = f\left(w_L y_{L-1}\right)$

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

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

- $\ldots$

Skip Connection: *Simple Example*



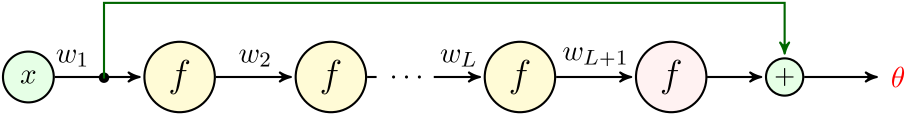
The backward pass looks the same up to the skip connection

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

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

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

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*
  - ↳ $y_1 = f(w_1 x)$
  - ↳ $\theta = y_{L+1} + w_1 x$

$$\frac{\mathrm{d}\hat{R}}{\mathrm{d}w_1} = \frac{\mathrm{d}\hat{R}}{\mathrm{d}y_1}\frac{\mathrm{d}y_1}{\mathrm{d}w_1} + \frac{\mathrm{d}\hat{R}}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}w_1}$$

$$= \overleftarrow{y}_1 x \dot{f}(w_1 x) + \overleftarrow{\theta} x = \overleftarrow{\theta} x \left(\dot{f}(w_1 x) \prod_{\ell=2}^{L+1} w_\ell \dot{f}(w_\ell y_{\ell-1}) + 1 \right)$$

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*

Skip Connection

Skip connection refers to links that carry information from layer $\ell - s$ to layer ℓ for $s > 1$

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*
  - ↳ *If fully-connected, $\mathbf{Z}_\ell$ and $\mathbf{Y}_\ell$ are vectors*

With a skip connection of depth s, the output of layer ℓ is

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

↳ $\mathbf{W}$ *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!

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 $\mathbf{Z}_{\ell-s}$*

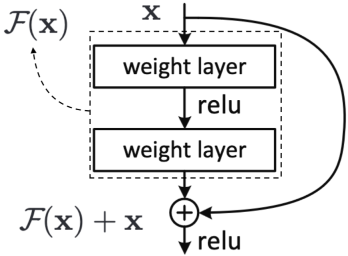
↳ *Similar to batch normalization, best combination is found by experiment*

Residual Unit: *New Building Block via Skip Connection*

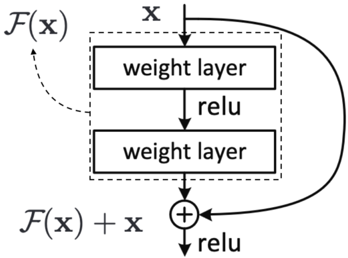
Skip connection allowed for training deeper NNs: *experiments showed that*

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

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*
  - ↳ *standard fully-connected layer*
- *a skip connection that adds input of the unit to the output*
  - ↳ *generally a weighted connection*

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

  - ↳ *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*

The idea was proposed by Microsoft to win ILSVRC in this paper and then expanded in this paper

Forward Pass through Residual Units

In original proposal, Residual Units are implemented by convolutional layers

1. *Input* $\mathbf{x} = \mathbf{X}$ *is a tensor with* C *channels*
2. $\mathbf{X}$ *is given to a convolutional layer with* C *output channels, i.e.,* C *filters*

$$\mathbf{Z}_1 = \mathrm{Conv}\left(\mathbf{X} | \mathbf{W}_1^1, \ldots, \mathbf{W}_C^1\right)$$

3. $\mathbf{Z}_1$ *is then activated* $\mathbf{Y}_1 = f\left(\mathbf{Z}_1\right)$
4. $\mathbf{Y}_1$ *is given to another convolutional layer with* C *output channels*

$$\mathbf{Z}_2 = \mathrm{Conv}\left(\mathbf{Y}_1 | \mathbf{W}_1^2, \ldots, \mathbf{W}_C^2\right)$$

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* $\dot{f}(\mathbf{Z}_2 + \mathbf{X})$
2. $\nabla_{\mathbf{Y}_1} \hat{R}$ *is computed by convolution*

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

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

$$\nabla_{\mathbf{X}} \hat{R} = \underbrace{\nabla_{\mathbf{Z}_1} \hat{R} \circ \nabla_{\mathbf{X}} \mathbf{Z}_1}_{\text{backward convolution}} + \nabla_{\mathbf{Y}} \hat{R} \underbrace{\circ}_{\odot} \underbrace{\nabla_{\mathbf{X}} \mathbf{Y}}_{\dot{f}(\mathbf{Z}_2 + \mathbf{X})}$$

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

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*

These kinds of NNs are called Residual Networks or shortly ResNet

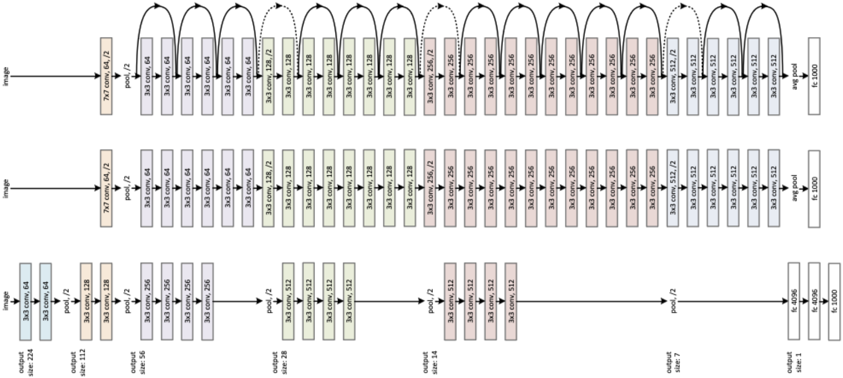
↳ *they were proposed in the original paper introduced Residual Unit*

↳ *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[1]

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



[1] Find the details in their paper

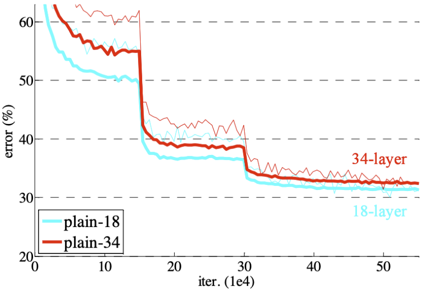
Residual Networks: *A Nice Experiment*

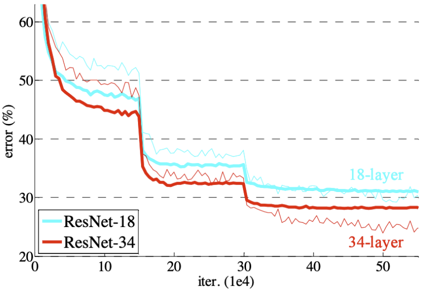
The results was interesting: *the depth challenge is now efficiently addressed*, *i.e., by going deeper we always get better in performance*

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!

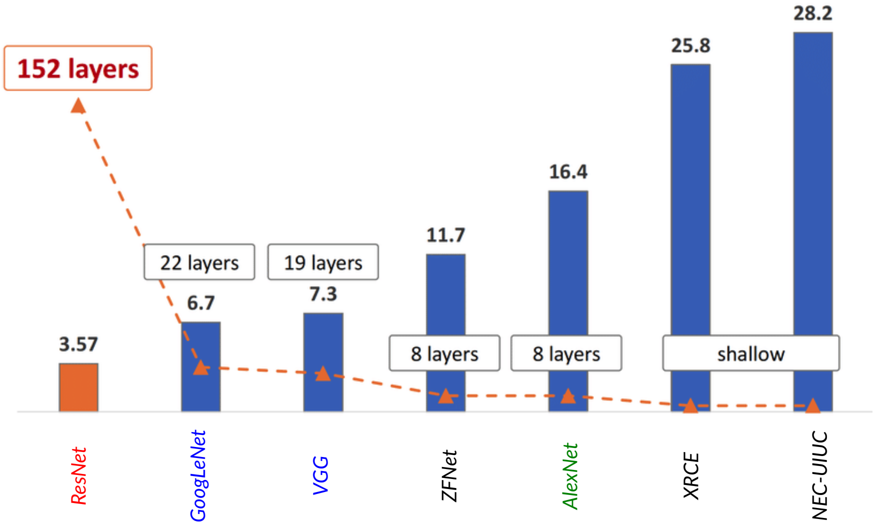
Residual Networks: *ILSVRC*

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!

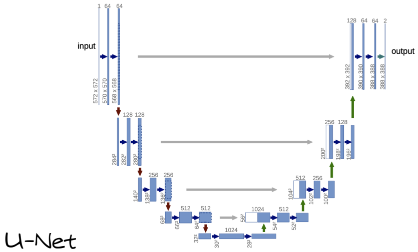
Depth vs Accuracy: *ILSVRC Winners till 2015*

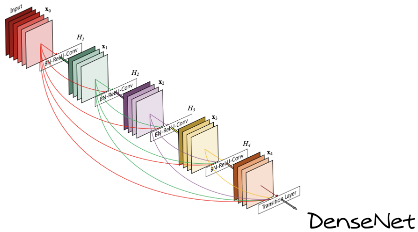


Other Architectures with Skip Connection

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*[2]
- *DenseNet uses long and short skip connections densely to go even deeper*[3]





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

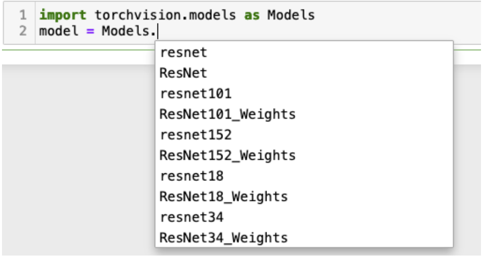
[3]Check the original proposal of DenseNet here

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 through `torchvision.models`



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 if 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*