

Seongok Ryu KAIST Chemistry

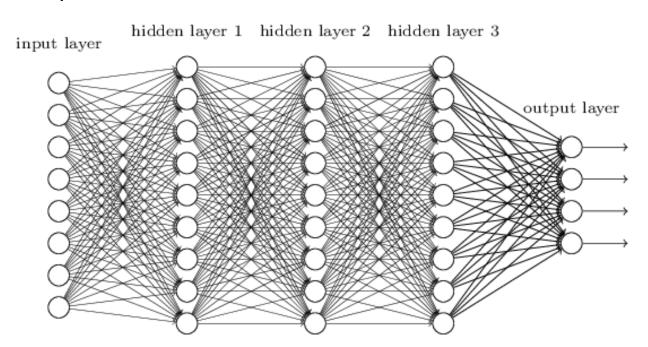


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- Convolution operation
- Convolutional neural networks
- Residual networks
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Weight sharing

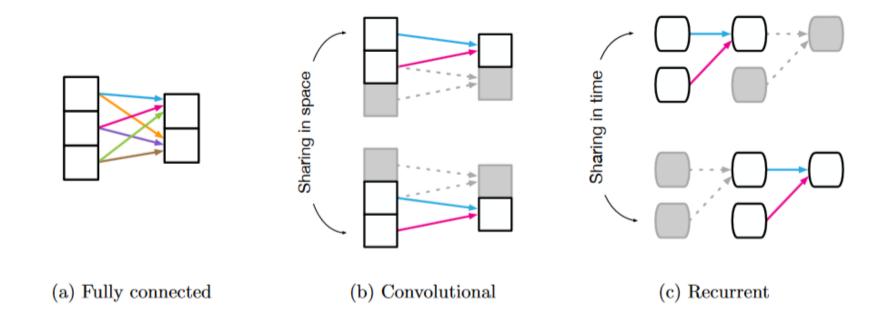
- Multi-layer perceptrons (or sometimes called as fully-connected neural networks) connect all the neurons between the layers.
- This model structure use too much number of parameters, vulnerable to over-fitting problems.
- For example, as an input with images having a dimensionality $H \times W \times C$ and hidden dimension d, a MLP uses total $H \times W \times C \times d$ number of weight parameters. If H = W = 32, C = 3 and d = 512, then total 1.57M number of parameters is required.





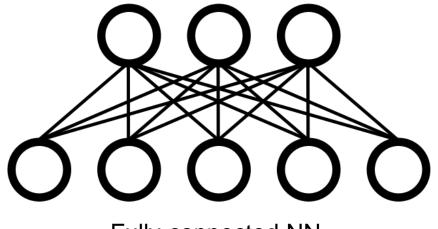
Weight sharing

- For many domains, a same operation can be applied on local regions of input data.
- Images: same convolution operations on different pixels in images.
- Languages: same recurrent/convolution operations on different words in sentences.
- Molecules: same graph convolution operations on different atoms in molecules.
- This makes designing a model architecture much simpler and helps using less number of parameters.

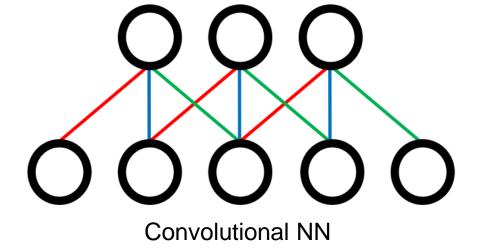


Convolution operation

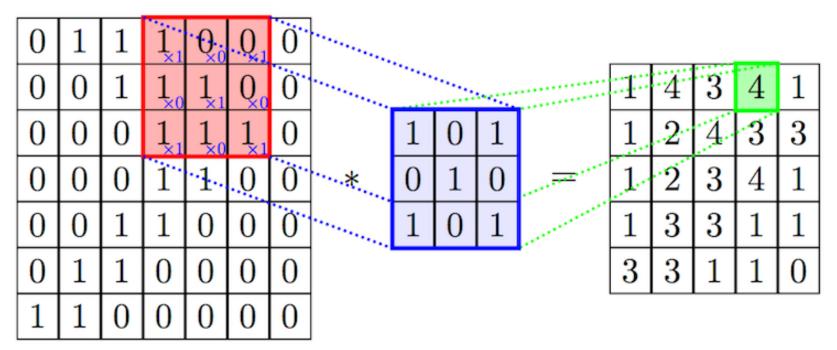
- Convolution is the most commonly used operation in modern deep neural networks.
- Using non-zero weight values on local regions.
- Sharing a same weight parameter (also referred to as a receptive field) for different regions.



Fully-connected NN



Convolution operation



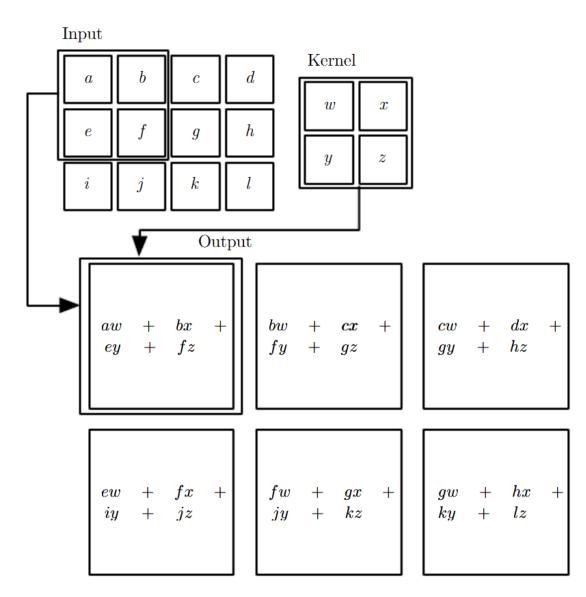
k = 1 for 3×3 convolution

$$X_{i}^{(l+1)} = \sigma(\sum_{j \in [i-k,i+k]} W_{j}^{(l)} X_{j}^{(l)} + b^{(l)})$$

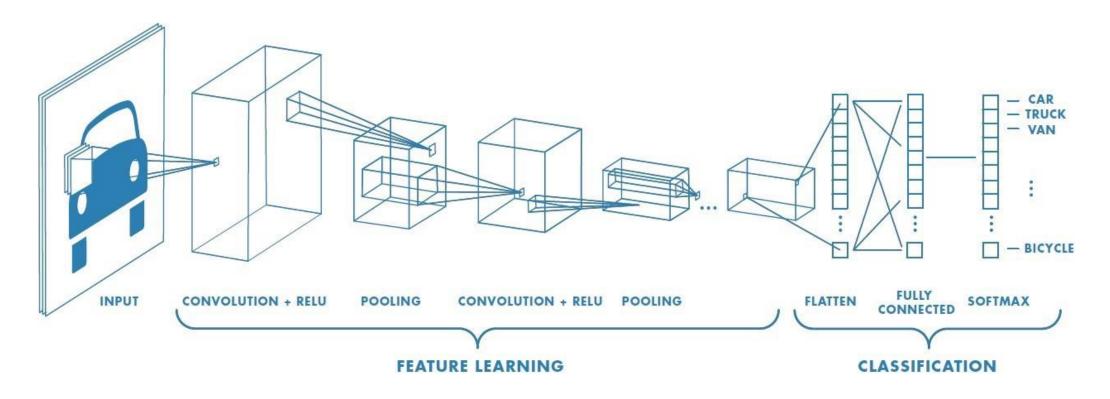
learnable parameters are shared

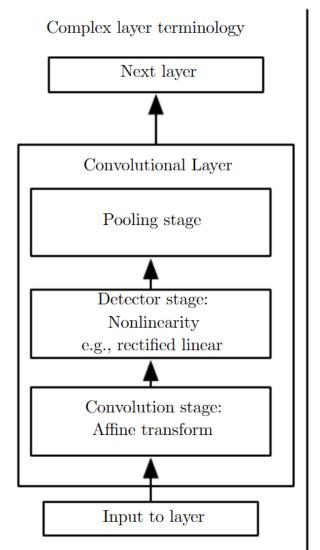
Convolution operation

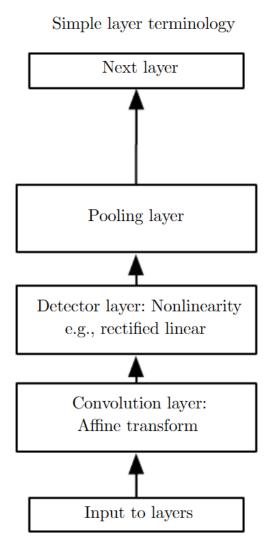
An example of 2-D convolution



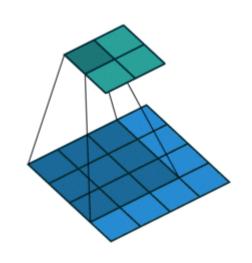
• "CNNs are simply neural networks that use convolution in place of general matrix multiplication in at least one of their layers." – Deep learning book

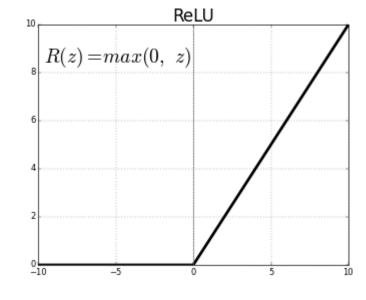


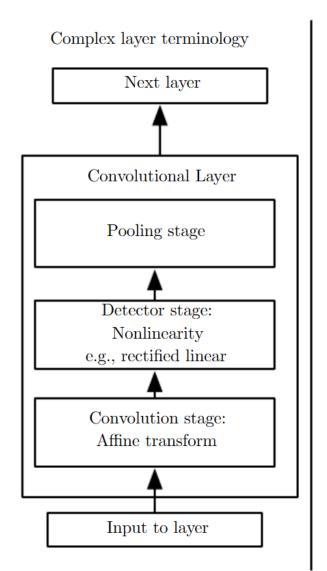


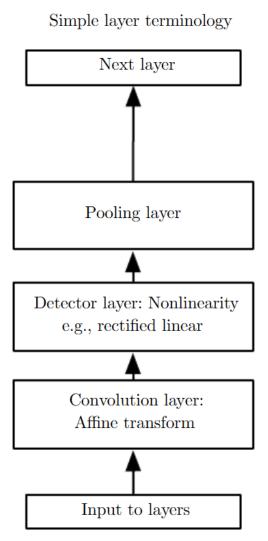


- Convolution operations compute the linear combination of pixel values.
- Then, non-linear activations computes output responses and detects large ones.





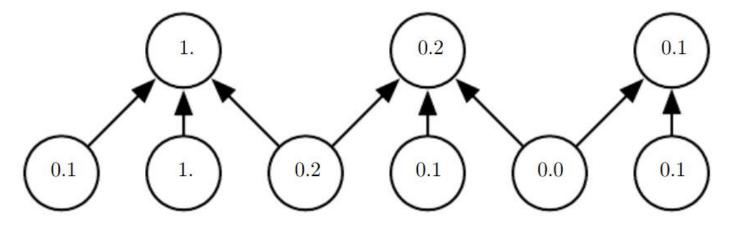




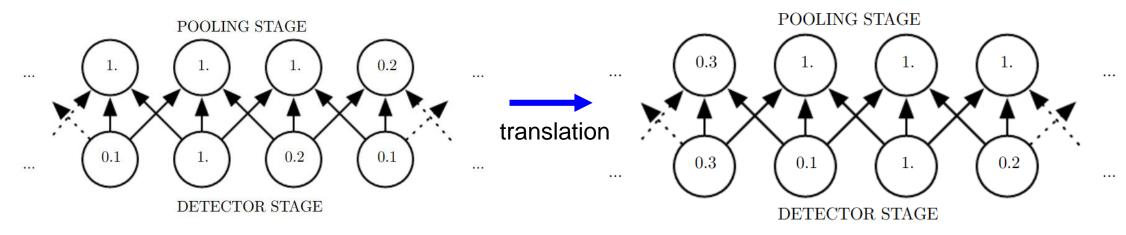
- Then, the pooling operation is applied to summarize the statistics of features.
- Max-pooling, L2-norm pooling, average pooling, ...

12	20	30	0			
8	12	2	0	2×2 Max-Pool	20	30
34	70	37	4		112	37
112	100	25	12			

Pooling operation with strides larger than 2 can provide down-sampling of images (feature-maps).



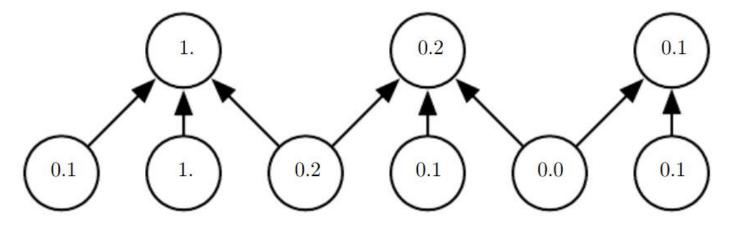
Pooling operation can approximate invariance to local translation



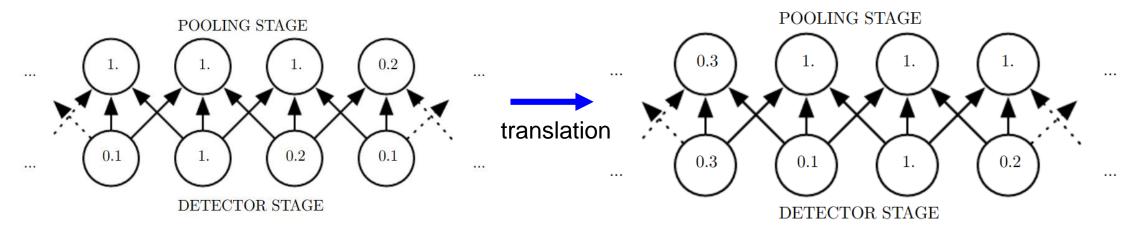
Every value in the botton row has changed, but only half of the values in the top row have changed.



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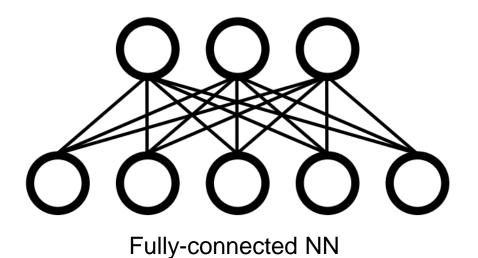
Pooling operation can approximate invariance to local translation

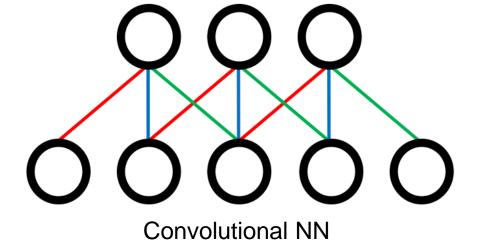


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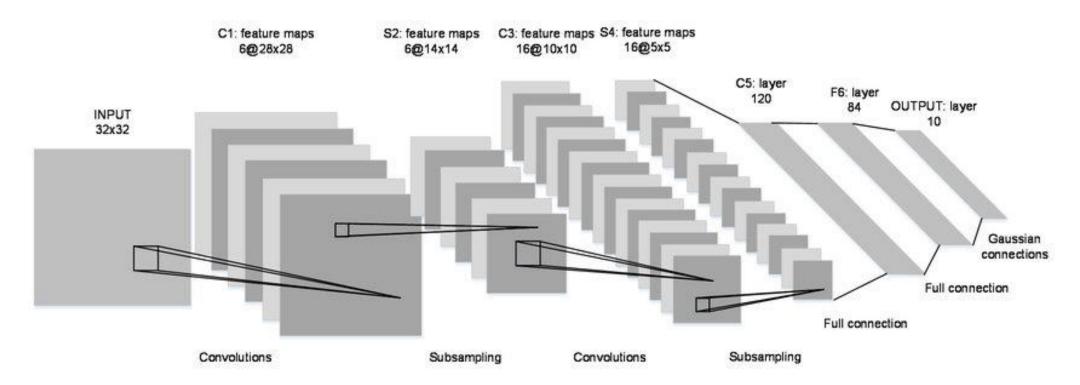


- We can understand convolution and pooling as an infinitely strong prior.
- An infinitely strong prior places zero probability on some parameters and says that theses parameter values are completely forbidden, regardless of how much support the data give to those values.
- Using those operations endue strong inductive biases on a hypothesis.

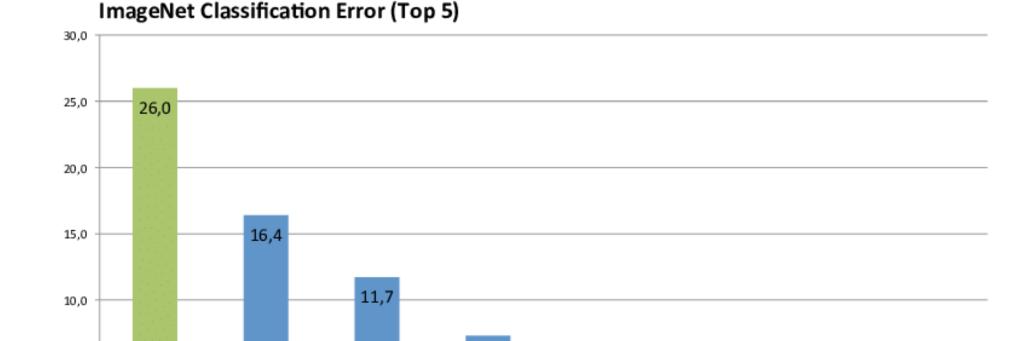




- In early 1990s, LeNet was invented by Yann Lecun, who is one of the pioneers of deep learning researches.
- Using simple convolution and pooling operations for featurizations and fully-connected layers for a classifier.
- CNN demo from 1993, https://www.youtube.com/watch?v=FwFduRA_L6Q



Representative CNN models wons ImageNet Challenge (ILSVRC)



7,3

2014 (VGG)

6,7

2014

(GoogLeNet)

5,0

Human

3,6

2015 (ResNet)

3,1

2016

(GoogLeNet-v4)



5,0

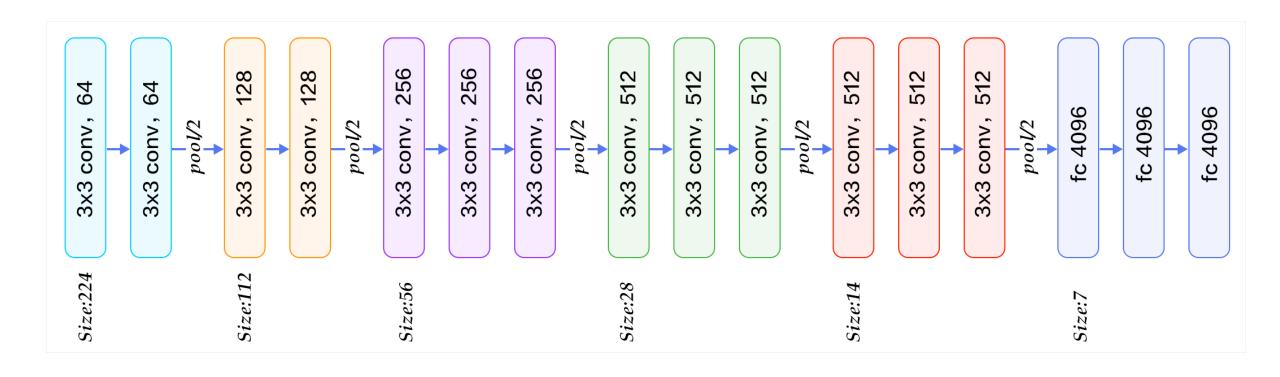
0,0

2011 (XRCE)

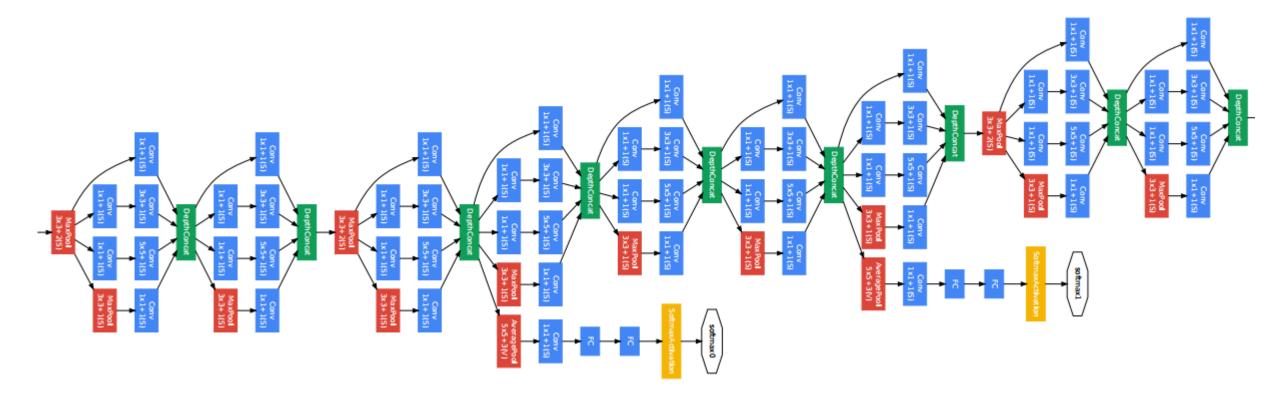
2012 (AlexNet)

2013 (ZF)

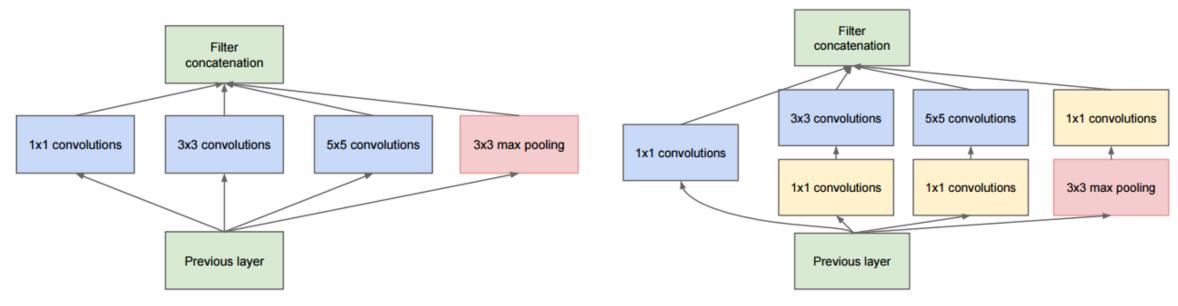
- VGG-Net
- Total 19 layers with a simple combination of convolution and pooling operations



- GoogLeNet (Inception network)
- Inception module is combined with different receptive fields and max-pooling operations.



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(a) Inception module, naïve version

(b) Inception module with dimension reductions

- Make CNN models wider as well as deeper.
- Efficient use of parameters: showing better performance with using less number of parameters than VGGNet.

Residual Networks

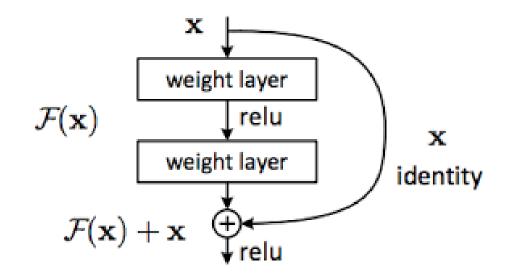
- Using residual blocks or skip-connections allows model to be much deeper.
- The residual block updates the feature by the amount of F(x):

$$x^{l+1} - x^l = F(x^l)$$

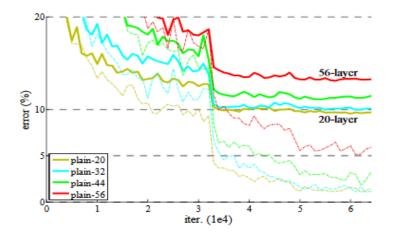
- Residual learning can mitigate vanishing gradient problems.
- Let y = x + F(x), then the gradient of loss is given by:

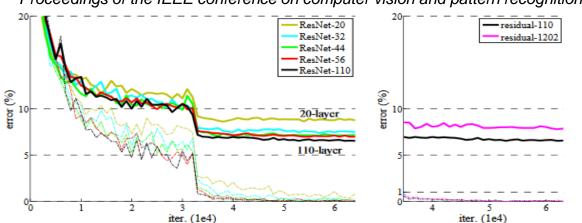
$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial y} \cdot \frac{\partial y}{\partial x} = \frac{\partial L}{\partial y} (1 + \frac{\partial F(x)}{\partial x})$$

In contrast to the gradient of plain networks is given by $\frac{\partial L}{\partial y} \cdot \frac{\partial F(x)}{\partial x}$.



 $\frac{\partial y}{\partial y} = \frac{\partial x}{\partial x}$ He, Kaiming, et al. "Deep residual learning for image recognition." Proceedings of the IEEE conference on computer vision and pattern recognition. 2016.





Residual Networks

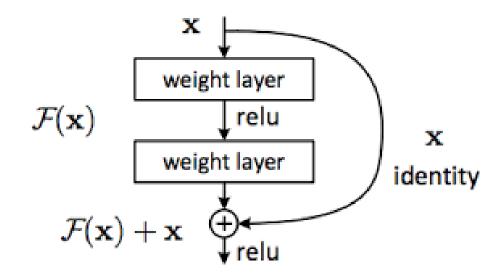
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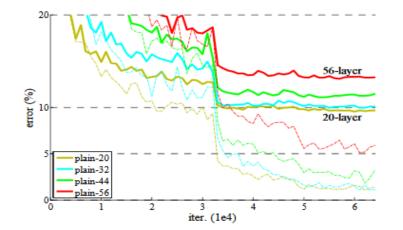
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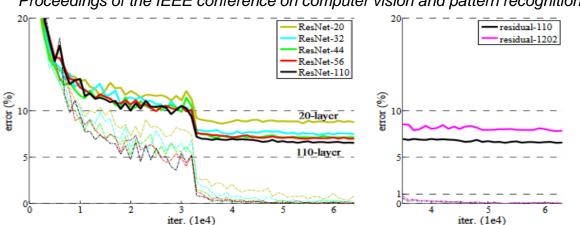
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Neural architecture search (NAS): searching model architectures by neural networks

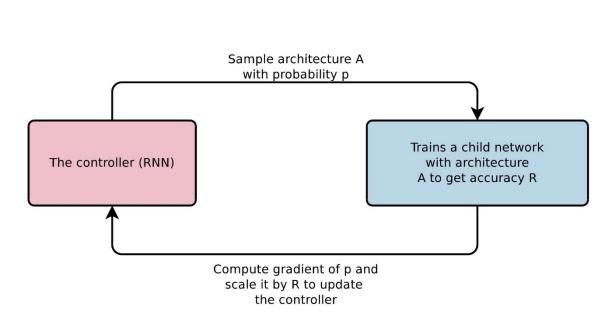
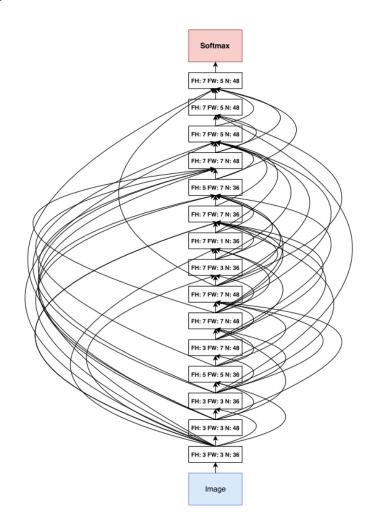
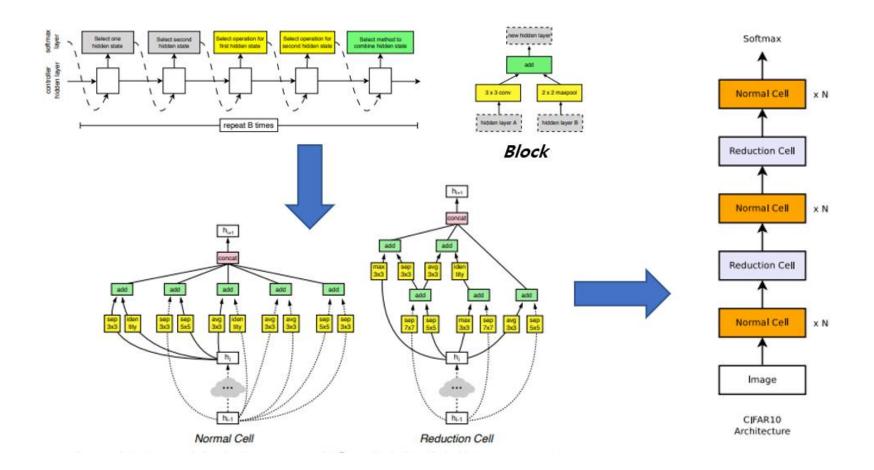


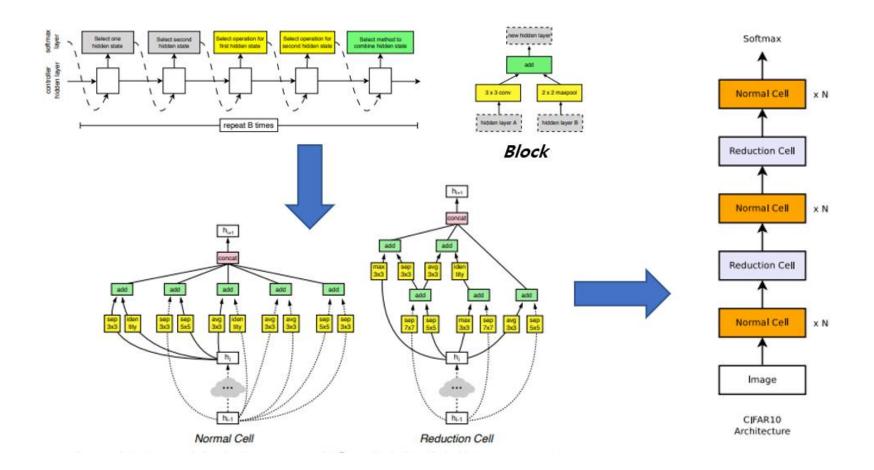
Figure 1: An overview of Neural Architecture Search.



Neural architecture search (NAS): searching model architectures by neural networks



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Improve parameter efficiency - very important for practical uses (time costs, electricity consumption, ...)

