Memo: Backpropagation in Convolutional Neural Network

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Note

Purpose

The purpose of this memo is trying to understand and remind the backpropagation algorithm in Convolutional Neural Network based on a discussion with Prof. Masayuki Tanaka.

Table of Contents

In this memo, backpropagation algorithms in different neural networks are explained in the following order.

Notation

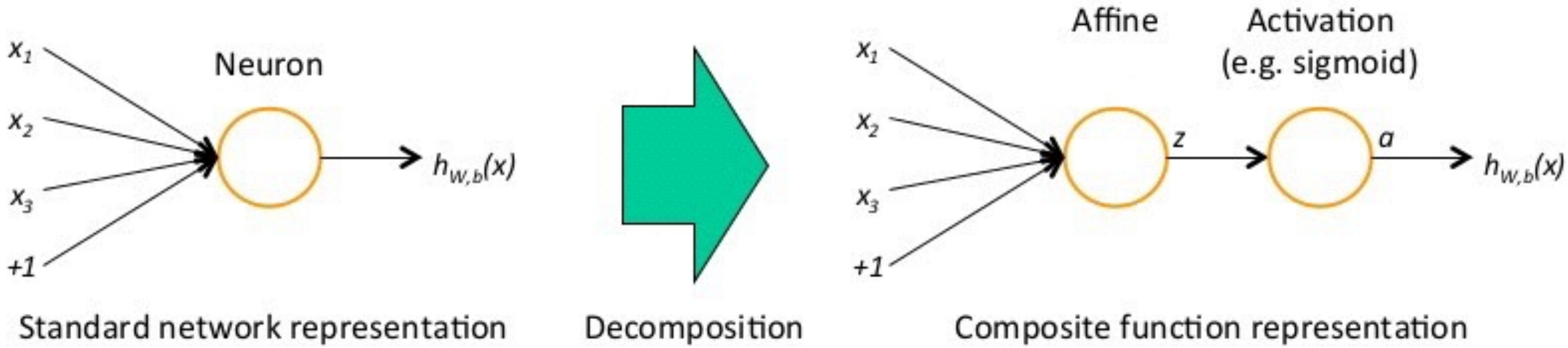
This memo follows the notation in UFLDL tutorial (http://ufldl.stanford.edu/tutorial)

Neural Network as a Composite Function

A neural network is decomposed into a composite function where each function element corresponds to a differentiable operation.

- Single neuron (the simplest neural network) example

A single neuron is decomposed into a composite function of an affine function element parameterized by *W* and *b* and an activation function element *f* which we choose to be the sigmoid function.



$$h_{W,b}(x) = f\left(W^T x + b\right) = \text{sigmoid}\left(\text{affine}_{W,b}(x)\right) = \left(\text{sigmoid} \circ \text{affine}_{W,b}\right)(x)$$

Derivatives of both affine and sigmoid function elements w.r.t. both inputs and parameters are known. Note that sigmoid function does not have neither parameters nor derivatives parameters.

Sigmoid function is applied element-wise. '•' denotes Hadamard product, or element-wise product.

$$\frac{\partial a}{\partial z} = a \bullet (1-a) \text{ where } a = h_{w,b}(x) = \text{sigmoid}(z) = \frac{1}{1+\exp(-z)}$$

$$\frac{\partial z}{\partial x} = W,\ \frac{\partial z}{\partial W} = x,\ \frac{\partial z}{\partial b} = I \text{ where } z = \text{affine}_{W,b}(x) = W^T x + b, \text{ and } I \text{ is identity matrix}$$

Chain Rule of Error Signals and Gradients

Error signals are defined as the derivatives of any cost function *J* which we choose to be the square error. Error signals are computed (propagated backward) by the chain rule of derivative and useful for computing the gradient of the cost function.

- Single neuron example

Suppose we have *m* labeled training examples $\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\}$. Square error cost function for each example is as follows. Overall cost function is the summation of cost functions over all examples.

$$J(W,b;x,y) = \frac{1}{2}\left\| y - h_{w,b}(x) \right\|^2$$

Error signals of the square error cost function for each example are propagated using derivatives of function elements w.r.t. inputs.

$$\delta^{(a)} = \frac{\partial}{\partial a} J(W,b;x,y) = -(y-a)$$

$$\delta^{(z)} = \frac{\partial}{\partial z} J(W,b;x,y) = \frac{\partial J}{\partial a}\frac{\partial a}{\partial z} = \delta^{(a)} \bullet a \bullet (\mathbf{1}-a)$$

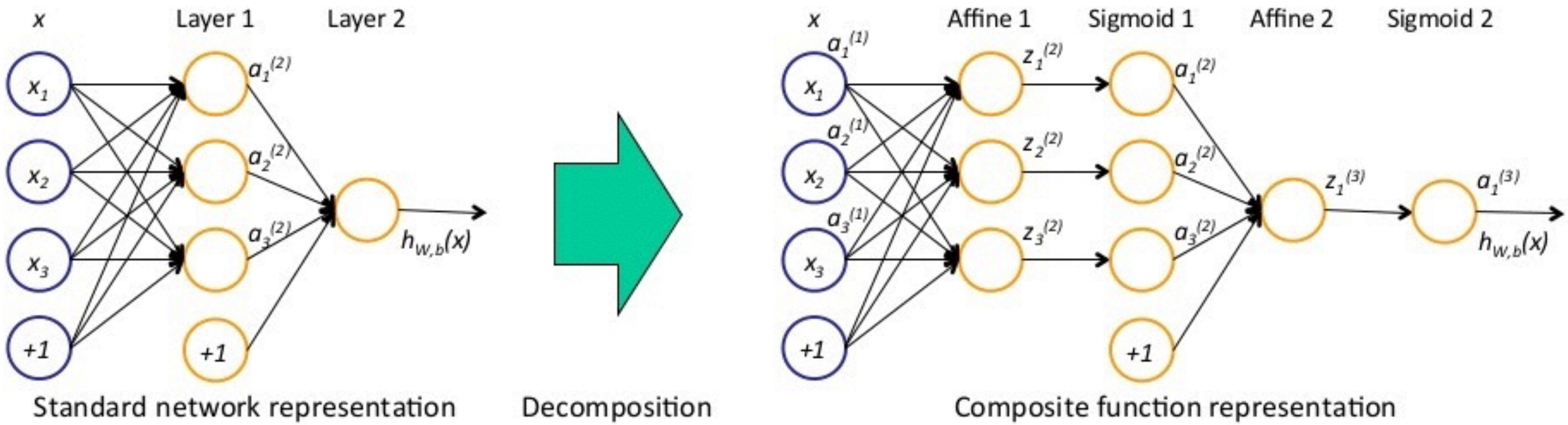
Gradient of the cost function w.r.t. parameters for each example is computed using error signals and derivatives of function elements w.r.t. parameters. Summing gradients for all examples gets overall gradient.

$$\nabla_W J(W,b;x,y) = \frac{\partial}{\partial W} J(W,b;x,y) = \frac{\partial J}{\partial z}\frac{\partial z}{\partial W} = \delta^{(z)} x^T$$

$$\nabla_b J(W,b;x,y) = \frac{\partial}{\partial b} J(W,b;x,y) = \frac{\partial J}{\partial z}\frac{\partial z}{\partial b} = \delta^{(z)}$$

Decomposition of Multi-Layer Neural Network

- Composite function representation of a multi-layer neural network



$$h_{W,b}(x) = \left(\text{sigmoid} \circ \text{affine}_{W^{(2)},b^{(2)}} \circ \text{sigmoid} \circ \text{affine}_{W^{(1)},b^{(1)}}\right)(x)$$

- Derivatives of function elements w.r.t. inputs and parameters

$$a^{(1)} = x,\ a^{(l_{\max})} = h_{w,b}(x)$$

$$\frac{\partial a^{(l+1)}}{\partial z^{(l+1)}} = a^{(l+1)} \bullet \left(1 - a^{(l+1)}\right) \text{ where } a^{(l+1)} = \text{sigmoid}\left(z^{(l+1)}\right) = \frac{1}{1+\exp\left(-z^{(l+1)}\right)}$$

$$\frac{\partial z^{(l+1)}}{\partial a^{(l)}} = W^{(l)},\ \frac{\partial z^{(l+1)}}{\partial W^{(l)}} = a^{(l)},\ \frac{\partial z^{(l+1)}}{\partial b^{(l)}} = I \text{ where } z^{(l+1)} = \left(W^{(l)}\right)^T a^{(l)} + b^{(l)}$$

Error Signals and Gradients in Multi-Layer NN

- Error signals of the square error cost function for each example

$$\delta^{\left(a^{(l)}\right)} = \frac{\partial}{\partial a^{(l)}} J(W,b;x,y) = \begin{cases} -\left(y - a^{(l)}\right) \text{ for } l = l_{\max} \\ \dfrac{\partial J}{\partial z^{(l+1)}} \dfrac{\partial z^{(l+1)}}{\partial a^{(l)}} = \left(W^{(l)}\right)^T \delta^{\left(z^{(l+1)}\right)} \text{ otherwise} \end{cases}$$

$$\delta^{\left(z^{(l)}\right)} = \frac{\partial}{\partial z^{(l)}} J(W,b;x,y) = \frac{\partial J}{\partial a^{(l)}} \frac{\partial a^{(l)}}{\partial z^{(l)}} = \delta^{\left(a^{(l)}\right)} \bullet a^{(l)} \bullet \left(\mathbf{1} - a^{(l)}\right)$$

- Gradient of the cost function w.r.t. parameters for each example

$$\nabla_{W^{(l)}} J(W,b;x,y) = \frac{\partial}{\partial W^{(l)}} J(W,b;x,y) = \frac{\partial J}{\partial z^{(l+1)}} \frac{\partial z^{(l+1)}}{\partial W^{(l)}} = \delta^{\left(z^{(l+1)}\right)} \left(a^{(l)}\right)^T$$

$$\nabla_{b^{(l)}} J(W,b;x,y) = \frac{\partial}{\partial b^{(l)}} J(W,b;x,y) = \frac{\partial J}{\partial z^{(l+1)}} \frac{\partial z^{(l+1)}}{\partial b^{(l)}} = \delta^{\left(z^{(l+1)}\right)}$$

Backpropagation in General Cases

1. Decompose operations in layers of a neural network into function elements whose derivatives w.r.t inputs are known by symbolic computation.

$$h_\theta(x) = \left(f^{(l_{\max})} \circ \ldots \circ f^{(l)}_{\theta^{(l)}} \circ \ldots \circ f^{(2)}_{\theta^{(2)}} \circ f^{(1)}\right)(x) \text{ where } f^{(1)} = x,\ f^{(l_{\max})} = h_\theta(x) \text{ and } \forall l : \frac{\partial f^{(l+1)}}{\partial f^{(l)}} \text{ is known}$$

2. Backpropagate error signals corresponding to a differentiable cost function by numerical computation (Starting from cost function, plug in error signals backward).

$$\delta^{(l)} = \frac{\partial}{\partial f^{(l)}} J(\theta; x, y) = \frac{\partial J}{\partial f^{(l+1)}} \frac{\partial f^{(l+1)}}{\partial f^{(l)}} = \delta^{(l+1)} \frac{\partial f^{(l+1)}}{\partial f^{(l)}} \text{ where } \frac{\partial J}{\partial f^{(l_{\max})}} \text{ is known}$$

3. Use backpropagated error signals to compute gradients w.r.t. parameters only for the function elements with parameters where their derivatives w.r.t parameters are known by symbolic computation.

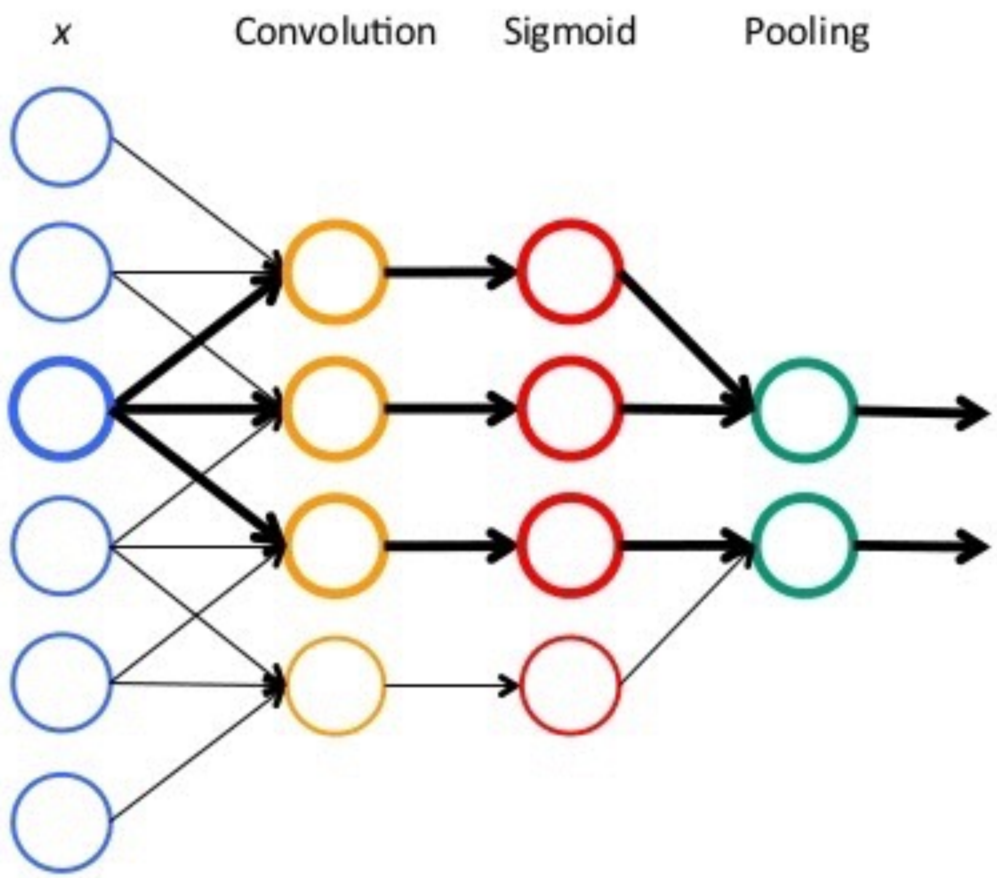
$$\nabla_{\theta^{(l)}} J(\theta; x, y) = \frac{\partial}{\partial \theta^{(l)}} J(\theta; x, y) = \frac{\partial J}{\partial f^{(l)}} \frac{\partial f^{(l)}_{\theta^{(l)}}}{\partial \theta^{(l)}} = \delta^{(l)} \frac{\partial f^{(l)}_{\theta^{(l)}}}{\partial \theta^{(l)}} \text{ where } \frac{\partial f^{(l)}_{\theta^{(l)}}}{\partial \theta^{(l)}} \text{ is known}$$

4. Sum gradients over all example to get overall gradient. $\nabla_{\theta^{(l)}} J(\theta) = \sum_{i=1}^{m} \nabla_{\theta^{(l)}} J\left(\theta; x^{(i)}, y^{(i)}\right)$

Convolutional Neural Network

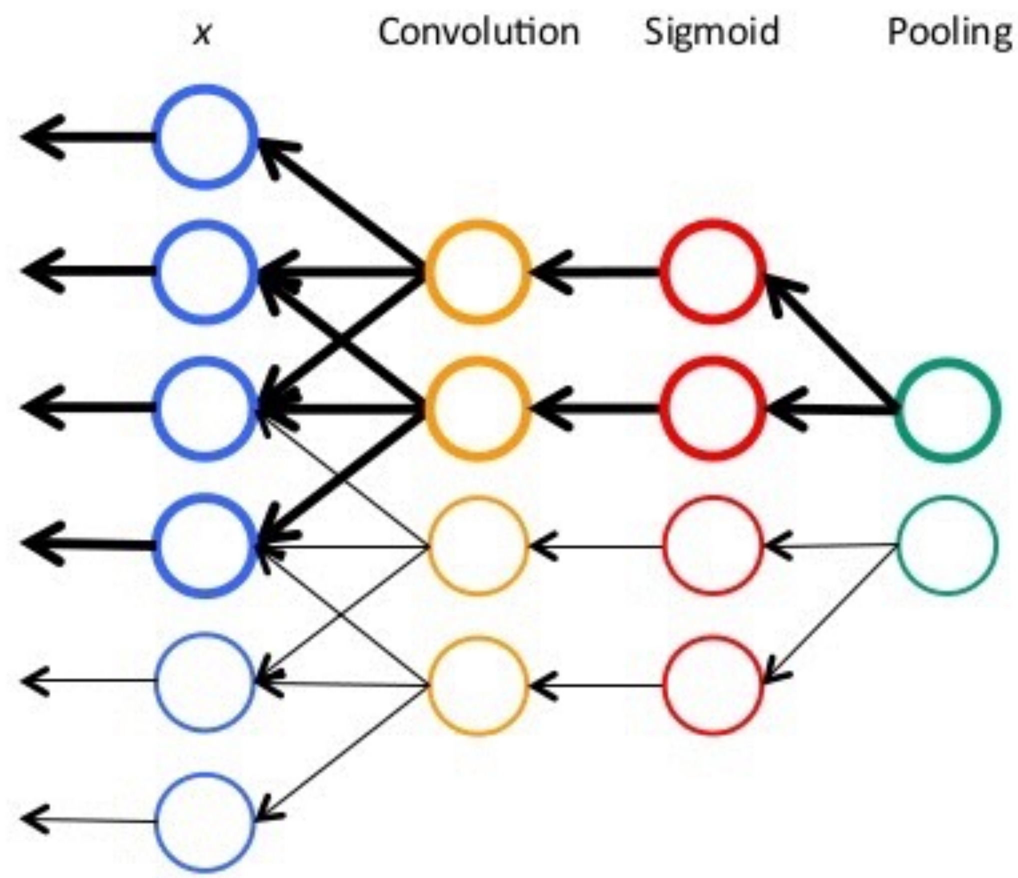
A convolution-pooling layer in Convolutional Neural Network is a composite function decomposed into function elements $f^{(conv)}$, $f^{(sigm)}$, and $f^{(pool)}$.

Let x be the output from the previous layer. Sigmoid nonlinearity is optional.



$$\left(f^{(pool)} \circ f^{(sigm)} \circ f_w^{(conv)}\right)(x)$$

Forward propagation



Backward propagation

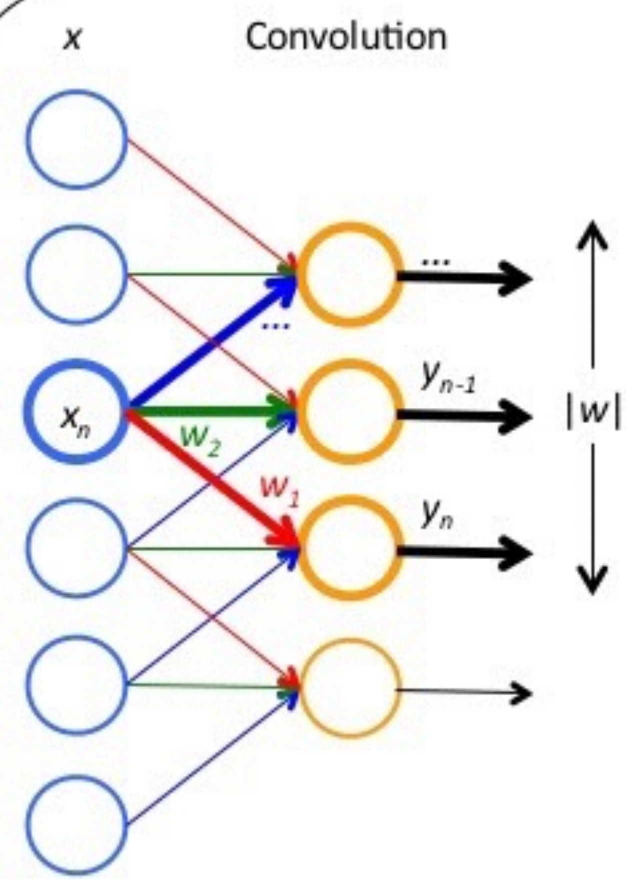
Derivatives of Convolution

- Discrete convolution parameterized by a feature *w* and its derivatives

Let *x* be the input, and *y* be the output of convolution layer. Here we focus on only one feature vector *w*, although a convolution layer usually has multiple features $W = [w_1\ w_2\ \dots\ w_n]$. *n* indexes *x* and *y* where $1 \le n \le |x|$ for x_n, $1 \le n \le |y| = |x| - |w| + 1$ for y_n. *i* indexes *w* where $1 \le i \le |w|$. $(f*g)[n]$ denotes the *n*-th element of $f*g$.

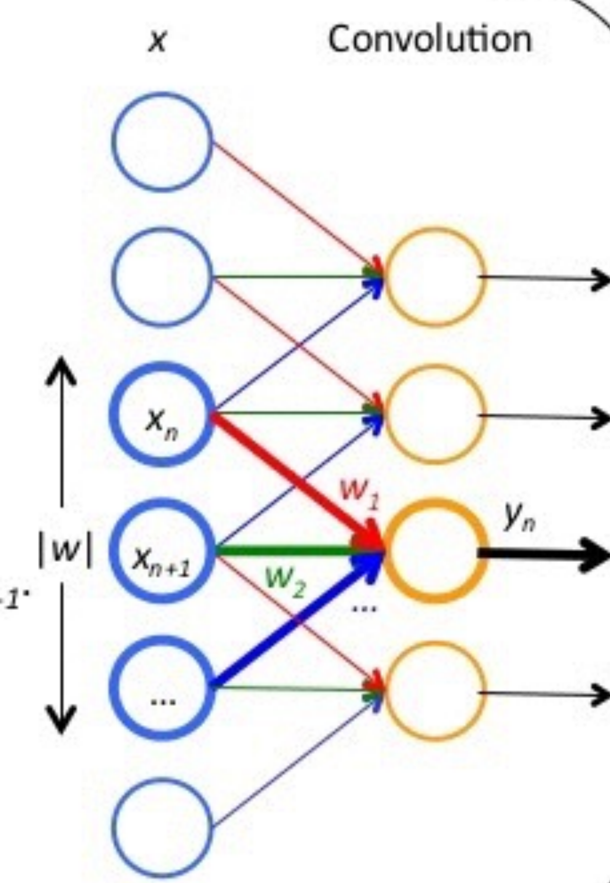
$$y = x * w = [y_n],\ y_n = (x * w)[n] = \sum_{i=1}^{|w|} x_{n+i-1} w_i = w^T x_{n:n+|w|-1}$$

$$\frac{\partial y_{n-i+1}}{\partial x_n} = w_i,\ \frac{\partial y_n}{\partial w_i} = x_{n+i-1} \text{ for } 1 \le i \le |w|$$



From a fixed x_n stand point, x_n has outgoing connections to $y_{n-|W|+1:n}$, i.e., all $y_{n-|W|+1:n}$ have derivatives w.r.t. x_n. Note that *y* and *w* indices are reverse order.

y_n has incoming connections from $x_{n:n+|W|-1}$.



Backpropagation in Convolution Layer

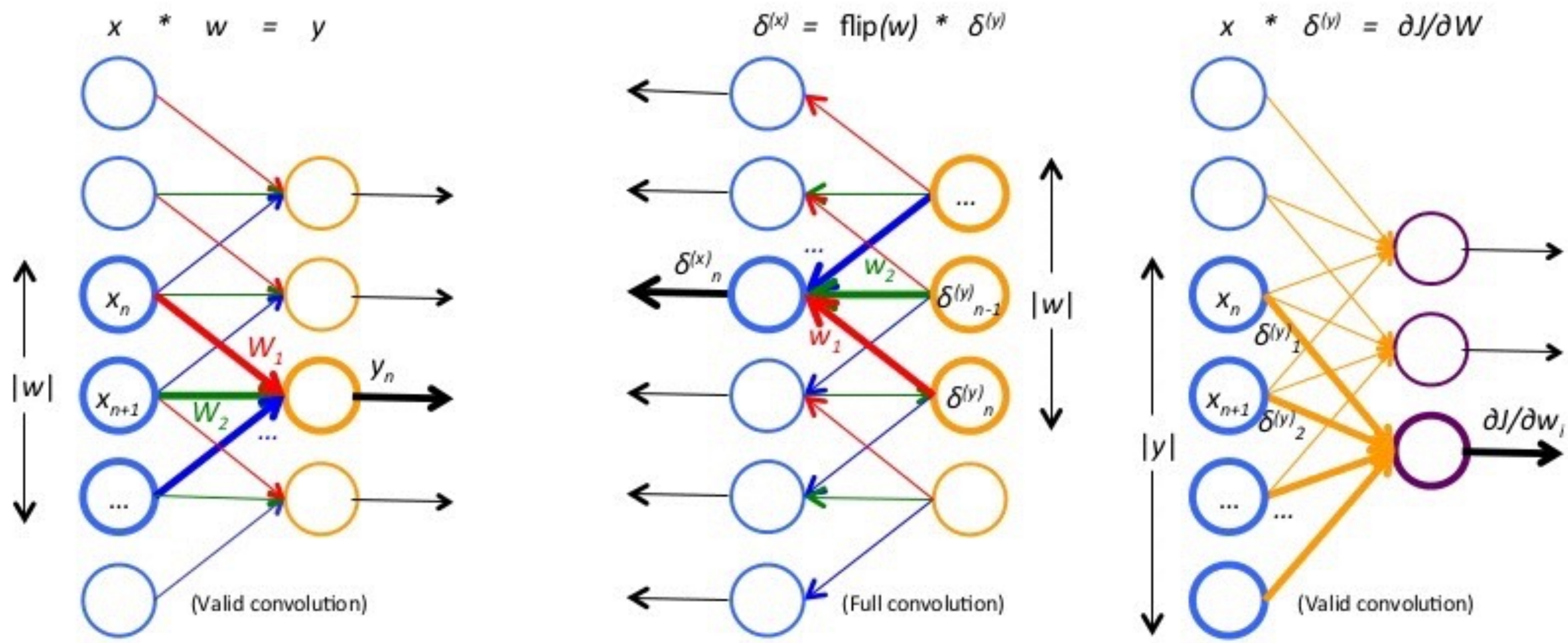
Error signals and gradient for each example are computed by convolution using the commutativity property of convolution and the multivariable chain rule of derivative.

Let's focus on single elements of error signals and a gradient w.r.t. *w*.

$$\delta^{(x)}_n = \frac{\partial J}{\partial x_n} = \frac{\partial J}{\partial y}\frac{\partial y}{\partial x_n} = \sum_{i=1}^{|w|}\frac{\partial J}{\partial y_{n-i+1}}\frac{\partial y_{n-i+1}}{\partial x_n} = \sum_{i=1}^{|w|}\delta^{(y)}_{n-i+1} w_i = \left(\delta^{(y)} * \mathrm{flip}(w)\right)[n],\ \delta^{(x)} = \left[\delta^{(x)}_n\right] = \delta^{(y)} * \mathrm{flip}(w)$$

↑ Reverse order linear combination

$$\frac{\partial J}{\partial w_i} = \frac{\partial J}{\partial y}\frac{\partial y}{\partial w_i} = \sum_{n=1}^{|x|-|w|+1}\frac{\partial J}{\partial y_n}\frac{\partial y_n}{\partial w_i} = \sum_{n=1}^{|x|-|w|+1}\delta^{(y)}_n x_{n+i-1} = \left(\delta^{(y)} * x\right)[i],\ \frac{\partial J}{\partial w} = \left[\frac{\partial J}{\partial w_i}\right] = \delta^{(y)} * x = x * \delta^{(y)}$$



Forward propagation (convolution) Backward propagation Gradient computation

Derivatives of Pooling

Pooling layer subsamples statistics to obtain summary statistics with any aggregate function (or filter) *g* whose input is vector, and output is scalar. Subsampling is an operation like convolution, however *g* is applied to disjoint (non-overlapping) regions.

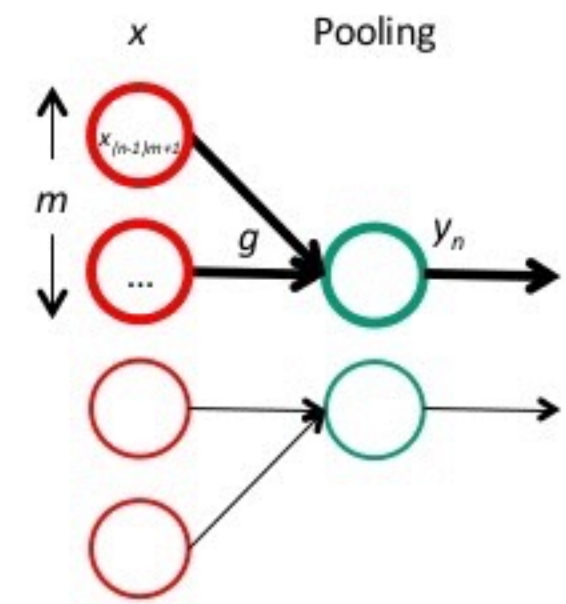
- Definition: *subsample* (or *downsample*)

  Let *m* be the size of pooling region, *x* be the input, and *y* be the output of the pooling layer. subsample(*f*, *g*)[*n*] denotes the *n*-th element of subsample(*f*, *g*).

$$y_n = \text{subsample}(x, g)[n] = g\left(x_{(n-1)m+1:nm}\right)$$

$$y = \text{subsample}(x, g) = [y_n]$$

$$g(x) = \begin{cases} \dfrac{\sum_{k=1}^{m} x_k}{m}, \ \dfrac{\partial g}{\partial x} = \dfrac{\mathbf{1}}{m} & \text{mean pooling} \\ \max(x), \ \dfrac{\partial g}{\partial x_i} = \begin{cases} 1 \text{ if } x_i = \max(x) \\ 0 \text{ otherwise} \end{cases} & \text{max pooling} \\ \|x\|_p = \left(\sum_{k=1}^{m} |x_k|^p\right)^{1/p}, \ \dfrac{\partial g}{\partial x_i} = \left(\sum_{k=1}^{m} |x_k|^p\right)^{1/p-1} |x_i|^{p-1} & \text{L}^{\text{p}} \text{ pooling} \\ \text{or any other differentiable } \mathbf{R}^m \to \mathbf{R} \text{ functions} \end{cases}$$



Backpropagation in Pooling Layer

Error signals for each example are computed by upsampling. Upsampling is an operation which backpropagates (distributes) the error signals over the aggregate function *g* using its derivatives $g'_n = \partial g / \partial x_{(n-1)m+1:nm}$. g'_n can change depending on pooling region *n*.

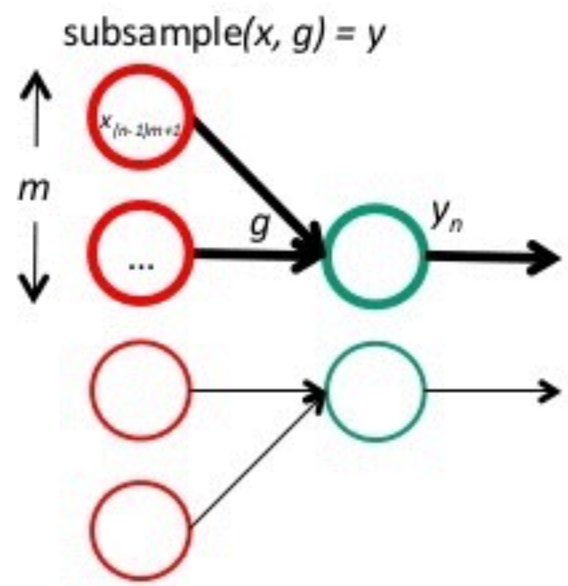
- In max pooling, the unit which was the max at forward propagation receives all the error at backward propagation and the unit is different depending on the region *n*.

- Definition: *upsample*

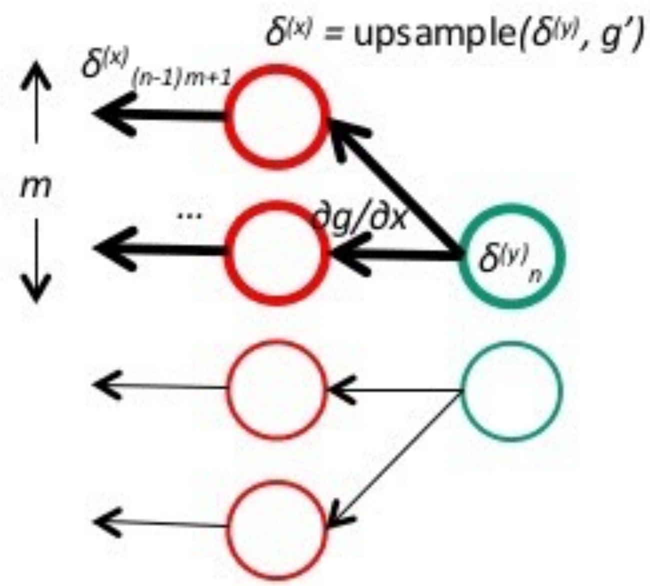
  upsample(*f*, *g*)[*n*] denotes the *n*-th element of upsample(*f*, *g*).

$$\delta^{(x)}_{(n-1)m+1:nm} = \text{upsample}\left(\delta^{(y)}, g'\right)[n] = \delta^{(y)}_n g'_n = \delta^{(y)}_n \frac{\partial g}{\partial x_{(n-1)m+1:nm}} = \frac{\partial J}{\partial y_n} \frac{\partial y_n}{\partial x_{(n-1)m+1:nm}} = \frac{\partial J}{\partial x_{(n-1)m+1:nm}}$$

$$\delta^{(x)} = \text{upsample}\left(\delta^{(a)}, g'\right) = \left[\delta^{(x)}_{(n-1)m+1:nm}\right]$$



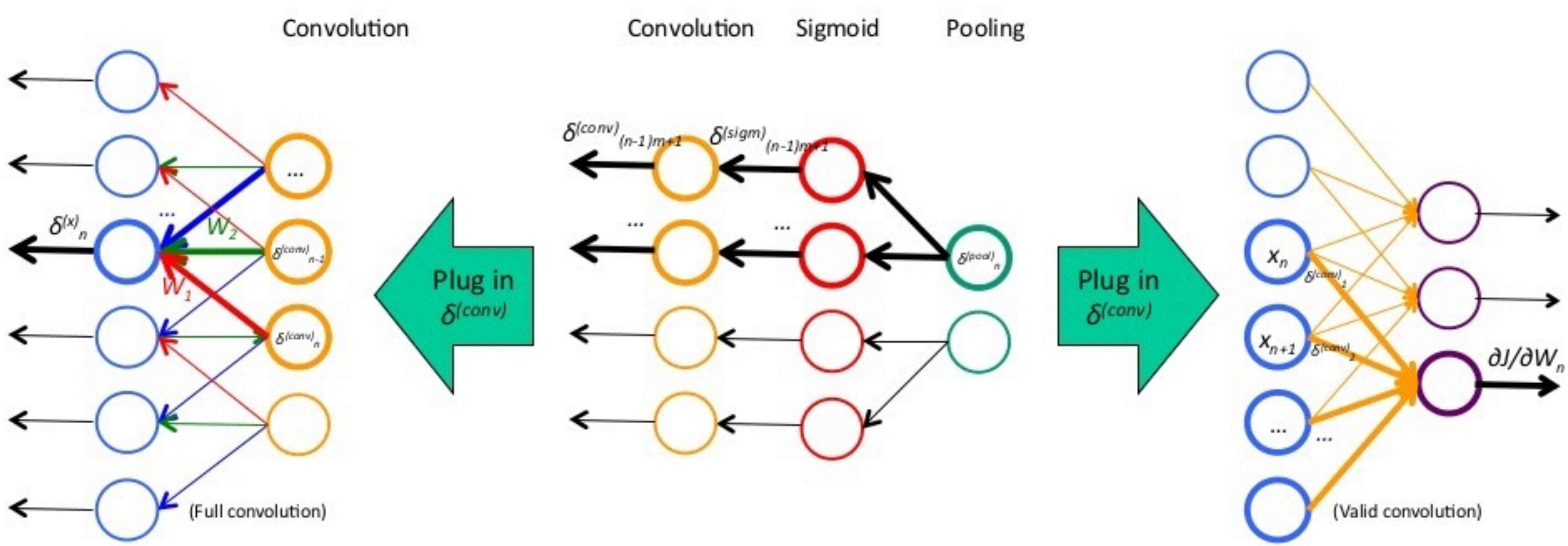
Forward propagation (subsapmling)



Backward propagation (upsapmling)

Backpropagation in CNN (Summary)

2. Propagate error signals $\delta^{(conv)}$ 1. Propagate error signals $\delta^{(pool)}$ 3. Compute gradient $\nabla_w J$



$$\delta^{(x)} = \delta^{(conv)} * \mathrm{flip}(w)$$

$$\delta^{(conv)} = \mathrm{upsample}\left(\delta^{(pool)}, g'\right) \underbrace{\bullet f^{(sigm)} \bullet \left(\mathbf{1} - f^{(sigm)}\right)}_{\text{Derivative of sigmoid}}$$

$$x * \delta^{(conv)} = \nabla_w J$$

Remarks

- References
  - ☐ UFLDL Tutorial, http://ufldl.stanford.edu/tutorial
  - ☐ Chain Rule of Neural Network is Error Back Propagation, http://like.silk.to/studymemo/ChainRuleNeuralNetwork.pdf

- Acknowledgement

This memo was written thanks to a good discussion with Prof. Masayuki Tanaka.