From Neural Networks To ...

(STATE-OF-ART NEURAL NETWORKS MODEL AND ALGORITHMS2019)

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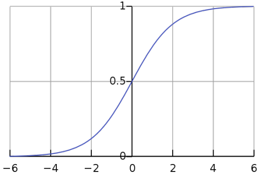
Contents

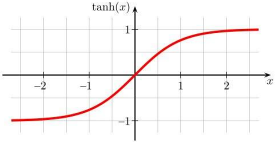
在我们讨论深度学习之前...

Check the **regression** notes on:

- revise on sigmoid and tanh function
- revise on logistic and softmax regression
- Then we talk about neural networks and multilayer perceptron



$$\sigma(z) = \frac{1}{1+e^{-z}}$$



$$\tanh u = \frac{e^u - e^{-u}}{e^u + e^{-u}}$$

Feedforward Neural Network in a nutshell

We begin Feedforward Neural networks, in a nutshell, comprised of the following steps:

- Feedforward

$$\mathrm{f}(\mathbf{x}) = \mathrm{f}_L(\ldots\mathrm{f}_2(\mathrm{f}_1(\mathbf{x};\theta_1);\theta_2)\ldots),\theta_L)$$

- The objective is to minimize the overall cost:

$$\mathrm{L}_\theta = \frac{1}{n}\sum_{i=1}^{n} l(\mathbf{y}_i, \mathrm{f}(\mathbf{x}_i;\theta))$$

- To put it in a gradient descent framework, i.e.,

$$\theta_{t+1} = \theta_t - \eta\frac{\partial \mathrm{f}}{\partial \theta}(\theta_t)$$

Something about $\frac{\partial f}{\partial \theta_t}$

We know all about it already from high school mathematics:

- Product rule:

$$\frac{\partial}{\partial \theta}(f(\theta)g(\theta)) = f(\theta)\frac{\partial}{\partial \theta}g(\theta) + \frac{\partial}{\partial \theta}g(\theta)f(\theta)$$

- Derivative of sums:

$$\frac{\partial}{\partial \theta}(f(\theta) + g(\theta)) = \frac{\partial f(\theta)}{\partial \theta} + \frac{\partial g(\theta)}{\partial \theta}$$

- Chain rule

$$\begin{aligned}\frac{\partial}{\partial \theta_l} &= \frac{\partial}{\partial \theta_l}\mathrm{f}_L(\ldots\mathrm{f}_2(\mathrm{f}_1(\mathbf{x};\theta_1);\theta_2)\ldots),\theta_L) \\ &= \frac{\partial f_L}{\partial f_{L-1}^T}\frac{\partial f_{L-1}}{\partial f_{L-2}^T}\cdots\frac{\partial f_{l+1}}{\partial f_l^T}\frac{\partial f_l}{\partial \theta_l}\end{aligned}$$

Multivariable Chain Rule

We know all about it already from high school mathematics:

- Product rule:

$$\frac{\partial}{\partial\theta}(f(\theta)g(\theta)) = f(\theta)\frac{\partial}{\partial\theta}g(\theta) + \frac{\partial}{\partial\theta}g(\theta)f(\theta)$$

- Derivative of sums:

$$\frac{\partial}{\partial\theta}(f(\theta)+g(\theta)) = \frac{\partial f(\theta)}{\partial\theta} + \frac{\partial g(\theta)}{\partial\theta}$$

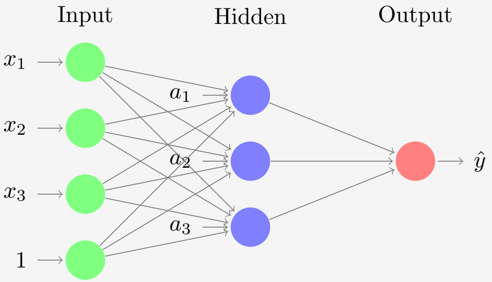
- Chain rule

$$\begin{aligned}\frac{\partial}{\partial\theta_l} &= \frac{\partial}{\partial\theta_l}\mathrm{f}_L(\ldots\mathrm{f}_2(\mathrm{f}_1(\mathbf{x};\theta_1);\theta_2)\ldots),\theta_L) \\ &= \frac{\partial f_L}{\partial f_{L-1}^T}\frac{\partial f_{L-1}}{\partial f_{L-2}^T}\cdots\frac{\partial f_{l+1}}{\partial f_l^T}\frac{\partial f_l}{\partial\theta_l}\end{aligned}$$

Look at Neural network systematically: Feed Forward (1)

$$
\begin{aligned}
\hat{y} &= U^T f(Wx+b) \\
&= \underbrace{U^T \underbrace{f(Wx+b)}_{z}}_{a} = U^T a
\end{aligned}
$$

let $\hat{y}$ be a **scalar** score instead of a **softmax** this time



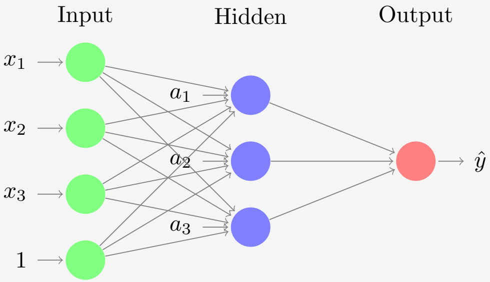
$$
\begin{aligned}
\hat{y} &= U^T f(Wx+b) \\
&= U^T f\left(\begin{bmatrix} w_{11} & w_{11} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)
\end{aligned}
$$

Look at Neural network systematically: Feed Forward (2)

$$z_1 = w_{1,:}^T x + b_1 = \sum_i w_{1,i}^T x_i + b_1$$
$$z_2 = w_{2,:}^T x + b_2 = \sum_i w_{2,i}^T x_i + b_2$$
$$z_3 = w_{3,:}^T x + b_3 = \sum_i w_{3,i}^T x_i + b_3$$

Therefore

$$W_{(\text{index of a, index of X})}$$



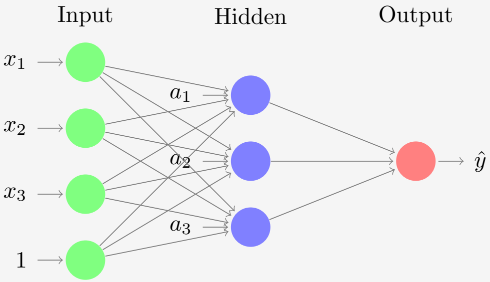
$$\begin{aligned}\hat{y} &= U^T f(Wx + b) \\ &= U^T f\left(\begin{bmatrix} w_{11} & w_{11} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)\end{aligned}$$

Neural Networks: Backpropagation

$$
\begin{aligned}
\hat{y} &= U^T f(Wx+b) \\
&= \underbrace{U^T \underbrace{f(Wx+b)}_{z}}_{a} = U^T a
\end{aligned}
$$

Careful of their dimensions:

$$
\begin{aligned}
\frac{\partial \hat{y}}{\partial W} &= \underbrace{\frac{\partial \hat{y}}{\partial a}\frac{\partial a}{\partial z}}_{columnvector} \times \underbrace{\frac{\partial z}{\partial W}}_{rowvector} \\
&= \underbrace{(U \odot f'(z))}_{columnvector} \times \underbrace{x}_{rowvector}
\end{aligned}
$$



$$
\begin{aligned}
\hat{y} &= U^T f(Wx+b) \\
&= U^T f\left(\begin{bmatrix} w_{11} & w_{11} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)
\end{aligned}
$$

Backpropagation for $W_{i,j}$

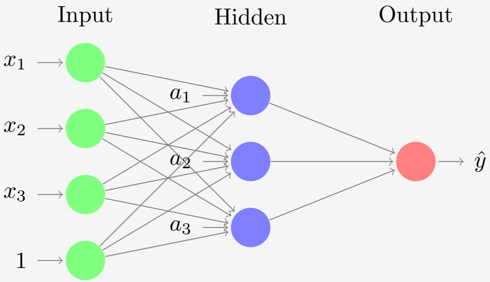
$$\hat{y} = u^T f(Wx + b)$$
$$= u^T \underbrace{f(\underbrace{Wx + b}_{z})}_{a} = u^T a$$

If dimensionality of derivative of W is too hard to see, then we perform derivative one element $W_{i,j}$ at the time:

$$W_{(\text{index of a, index of X})}$$

If we were to compute $\frac{\partial S}{W_{i,j}}$:

$$\frac{\partial \hat{y}}{\partial W} = \frac{\partial \hat{y}}{\partial a}\frac{\partial a}{\partial z}\frac{\partial z}{\partial W}$$
$$\Rightarrow \frac{\partial \hat{y}}{\partial W_{i,j}} = \frac{\partial \hat{y}}{\partial a}\frac{\partial a}{\partial z}\frac{\partial z}{\partial W_{i,j}}$$
$$= \underbrace{u_i f'(z_i)}_{\delta_i} x_j$$
$$= \underbrace{u_i f'(W_{i,:}^T X + b_i)}_{\delta_i} x_j$$



$$\hat{y} = u^T f(Wx + b)$$
$$= u^T f\left(\begin{bmatrix} w_{11} & w_{11} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)$$

important to remember:

$$z_i = W_{i,:}^T X + b_i = (WX + b)_i$$

Backpropagation for W

If we were to compute $\frac{\partial S}{W_{i,j}}$:

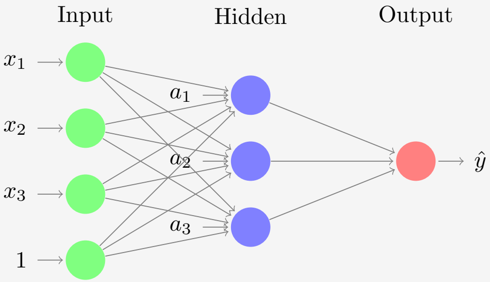
$$\frac{\partial \hat{y}}{\partial W} = \underbrace{U_i f'(W_{i,:}^T X + b_i)}_{\delta_i} X_j$$

$$\delta = \begin{bmatrix} U_1 f'(W_{1,:}^T X + b_1) \\ U_2 f'(W_{2,:}^T X + b_2) \\ U_2 f'(W_{3,:}^T X + b_3) \end{bmatrix}$$

$$= U \odot f'(WX + B)$$

$$\frac{\partial \hat{y}}{\partial W} = \begin{bmatrix} U_1 f'(W_{1,:}^T X + b_1) \\ U_2 f'(W_{2,:}^T X + b_2) \\ U_2 f'(W_{3,:}^T X + b_3) \end{bmatrix}$$

$$= \delta X^T$$



$$\hat{y} = U^T f(Wx + b)$$

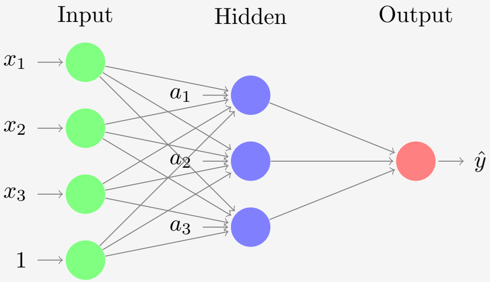
$$= U^T f\left(\begin{bmatrix} w_{11} & w_{11} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)$$

Something about δ

$$\delta = \begin{bmatrix} U_1 f'(W_{1,:}^T X + b_1) \\ U_2 f'(W_{2,:}^T X + b_2) \\ U_2 f'(W_{3,:}^T X + b_3) \end{bmatrix}$$
$$= U \odot f'(WX + B)$$

$$\frac{\partial \hat{y}}{\partial W} = \begin{bmatrix} U_1 f'(W_{1,:}^T X + b_1) \\ U_2 f'(W_{2,:}^T X + b_2) \\ U_2 f'(W_{3,:}^T X + b_3) \end{bmatrix}$$
$$= \delta X^T$$

- δ is the error signal, i.e., $\frac{\partial \hat{y}}{\partial z}$
- δ involves the derivatives of all the activationfunction $\{a_i = f(z_i)\}$

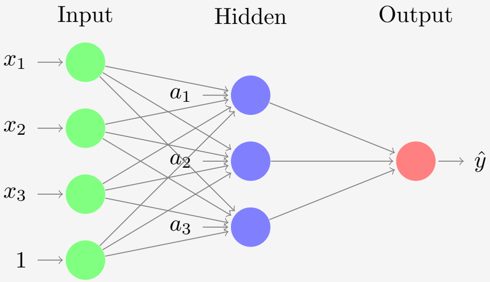


$$\hat{y} = U^T f(Wx + b)$$
$$= U^T f\left(\begin{bmatrix} w_{11} & w_{11} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)$$

Backpropagation for b

$$\frac{\partial \hat{y}}{\partial b_i} = \underbrace{u_i f'(w_{i,:}^T x + b_i)}_{\delta_i} 1$$

$$= \delta_i$$



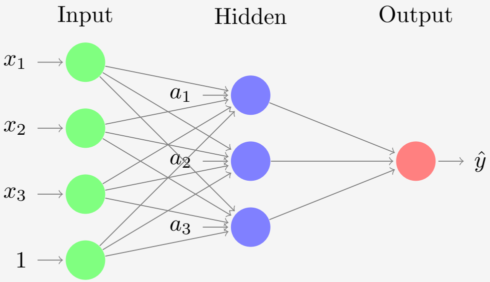
$$\hat{y} = u^T f(Wx + b)$$

$$= u^T f\left(\begin{bmatrix} w_{11} & w_{11} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}\right)$$

Backpropagation for x_j

Note each x_j is contributed by all $\{a_j\}$

$$
\begin{aligned}
\frac{\partial \hat{y}}{\partial x_j} &= \sum_{i=1}^{3} \frac{\partial \hat{y}}{\partial a_i} \frac{\partial a_i}{\partial x_j} \\
&= \sum_{i=1}^{3} \frac{\partial \hat{U}^T a}{\partial a_i} \frac{\partial a_i}{\partial x_j} \\
&= \sum_{i=1}^{3} U_i \frac{\partial f(W_{i,:}x + b)}{\partial x_j} \\
&= \sum_{i=1}^{3} \underbrace{U_i f'(W_{i,:}x + b)}_{\delta_i} \frac{\partial W_{i,:}x}{\partial x_j} \\
&= \sum_{i=1}^{3} \delta_i W_{i,j} \\
&= \delta^T W_{:,j}
\end{aligned}
$$



$$
\begin{aligned}
\hat{y} &= U^T f(Wx + b) \\
&= U^T f\left(\begin{bmatrix} w_{11} & w_{11} & w_{13} \\ w_{21} & w_{22} & w_{23} \\ w_{31} & w_{32} & w_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)
\end{aligned}
$$

Backpropagation for two layers with respect to $W^{(2)}$

$$
\begin{aligned}
a^{(0)} &= x && \text{(input)} \\
z^{(1)} &= W^{(1)} a^{(0)} + b^{(1)} && \text{(linear)} \\
a^{(1)} &= f(z^{(1)}) && \text{(non-linear)} \\
z^{(2)} &= W^{(2)} a^{(1)} + b^{(2)} && \text{(linear)} \\
a^{(2)} &= f(z(2)) && \text{(non-linear)} \\
\hat{y} &= U^T a^{(2)} && \text{(output)}
\end{aligned}
$$

$$\hat{y} = U^T f(W^{(2)} f(W^{(1)} x + b^{(1)}) + b^{(2)})$$

$$
\begin{aligned}
\frac{\partial \hat{y}}{\partial W_{i,j}} &= \underbrace{U_i f'(z_i)}_{\delta_i} x_j && \text{(one layer case)} \\
\Rightarrow \frac{\partial \hat{y}}{\partial W_{i,j}^{(2)}} &= \underbrace{U_i f'(z_i^{(2)})}_{\delta_i^{(2)}} a_j^{(2)} \\
\Rightarrow \frac{\partial \hat{y}}{\partial W^{(2)}} &= \delta_i^{(2)} a^{(2)T} && (\text{where } \delta^{(2)} = U \odot f'(z^{(2)}))
\end{aligned}
$$

Backpropagation for two layers with respect to $W^{(1)}$

$$
\begin{aligned}
a^{(0)} &= x && \text{(input)}\\
z^{(1)} &= W^{(1)}a^{(0)} + b^{(1)} && \text{(linear)}\\
a^{(1)} &= f(z^{(1)}) && \text{(non-linear)}\\
z^{(2)} &= W^{(2)}a^{(1)} + b^{(2)} && \text{(linear)}\\
a^{(2)} &= f(z(2)) && \text{(non-linear)}\\
\hat{y} &= U^T a^{(2)} && \text{(output)}
\end{aligned}
$$

$$
\begin{aligned}
\hat{y} &= U^T f(W^{(2)} f(W^{(1)}x + b^{(1)}) + b^{(2)})\\
&= U^T f(\underbrace{W^{(2)} f(\underbrace{W^{(1)}x + b^{(1)}}_{z^{(1)}}) + b^{(2)}}_{z^{(2)}})
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \hat{y}}{\partial W^{(1)}} &= \underbrace{Uf'(W^{(2)} f(W^{(1)}x + b^{(1)}))}_{\frac{\partial \hat{y}}{\partial a^{(2)}}\frac{\partial a^{(2)}}{\partial z^{(2)}}} \underbrace{W^{(2)}}_{\frac{\partial z^{(2)}}{\partial a^{(1)}}} \underbrace{f'(W^{(1)}x + b^{(1)})}_{\frac{\partial a^{(1)}}{\partial z^{(1)}}} \underbrace{x}_{\frac{\partial z^{(1)}}{\partial w^{(1)}}}\\
&= \underbrace{\underbrace{\frac{\partial \hat{y}}{\partial a^{(2)}}\frac{\partial a^{(2)}}{\partial z^{(2)}}}_{\delta^{(2)}} \frac{\partial z^{(2)}}{\partial a^{(1)}} \frac{\partial a^{(1)}}{\partial z^{(1)}}}_{\delta^{(1)}} \frac{\partial z^{(1)}}{\partial w^{(1)}}\\
&= \underbrace{\delta^{(2)} W^{(2)} f'(z^{(2)})}_{\delta^{(1)}} X
\end{aligned}
$$

Generalisation

Putting them in the ”correct” form of the matrix operations and generalise:

$$
\begin{aligned}
&= \underbrace{\left(W^{(2)T}\delta^{(2)}\right) \odot f'\left(z^{(2)}\right)}_{\delta^{(1)}} X^T \\
&\Rightarrow \delta^{(2)} = W^{(2)T}\delta^{(2)} \odot f'\left(z^{(2)}\right) \\
&\Rightarrow \delta^{(l)} = W^{(l)T}\delta^{(l)} \odot f'\left(z^{(l)}\right)
\end{aligned}
$$

Backpropagation in action!

$$a^{(0)} = x \qquad \text{(input)}$$

$$z^{(1)} = W^{(1)} a^{(0)} + b^{(1)} \qquad \text{(linear)}$$

$$a^{(1)} = f(z^{(1)}) \qquad \text{(non-linear)}$$

$$z^{(2)} = W^{(2)} a^{(1)} + b^{(2)} \qquad \text{(linear)}$$

$$a^{(2)} = f(z(2)) \qquad \text{(non-linear)}$$

$$\hat{y} = U^T a^{(2)} \qquad \text{(output)}$$

To generalise this:

$$\delta^{(l)} = W^{(l)T} \delta^{(l)} \odot f'(z^{(l)})$$

- step 1: compute δ of the last layer L:

$$\delta^{(L)} = U \odot \underbrace{f'(z^{(L)})}_{fromfeed-forward}$$

- step 2: Generate the whole sequence of $\{\delta^{(l)}\}_1^L$

$$\delta^{(l)} = W^{(l)T} \delta^{(l)} \odot f'(z^{(l)})$$

- step 3: compute gradients at each $\frac{\partial s}{\partial W^{(l)}}{}_1^{(L-1)}$:

$$\frac{\partial \hat{y}}{\partial W^{(l)}} = \delta^{(l+1)} a^{(l)T}$$

Note that $\frac{\partial \hat{y}}{\partial W^{(l)}}$ can be obtained as soon as $\delta^{(l+1)}$ becomes available.

Contents

Good old Feedforward Neural Network with Many layers

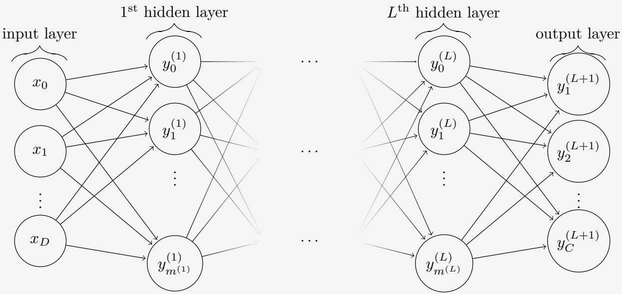
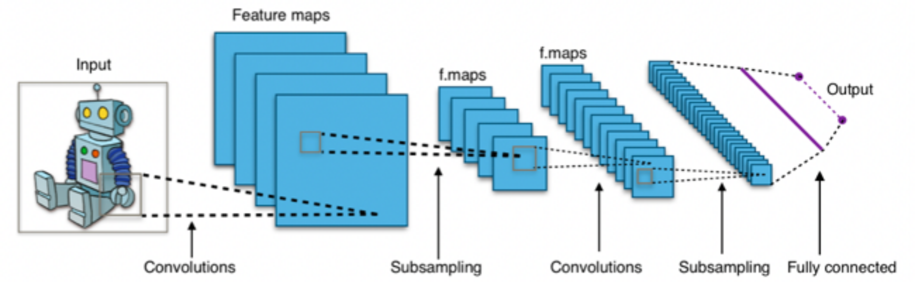


Figure: Network graph of a $(L+1)$-layer perceptron with D input units and C output units. The l^{th} hidden layer contains $m^{(l)}$ hidden units.

Feedforward Neural Network with Many layers

- For complicated problem, one hidden layer may NOT be enough.
- σ Layers can be flexibly designed: linear, Softmax, ReLU or any other
- Each layers may have their own parameters $\theta(l)$
- There are many such layers, hence many parameters
- Think about the case of **one meg pixel image**.
- How may we reduce the number of parameters from the fully connected network?
- keyword of the day: parameter sharing

A high level view of Convolution Neural Network (CNN)



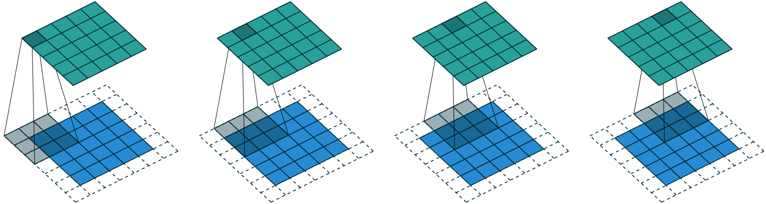
Convolution Neural Networks: What is a convolution?

- from a signal processing perspective:

$$(f * g)(t) \stackrel{\text{def}}{=} \int_{-\infty}^{\infty} f(\tau)g(t-\tau)d\tau = \int_{-\infty}^{\infty} f(t-\tau)g(\tau)d\tau$$

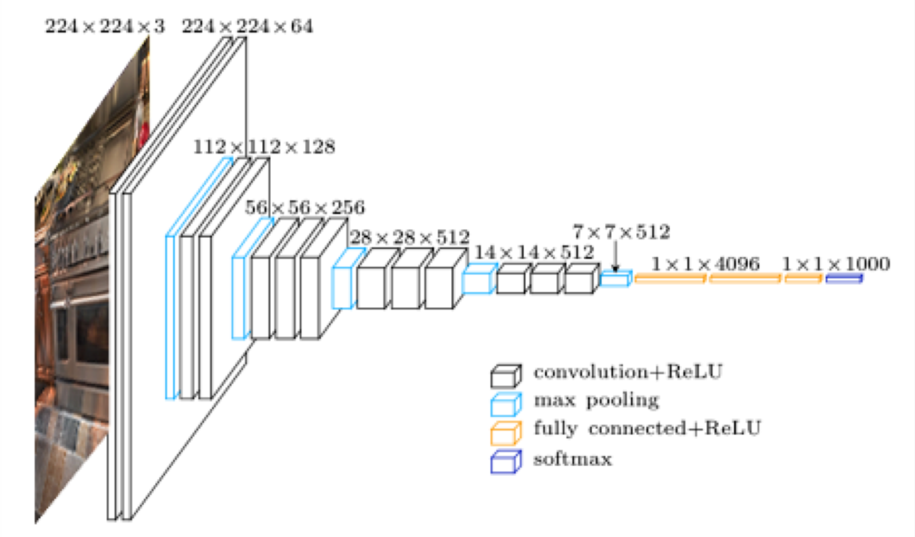
What is a 2D Convolution in Discrete Imaging?

An example of Convolving a 3×3 kernel over a 5×5 input with padding1.

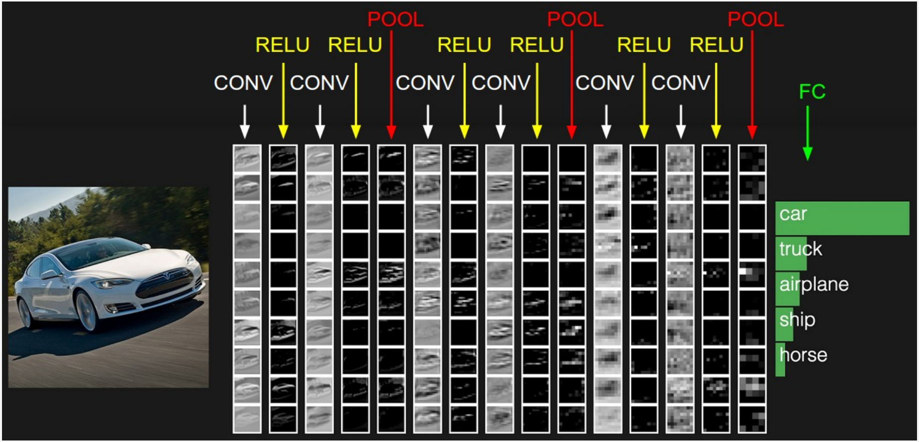


- Exploiting the strong spatially local correlation present in natural images.
- In term of number of parameters, assume in a layer, you have 128 convolution Kernels (the grey square), you create 64 “copies” of the image.
- Assume in a layer, if each kernel is 5×5 in size, we have something like $128x5x5 = 3200$ parameters.
- A lot less than fully connected neural networks

CNN for image classification: look at it again



What does the ”learnt” image feature represent?



CNN Feed-forward: convolution as a linear operator

- Let’s forget about only considers:

$$x_{i,j}^{(l)} = W * (y^{(l-1)}) \quad y_{ij}^{(l)} = \sigma(x_{ij}^{(l)})$$

- as matter of fact, in 1 - D convolution, one may replace convolution by matrix multiplication:

$$x^{(l)} = W * (y^{(l-1)}) = \begin{bmatrix} w_1 & 0 & \cdots & 0 & 0 \\ w_2 & w_1 & \cdots & \vdots & \vdots \\ w_3 & w_2 & \cdots & 0 & 0 \\ \vdots & w_3 & \cdots & w_1 & 0 \\ w_{m-1} & \vdots & \cdots & w_2 & w_1 \\ w_m & w_{m-1} & \vdots & \vdots & w_2 \\ 0 & w_m & \cdots & w_{m-2} & \vdots \\ 0 & 0 & \cdots & w_{m-1} & w_{m-2} \\ \vdots & \vdots & \vdots & w_m & w_{m-1} \\ 0 & 0 & 0 & \cdots & w_m \end{bmatrix} \begin{bmatrix} y_1^{(l-1)} \\ y_2^{(l-1)} \\ y_3^{(l-1)} \\ \vdots \\ y_n^{(l-1)} \end{bmatrix}$$

CNN Feed-forward: looking at one layer only

- say at layer $(l-1)$: $y^{(l-1)}$ has $N \times N$ square neurons
- use $m \times m$ filter ω
- when stride 0 used, $x^{(l)}$ will be of size $(N-m+1) \times (N-m+1)$
- for simplicity - shift the centre by $(\frac{m}{2}, \frac{m}{2})$

$$
\begin{aligned}
x_{ij}^{(l)} &= \sum_{a=0}^{m-1} \sum_{b=0}^{m-1} \omega_{ab} y_{(i+a)(j+b)}^{(l-1)} \\
y_{ij}^{(l)} &= \delta(x_{ij}^{(l)})
\end{aligned}
$$

CNN back-propagation

- we need four derivative quantities:
  - $\frac{\partial y_{ij}^{(l)}}{\partial x_{ij}^{(l)}} = \sigma'(x_{ij}^{(l)})$
  - $\frac{\partial x_{ij}^{(l)}}{\partial w_{a,b}^{(l)}} = y_{i_a,j+b}^{(l-1)}$
  - $\frac{\partial x_{(i-a)(j-b)}^{(l)}}{\partial y_{ij}^{(l-1)}} = \omega_{a,b}$
- say we already knew $\frac{\partial E}{\partial y_{ij}^{(l)}}$

find $\frac{\partial E}{\partial y_{ij}^{(l-1)}}$: it involves a "filter-window" of $x^{(l)}$

$$\frac{\partial E}{\partial y_{ij}^{(l-1)}} = \sum_{a=0}^{m-1}\sum_{b=0}^{m-1} \frac{\partial E}{\partial x_{(i-a)(j-b)}^{(l)}} \frac{\partial x_{(i-a)(j-b)}^{(l)}}{\partial y_{ij}^{(l-1)}}$$
$$= \sum_{a=0}^{m-1}\sum_{b=0}^{m-1} \frac{\partial E}{\partial y_{ij}^{(l)}} \sigma'(x_{(i-a)j-b}^{(l)})\omega_{a,b}$$

sum over a filter window

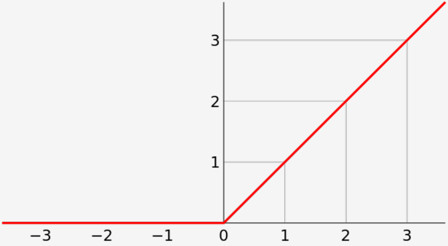
find $\frac{\partial E}{\partial w_{a,b}}$: it involves entire $x_{ij}^{(l)}$

$$\frac{\partial E}{\partial y_{ij}^{(l-1)}} = \sum_{i=0}^{N-m+1}\sum_{j=0}^{N-m+1} \frac{\partial E}{\partial x_{ij}^{(l)}} \frac{\partial x_{ij}^{(l)}}{\partial w_{a,b}}$$
$$= \sum_{i=0}^{N-m+1}\sum_{j=0}^{N-m+1} \frac{\partial E}{\partial y_{ij}^{(l)}} \sigma'(x_{i,j}^{(l)}) y_{i+a,j+b}^{(l-1)}$$

sum over an entire image

The winning ingredient: Rectified Linear Unit

- How to combine the different "convolved" images together?
- A Linear + **Activation function** $f(x) = \max(0, x)$



- High school mathematics is useful
- its derivative can only be $\{0, 1\}$. This is useful to prevent gradient vanishing and exploding
- They do not require any exponential computation (such as those required in sigmoid)
- reported around 6X speed over existing activation functions