△ 反向传播.　　KEYWORDS: Forward Pass . Backward Pass .

train 一个神经网络的时候其实就在优化一个 loss function.

e.g. 数字识别. input 为 256-dim vector, output 为 10-dim vector.

用交叉熵 $C(y,\hat{y}) = -\sum_{i=1}^{10} \hat{y}_i \ln y_i$ 定义 loss function: ($\hat{y}$ 目标)

相当于 $L(\theta) = \sum_{n=1}^{N} C^n(\theta)$.　(相当于 $y, \hat{y}$ 间距离)

"1": $y = \begin{bmatrix} y_1 \\ \vdots \\ y_{10} \end{bmatrix}_{10\times 1}$　$\hat{y} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}_{10\times 1}$.　$\theta = \begin{bmatrix} w_1 \\ \vdots \\ b_1 \\ \vdots \end{bmatrix}$　$\nabla L(\theta) = \begin{bmatrix} \frac{\partial L}{\partial w_1} \\ \vdots \\ \frac{\partial L}{\partial b_1} \\ \vdots \end{bmatrix}$

$\theta^* = \arg\min_\theta L(\theta)$.

gradient descent: $\theta^i \leftarrow \theta^{i-1} - \eta \nabla L(\theta^{i-1})$　(η: learning rate.)

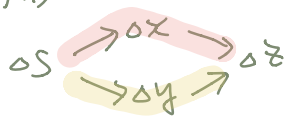
Backpropagation: 算 $\frac{\partial L}{\partial w_1} \cdots \frac{\partial L}{\partial b_1} \cdots$ 的高效方式. (因为参数可能有百万个. 直接算太多).

Chain Rule:

① $y = g(x)$　$z = h(y)$　$\Delta x \to \Delta y \to \Delta z$

$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$ (将路径从后往前算)

② $x = g(s)$　$y = h(s)$　$z = k(x,y)$



$\frac{dz}{ds} = \frac{\partial z}{\partial x}\frac{dx}{ds} + \frac{\partial z}{\partial y}\frac{dy}{ds}$

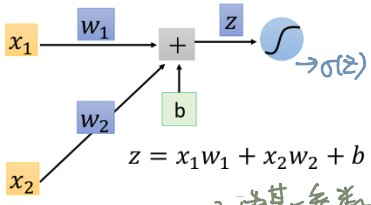
这里是偏导, 因为 z 有2个参数.

$L(\theta) = \sum_{n=1}^{N} C^n(\theta)$　$\frac{\partial L(\theta)}{\partial w} = \sum_{n=1}^{N} \frac{\partial C^n(\theta)}{\partial w}$

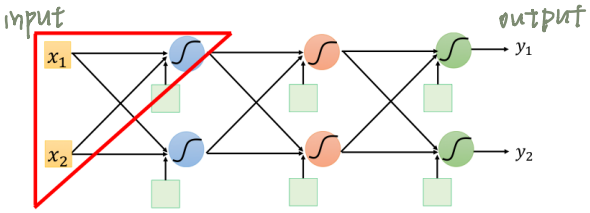
$C(\theta)$ 相当于 $C(y_1, \ldots, y_{10})$

我们的目标: 算 C 对一个参数的偏微分.

一个 neuron:



w 为某一个参数:



$z = z(w)$
$C = C(z)$

$\Delta w \to \Delta z \to \Delta C$

$\therefore \frac{dC}{dw} = \frac{dC}{dz}\frac{dz}{dw}$

$\frac{dC}{dz}$ 难算　$\frac{dz}{dw}$ 好算 (有流过)

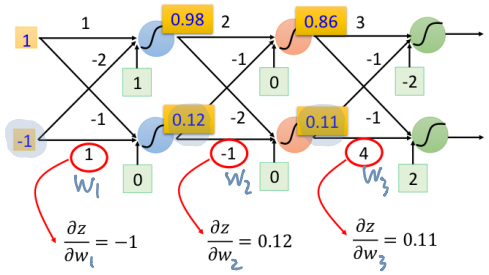
- **Forward Pass**：算 $\frac{\partial z}{\partial w}$

$\frac{\partial z}{\partial w_1} = x_1$，$\frac{\partial z}{\partial w_2} = x_2$。即看参数 w 前连的 input 是什么，结果就是什么。

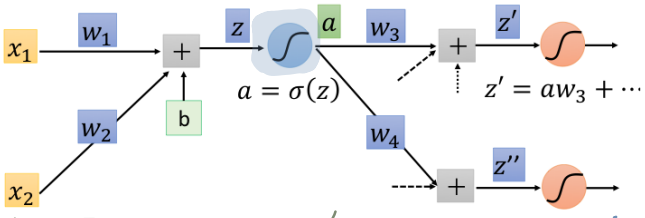
正向计算出所有 neuron 的 output (z) 后 ✓

∴给定了一组 input (x) 和参数 θ，可以直接读出 $\frac{\partial z}{\partial w}$。

（z 是相对于 neuron 来说的）。



- **Backward Pass**：算 $\frac{\partial C}{\partial z}$



$a = \sigma(z)$，$C = C(a)$ ⇒ $\frac{\partial C}{\partial z} = \frac{\partial C}{\partial a}\frac{\partial a}{\partial z}$，$\frac{\partial a}{\partial z} = \sigma'(z)$

→ 用 chain rule 表示时，不一定要把中间每层参数都拆出来，因为想拆多少都是能拆出来的。重要的是能不拆出一部分可求导的。

$\frac{\partial C}{\partial a}$ 链算。

$\sigma'(z)$ 是常数，因为 z 已被计算出值。

$z' = z'(a)$，$z'' = z''(a)$，$C = C(z', z'')$。

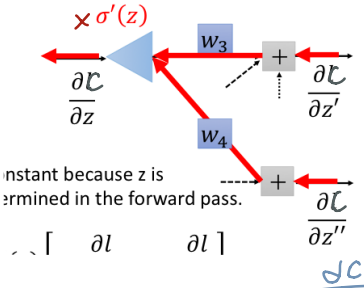
$\Delta a \to \Delta z', \Delta z'' \to \Delta C$

$\frac{\partial C}{\partial a} = \frac{\partial C}{\partial z'}\frac{\partial z'}{\partial a} + \frac{\partial C}{\partial z''}\frac{\partial z''}{\partial a}$，$\frac{\partial z'}{\partial a} = w_3$，$\frac{\partial z''}{\partial a} = w_4$

∴ $\frac{\partial C}{\partial a} = w_3\frac{\partial C}{\partial z'} + w_4\frac{\partial C}{\partial z''}$。

$\frac{\partial C}{\partial z} = \sigma'(z)\left[w_3\frac{\partial C}{\partial z'} + w_4\frac{\partial C}{\partial z''}\right]$。

用下一个倒过来的 neuron 表示：



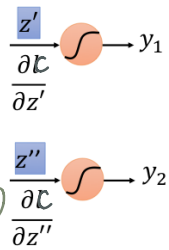
$\left[\frac{\partial l}{\partial} \quad \frac{\partial l}{\partial}\right]$

→ ① 当 z'、z'' 不在 output layer：

求 $\frac{\partial C}{\partial z'}$、$\frac{\partial C}{\partial z''}$ 和求 $\frac{\partial C}{\partial z}$ 相同。

② 当 z'、z'' 在 output layer：

$y_1 = \sigma(z')$，$C = C(y_1)$ ⇒ $\frac{\partial C}{\partial z'} = \frac{\partial C}{\partial y_1}\frac{\partial y_1}{\partial z'}$，$\frac{\partial y_1}{\partial z'} = \sigma'(z')$



同理，$\frac{\partial C}{\partial z''} = \frac{\partial C}{\partial y_2}\frac{\partial y_2}{\partial z''}$，$\frac{\partial y_2}{\partial z''} = \sigma'(z'')$。

$\frac{\partial C}{\partial y}$ 用 C 的定义直接求。

Framework

$\because L(\theta) = \sum_{n=1}^{N} C^n(\theta)$ $\quad \therefore \frac{\partial L(\theta)}{\partial w} = \sum_{n=1}^{N} \frac{\partial C^n(\theta)}{\partial w}$

$\frac{\partial C(\theta)}{\partial w} = \frac{\partial C}{\partial z}\frac{\partial z}{\partial w}$ （z为w所在neuron的线性组合值）

$\frac{\partial z}{\partial w}$ → Forward Pass，直接读input.

$\frac{\partial C}{\partial z}$ → Backward Pass

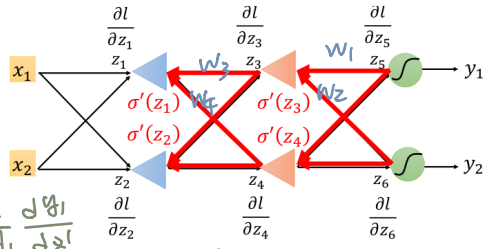
$\frac{\partial C}{\partial z} = \frac{\partial C}{\partial a}\frac{\partial a}{\partial z} = \sigma'(z)$

（z', z''为以$\sigma(z)$为input的neuron的线性组合值）.

$\frac{\partial C}{\partial z'}\frac{\partial z'}{\partial a} + \frac{\partial C}{\partial z''}\frac{\partial z''}{\partial a}$ （$\frac{\partial z'}{\partial a} = w_3$, $\frac{\partial z''}{\partial a} = w_4$）

z', z''在output layer：$\begin{cases} \frac{\partial C}{\partial z'} = \frac{\partial C}{\partial y_1}\frac{\partial y_1}{\partial z'} \\ \frac{\partial C}{\partial z''} = \frac{\partial C}{\partial y_2}\frac{\partial y_2}{\partial z''} \end{cases}$ 均易求.

z', z''不在output layer：继续递归



可导出：

$\frac{\partial l}{\partial z_5} = \frac{\partial l}{\partial y_1}\frac{\partial y_1}{\partial z_5}$

$\frac{\partial l}{\partial z_3} = \sigma'(z_3)\left(w_1\frac{\partial l}{\partial z_5} + w_2\frac{\partial l}{\partial z_6}\right)$

$\frac{\partial l}{\partial z_1} = \sigma'(z_1)\left(w_3\frac{\partial l}{\partial z_3} + w_4\frac{\partial l}{\partial z_4}\right)$