Autograd

What AutoDiff Is Not

* Finite differences

→ One sided:

$$\frac{\partial}{\partial x_i} f(x_1, \dots, x_N) \approx \frac{f(x_1, \dots x_i + h, \dots) - f(x_1, \dots x_i, x_N)}{h}$$

→ Or Two sided

$$\frac{\partial}{\partial x_i} f(x_1, \dots, x_N) \approx \frac{f(x_1, \dots x_i + h, \dots) - f(x_1, \dots, x_i - h, \dots)}{2h}$$

* Challenges with finite differences

  - Expensive: compute forward pass for each variable

  - Numerically unstable

Computational Graphs

* Nodes : operations (+, *, ...)

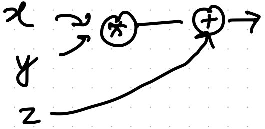
* Edges : variables | Tensors

Computational Graphs

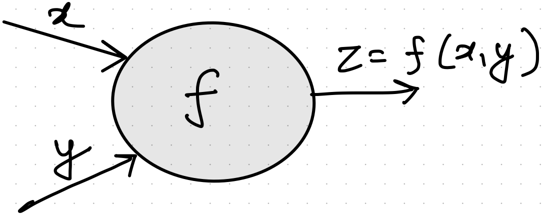
* Nodes : operations $(+, *, \ldots)$

* Edges : variables | Tensors
  (and data dependencies)

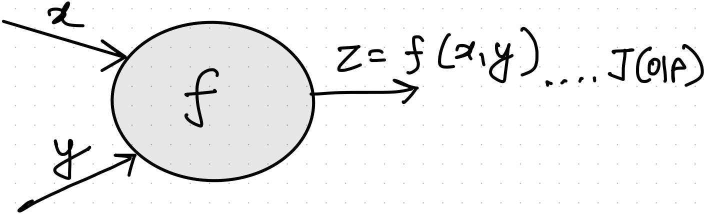
Example: $(x * y) + z$



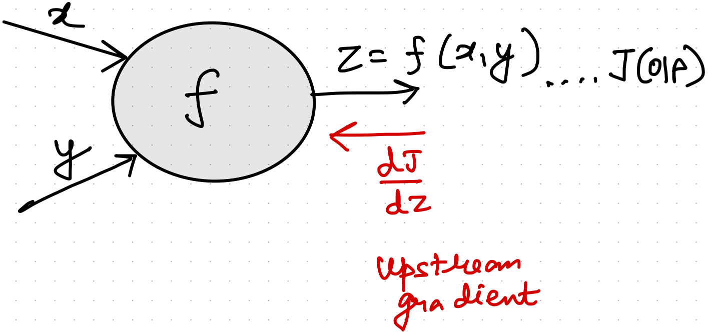
Back Prop Through Computational Graph



Back Prop Through Computational Graph

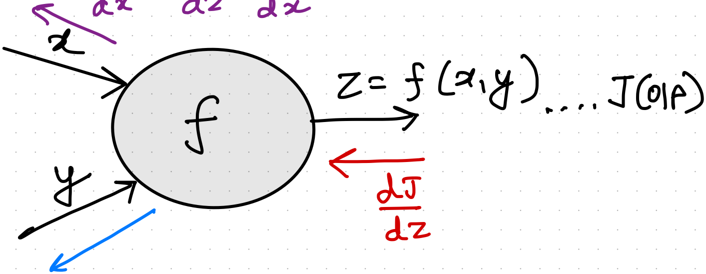


Back Prop Through Computational Graph



Back Prop Through Computational Graph

$$\frac{dJ}{dx} = \frac{dJ}{dz} \cdot \frac{dz}{dx}$$



$$\frac{dJ}{dy} = \frac{dJ}{dz} \cdot \frac{dz}{dy}$$

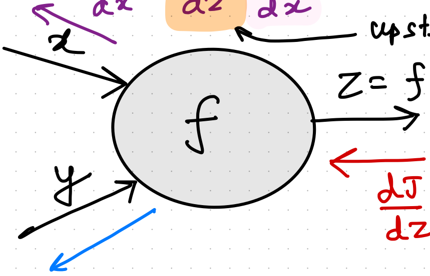
upstream gradient

Back Prop Through Computational Graph

$$\frac{dJ}{dx} = \frac{dJ}{dz} \cdot \frac{dz}{dx}$$

← Local grad.

upstream grad.



$z = f(x, y)$ .... $J(O/P)$

$\frac{dJ}{dz}$

upstream gradient

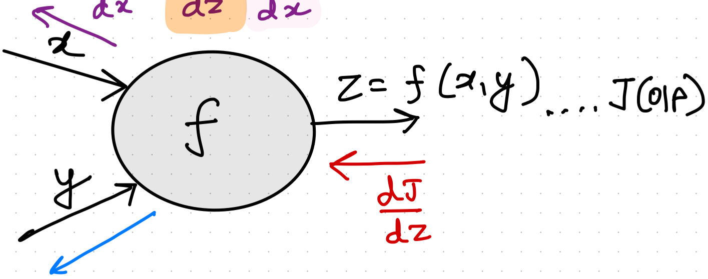
$$\frac{dJ}{dy} = \frac{dJ}{dz} \cdot \frac{dz}{dy}$$

upstream gradient

Local grad.

Back Prop Through Computational Graph

$$\frac{dJ}{dx} = \boxed{\frac{dJ}{dz}} \cdot \frac{dz}{dx}$$



Upstream gradient

$$\frac{dJ}{dy} = \boxed{\frac{dJ}{dz}} \cdot \frac{dz}{dy}$$

DOWNSTREAM GRADIENT
= UPSTREAM GRADIENT * LOCAL GRADIENT

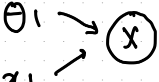
$$\hat{y} = \frac{1}{1+e^{-(\theta_0 + \theta_1 x_1 + \theta_2 x_2)}}$$

$$y = 1$$

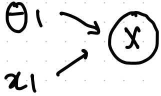
$$\text{LOSS} = -y \log \hat{y} - (1-y) \log (1-\hat{y})$$

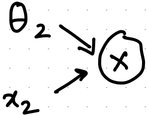
$$= -\log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1 + \theta_2 x_2)}} \right)$$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$

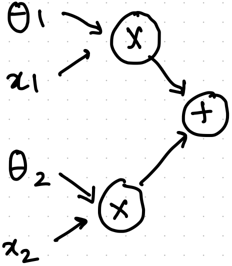


$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$

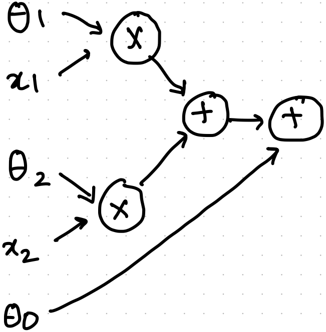




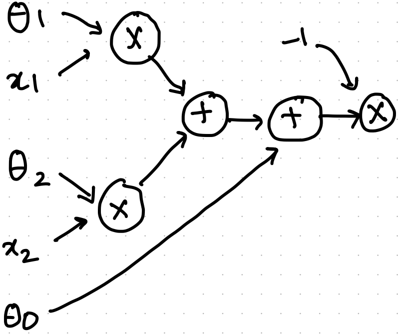
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



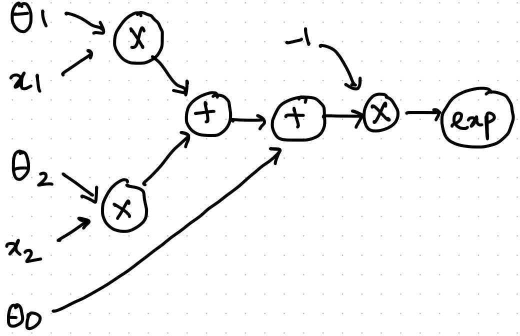
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



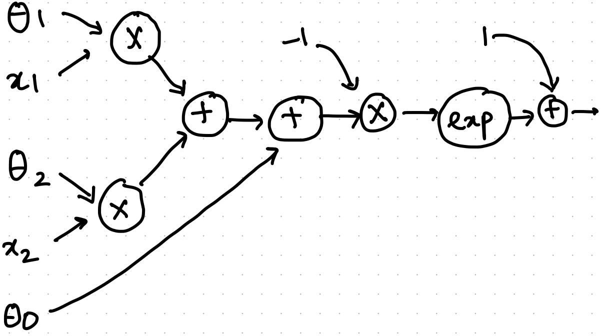
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



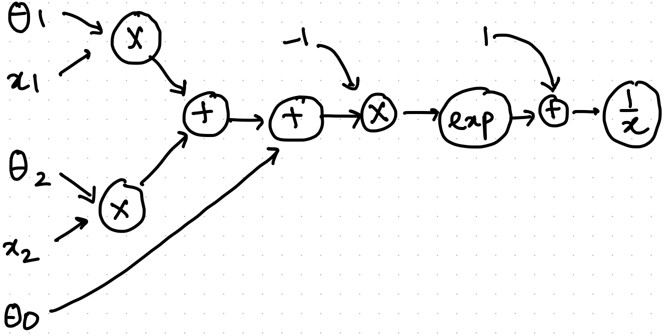
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



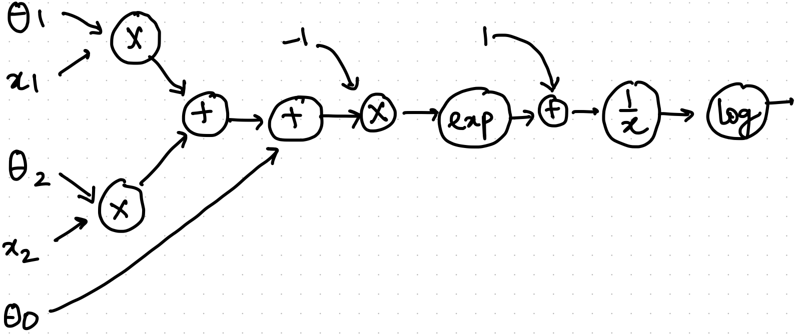
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



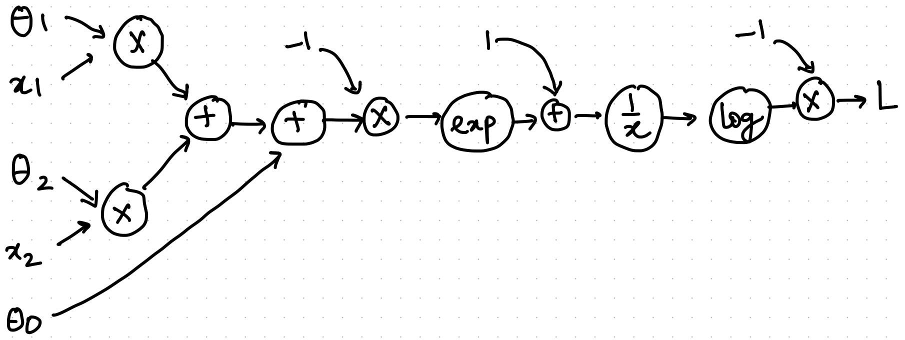
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



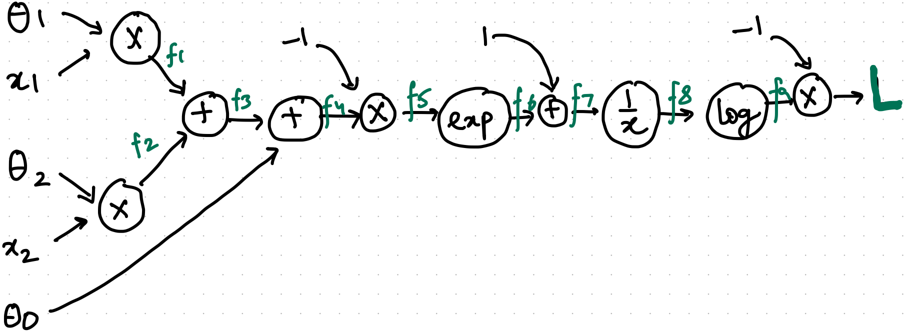
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}} \right)$$



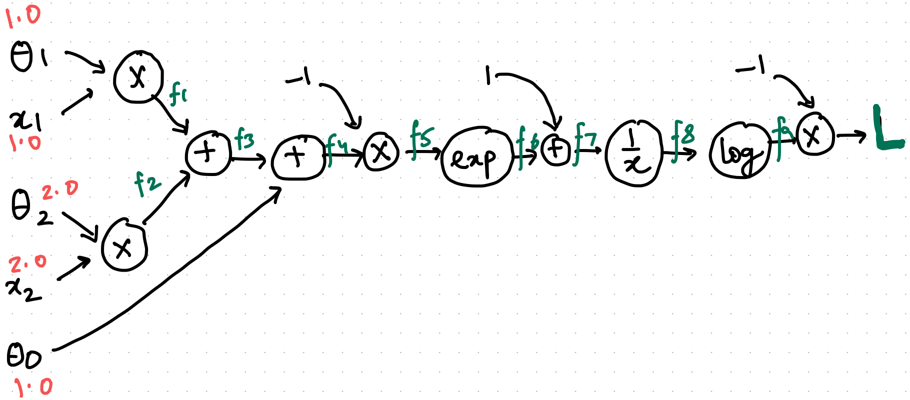
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}} \right)$$



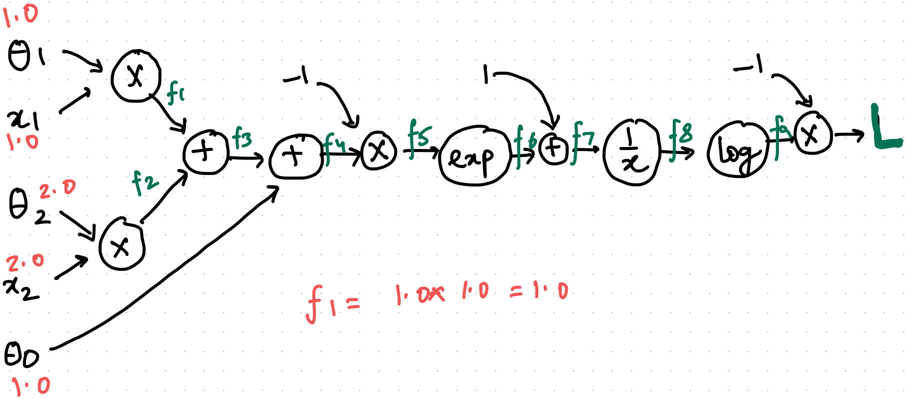
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$

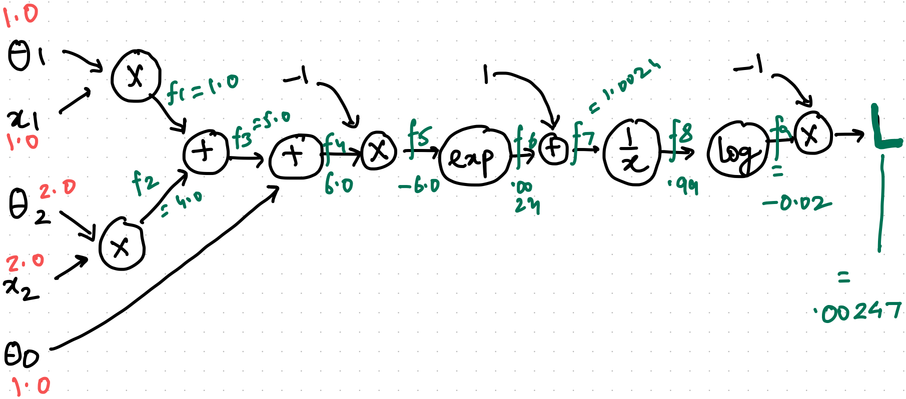


$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$

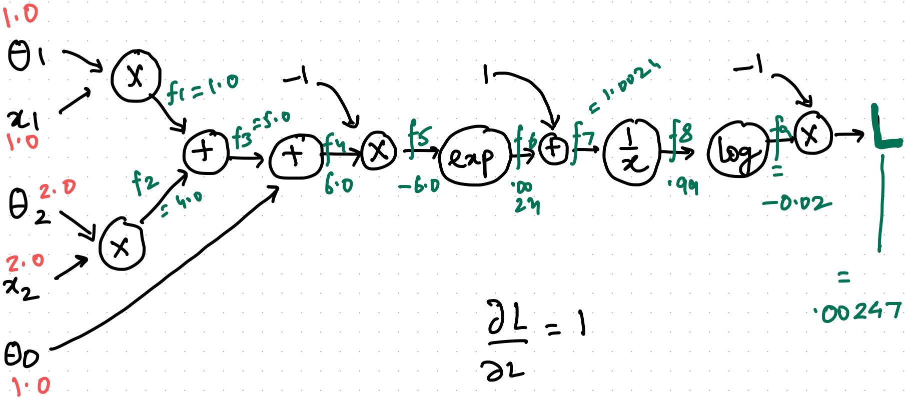


$f_1 = 1.0 \times 1.0 = 1.0$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$

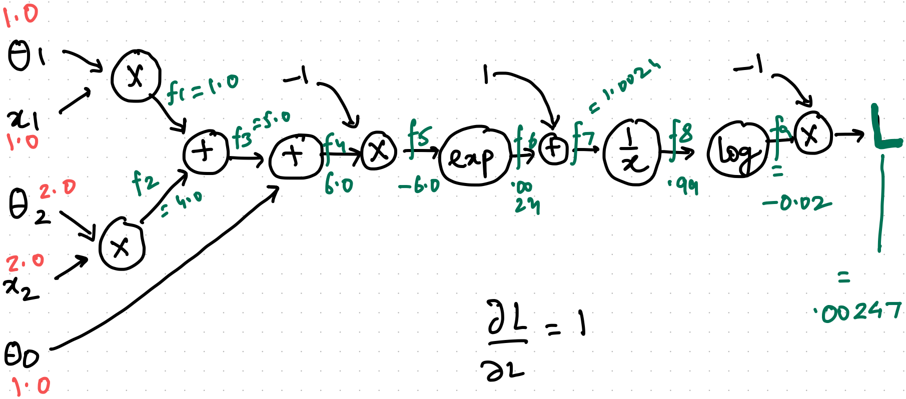


$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



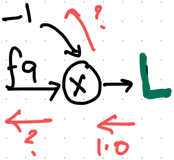
$$\frac{\partial L}{\partial L} = 1$$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



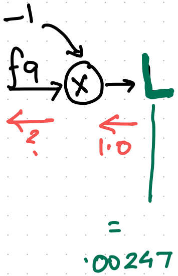
$$\frac{\partial L}{\partial L} = 1$$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



$$\frac{\partial L}{\partial L} = 1$$

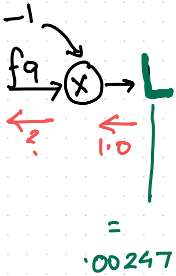
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



$$\frac{\partial L}{\partial L} = 1$$

upstream gradient = 1.0

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



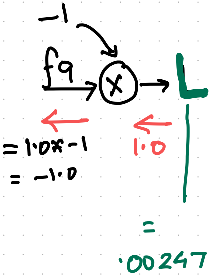
$$\frac{\partial L}{\partial L} = 1$$

upstream gradient = 1.0

$$L = fq * -1$$

$$\frac{\partial L}{\partial fq} = -1 \qquad \text{LOCAL GRADIENT} = -1$$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



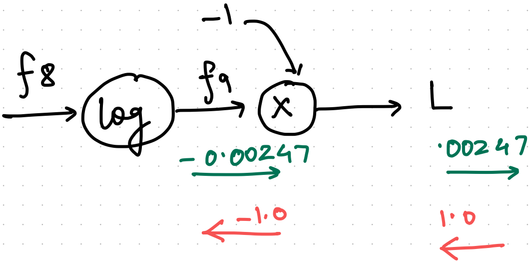
$$\frac{\partial L}{\partial L} = 1$$

upstream gradient = 1.0

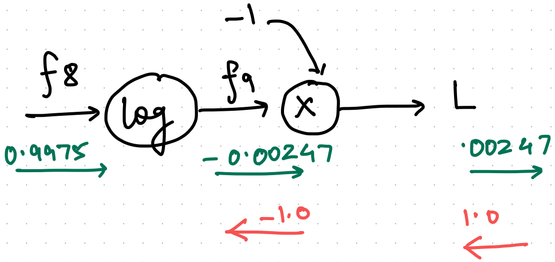
$$L = fq * -1$$

$$\frac{\partial L}{\partial fq} = -1$$ LOCAL GRADIENT = -1

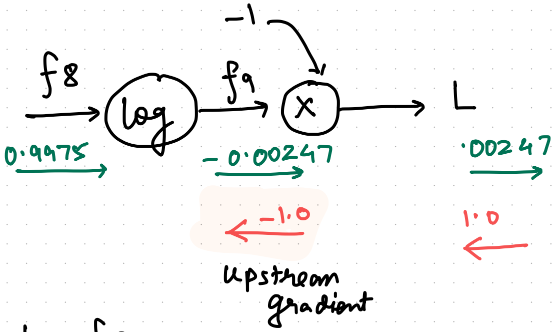
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



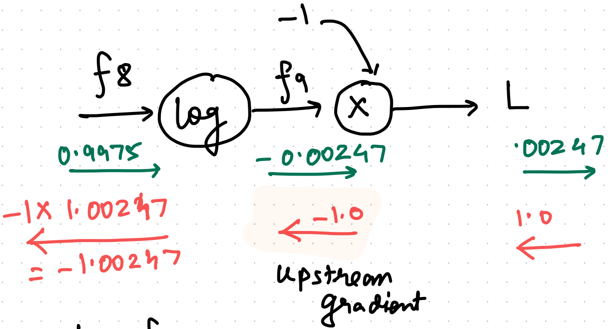
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



$$f9 = \log f8$$

$$\frac{\partial f9}{\partial f8} = \frac{1}{f8} = \frac{1}{.9975} = 1.00247 = \text{Local gradient}$$

$$\text{Loss} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



$$f9 = \log f8$$

$$\frac{\partial f9}{\partial f8} = \frac{1}{f8} = \frac{1}{.9975} = 1.00247 = \text{local gradient}$$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$

$$f_7 \longrightarrow \frac{1}{x} \longrightarrow f_8 \;\cdots\cdots$$

$$\xrightarrow[1.00247]{} \qquad\qquad \xrightarrow{0.9975}$$

$$\xleftarrow[-1.00247]{}$$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1 + e^{-(\theta_0 + \theta_1 x_1 + \theta_2 x_2)}} \right)$$

$$f_7 \xrightarrow[1.00247]{} \boxed{\frac{1}{x}} \xrightarrow[]{0.9975} f_8 \; \ldots\ldots$$

$\xleftarrow[-1.00247]{}$ upstream gradient

$$f_8 = \frac{1}{f_7} \qquad \frac{\partial f_8}{\partial f_7} = \frac{-1}{f_7^{\,2}} = -0.9951$$

$= \text{Local gradient}$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$

$$f_7 \longrightarrow \boxed{\tfrac{1}{x}} \longrightarrow f_8 \;\cdots\cdots$$

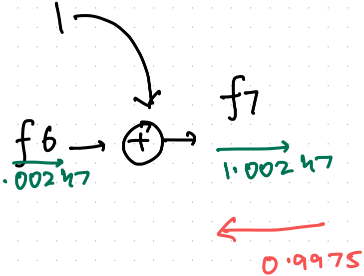
$\longrightarrow$ 1.00247 $\qquad\qquad$ 0.9975 $\longrightarrow$

$\longleftarrow$ $-0.9951 * -1.00247 = 0.9975$ $\qquad\qquad$ $\longleftarrow$ -1.00247 upstream gradient

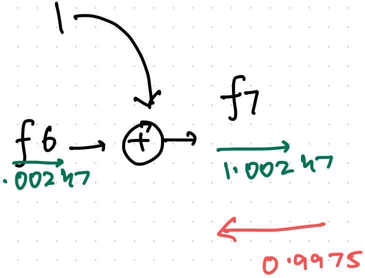
$$f_8 = \frac{1}{f_7} \qquad \frac{\partial f_8}{\partial f_7} = \frac{-1}{f_7^{\,2}} = -0.9951$$

$= $ Local gradient

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}} \right)$$



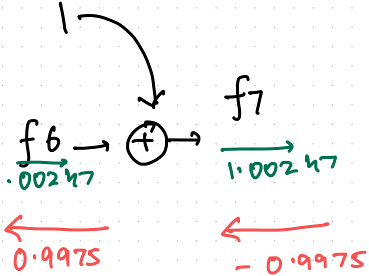
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



upstream grad. = 0.9975

local grad. = 1

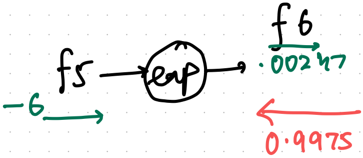
$$\text{Loss} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



upstream grad. = 0.9975

local grad. = 1

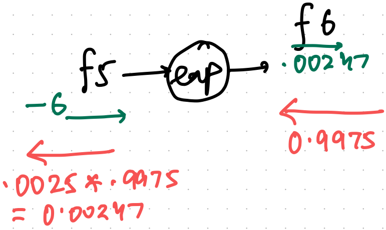
$$\text{LOSS} = -1*\log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



upstream grad. = 0.9975

$$\text{local grad.} = \frac{\partial f_6}{\partial f_5} = \frac{\partial e^{f_5}}{\partial f_5} = e^{f_5} = e^{-6} = 0.0025$$

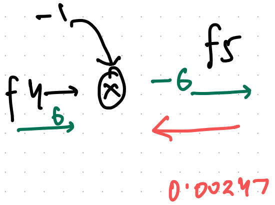
$$\text{Loss} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



upstream grad. = 0.9975

local grad. $= \dfrac{\partial f_6}{\partial f_5} = \dfrac{\partial e^{f_5}}{\partial f_5} = e^{f_5} = e^{-6} = 0.0025$

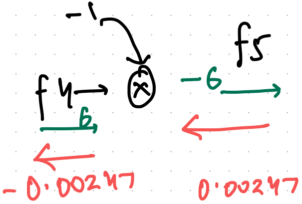
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



upstream grad. = 0.00247

local grad. = -1

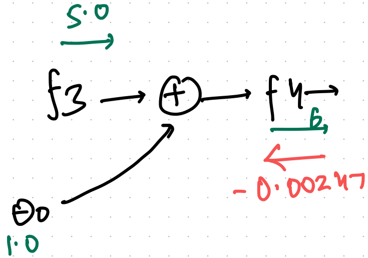
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



upstream grad. = 0·00247

local grad. = -1

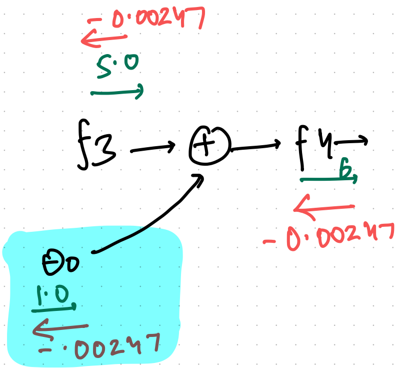
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



upstream grad. $= -0.00247$

local grad. $(\theta_0) = \dfrac{\partial f_4}{\partial \theta_0} = 1$; local grad for $f_3 = 1$

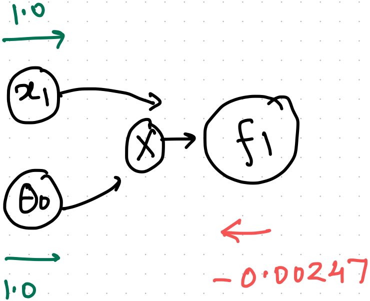
$$LOSS = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}} \right)$$



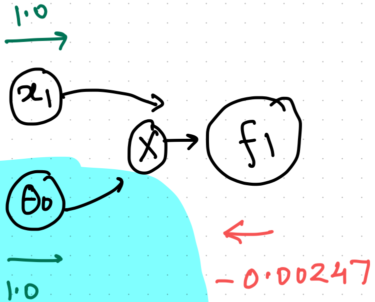
upstream grad. $= -0.00247$

local grad. $(\theta_0) = \frac{\partial f_4}{\partial \theta_0} = 1$; local grad for $f_3 = 1$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



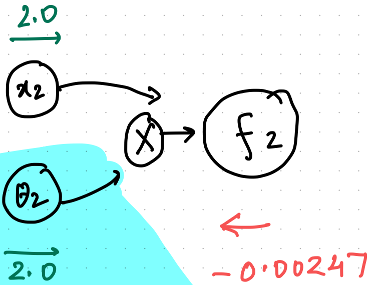
$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



$-0.00247 * x_1$ (1.0)

$= -.00247$

$$\text{LOSS} = -1 * \log\left(\frac{1}{1+e^{-(\theta_0+\theta_1 x_1+\theta_2 x_2)}}\right)$$



$$= -.00247 * \underset{(2.0)}{x_2}$$

$$= -.0049$$

What autodiff library needs to know

(i) $f = a * b$; $\frac{\partial f}{\partial a} = b$; $\frac{\partial f}{\partial b} = a$

(ii) $f = a + b$; $\frac{\partial f}{\partial a} = \frac{\partial f}{\partial b} = 1$

(iii) $f = e^a$; $\frac{\partial f}{\partial a} = e^a$

(iv) $f = \frac{1}{a}$; $\frac{\partial f}{\partial a} = -1/a^2$

$\vdots$