Automatic Differentiation

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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

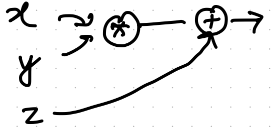
* Nodes : operations $(+, *, \ldots)$
* Edges : variables | Tensors

Computational Graphs

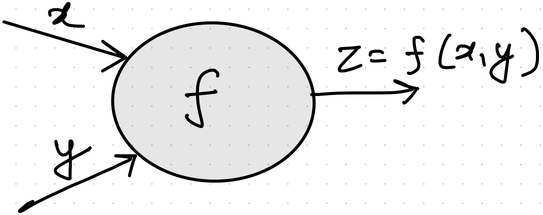
* Nodes : operations (+, *, ...)

* Edges : variables | Tensors
  (and data dependencies)

Example : $(x * y) + z$



Back Prop Through Computational Graph



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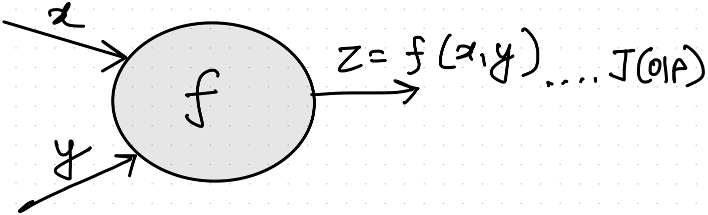

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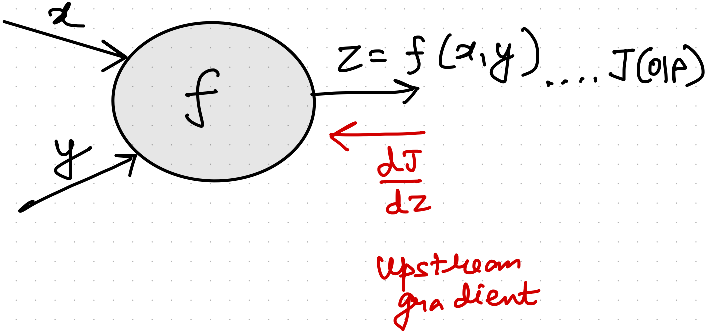
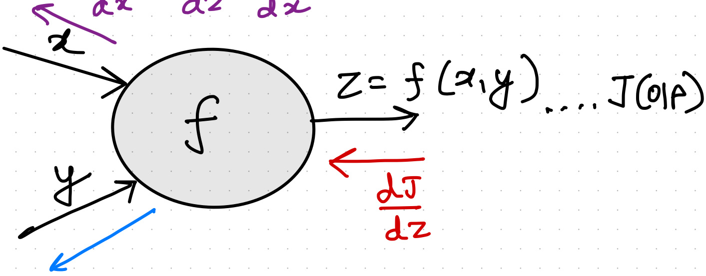


Back Prop Through Computational Graph

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



Upstream gradient

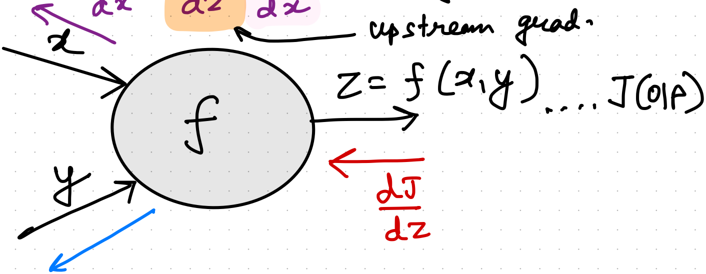
$$\frac{dJ}{dy} = \frac{dJ}{dz} \cdot \frac{dz}{dy}$$

Back Prop Through Computational Graph

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

← Local grad.

upstream grad.



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Back Prop Through Computational Graph

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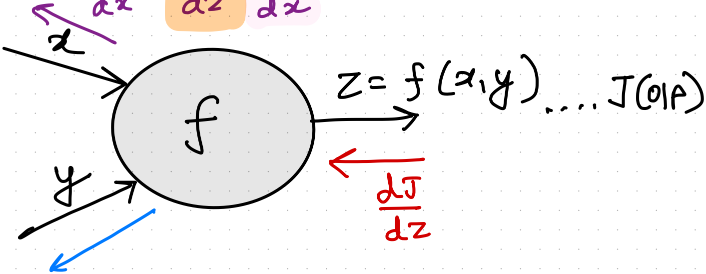

upstream gradient

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

$$\boxed{\text{DOWNSTREAM GRADIENT} = \text{UPSTREAM GRADIENT} * \text{LOCAL GRADIENT}}$$

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

$$y = 1$$

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

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

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

$$\begin{tikzcd} \theta_1 \arrow[dr] & \\ & \times \\ x_1 \arrow[ur] & \end{tikzcd}$$

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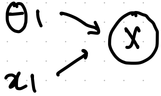

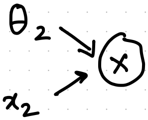

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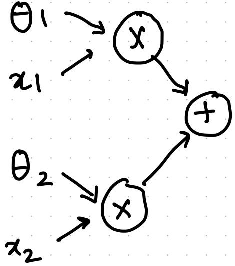

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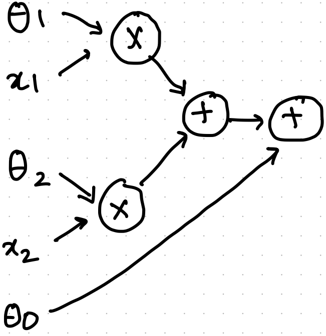

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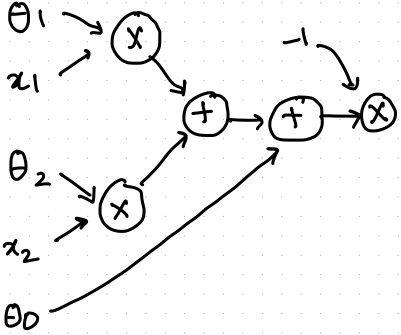

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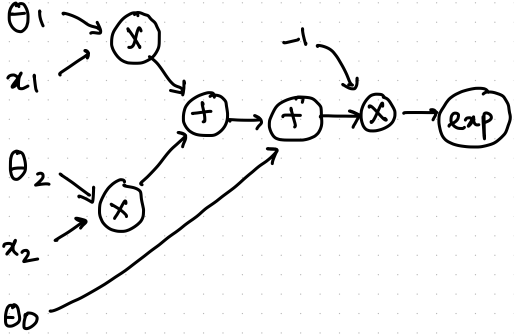

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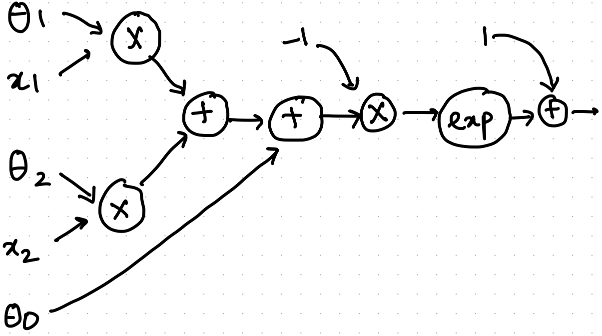

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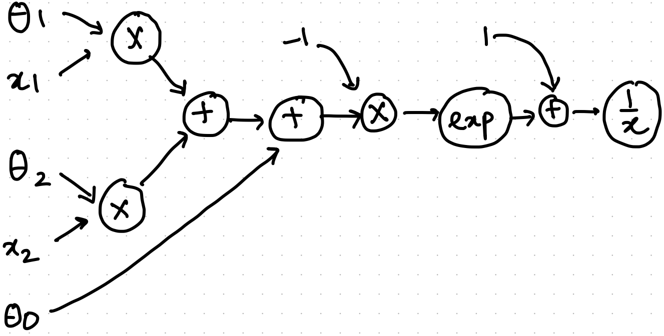

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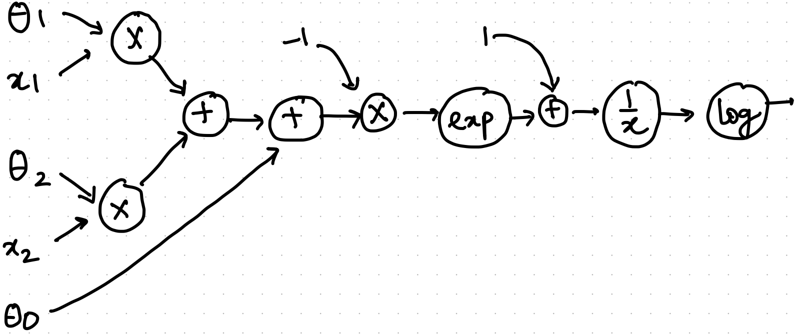

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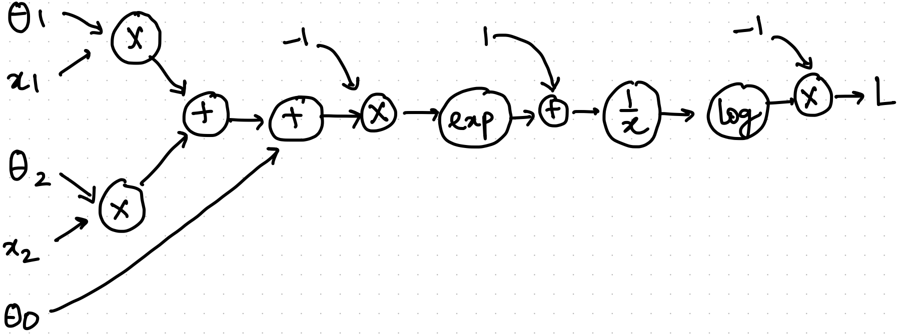

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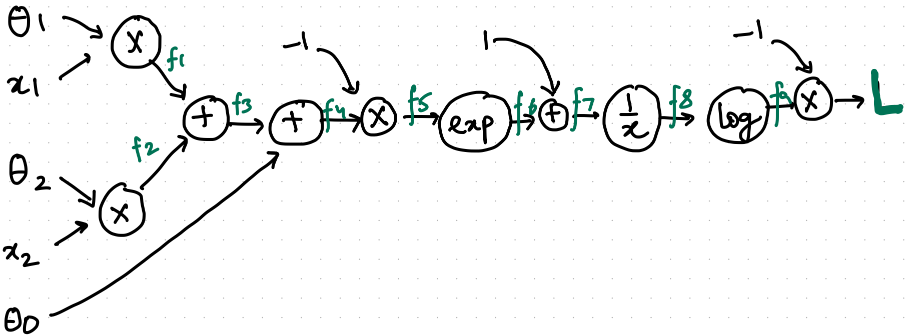

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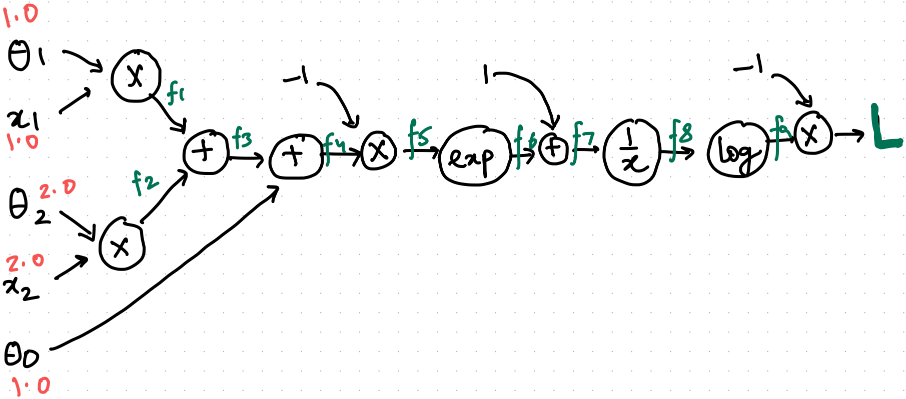

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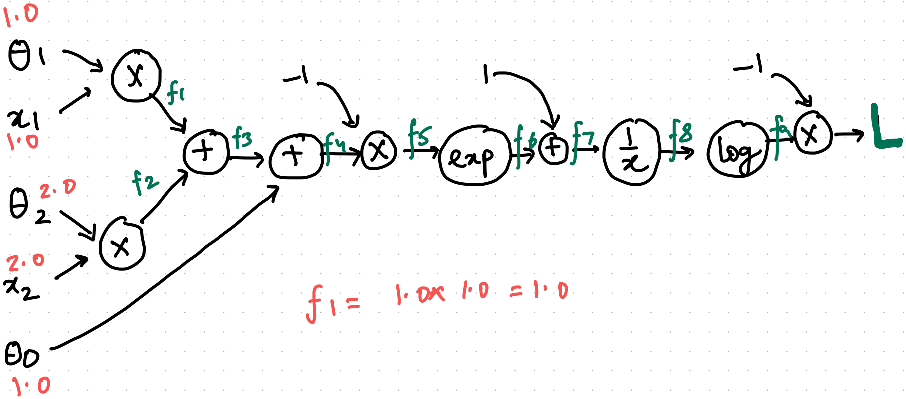
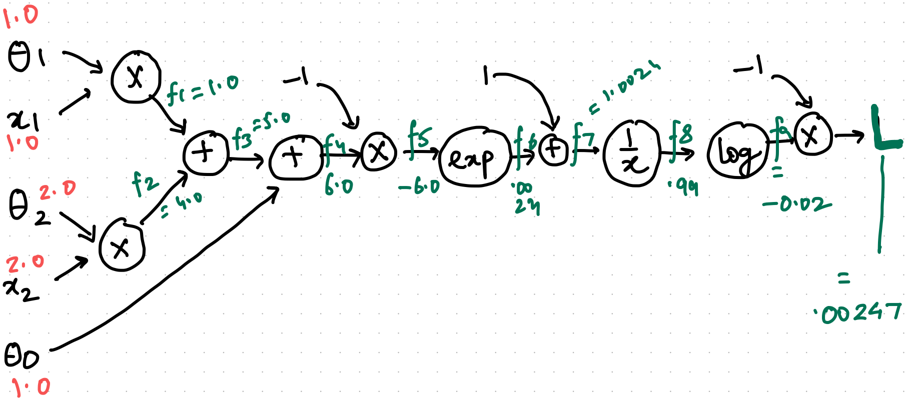


$f_1 = 1.0 \times 1.0 = 1.0$

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



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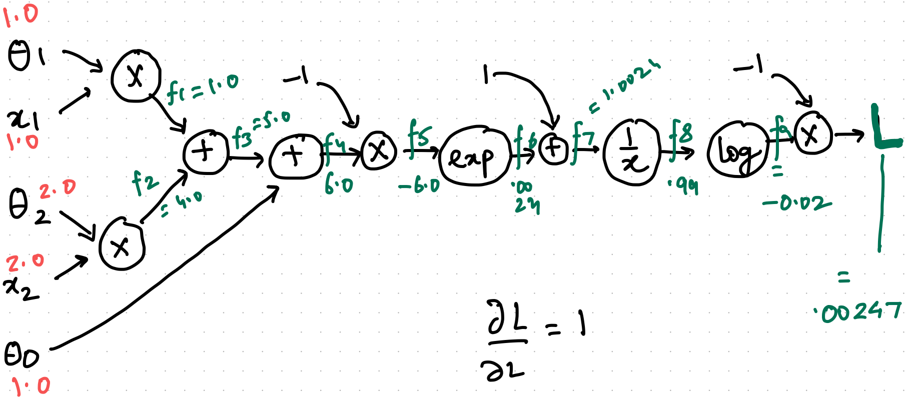
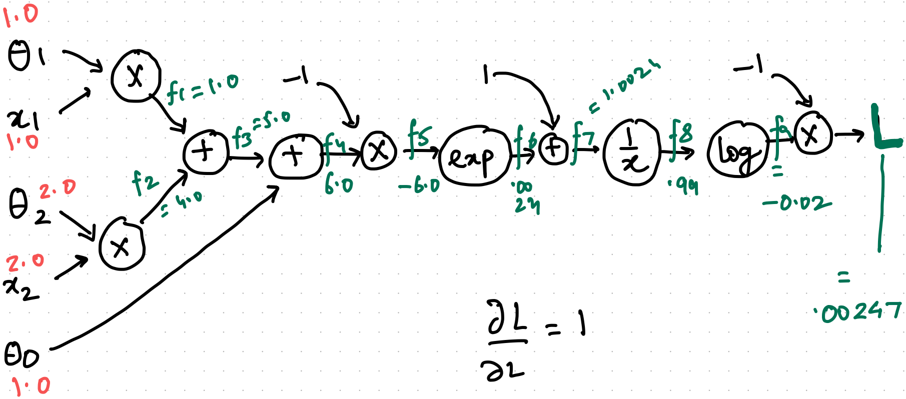


$$\frac{\partial L}{\partial L} = 1$$

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



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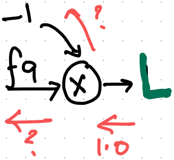

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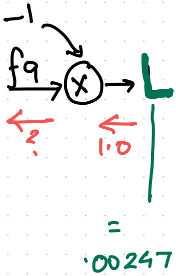

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upstream gradient = 1.0

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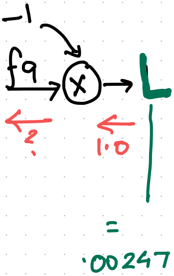

$$\frac{\partial L}{\partial L} = 1$$

upstream gradient = 1.0

$$L = fq * -1$$

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

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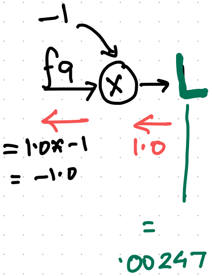

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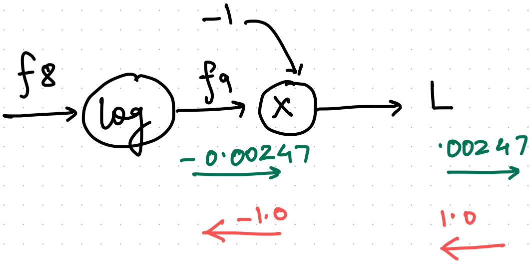

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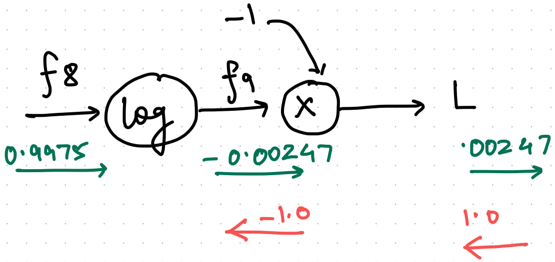

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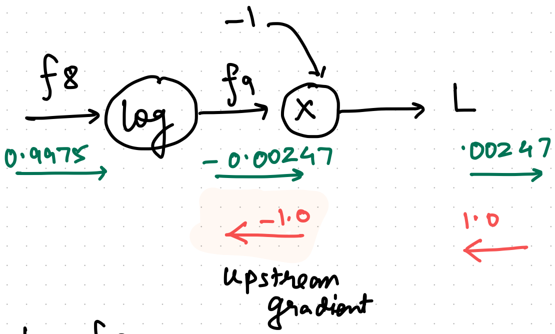
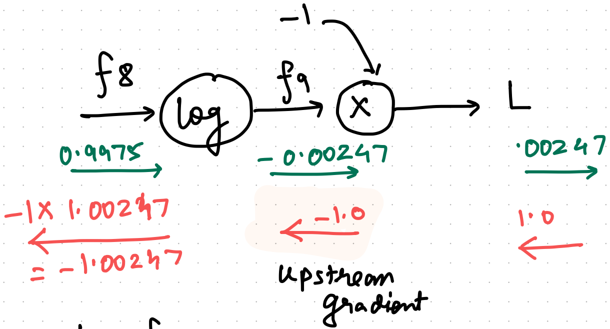


$$f9 = \log f8$$

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

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



$$f_9 = \log f_8$$

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$$f7 \longrightarrow \frac{1}{x} \longrightarrow f8 \cdots\cdots$$

$\xrightarrow{\hspace{2em}}$ 1.00247

0.9975 $\xrightarrow{\hspace{2em}}$

$\xleftarrow{\hspace{2em}}$ −1.00247

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

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

$\xrightarrow{}$ 1.00247

0.9975 $\xrightarrow{}$

$\xleftarrow{}$ −1.00247 upstream gradient

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

$= \text{Local gradient}$

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

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

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

$\xleftarrow{}$ $-0.9951 * -1.00247$ $= 0.9975$ $\qquad\qquad$ $\xleftarrow{}$ -1.00247 upstream gradient

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

= Local gradient

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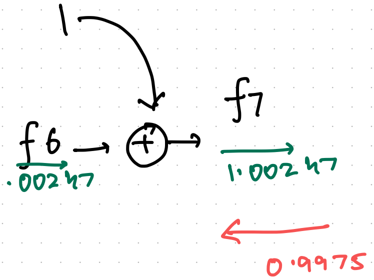

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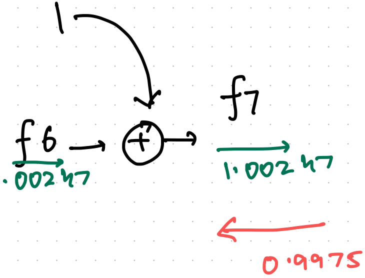
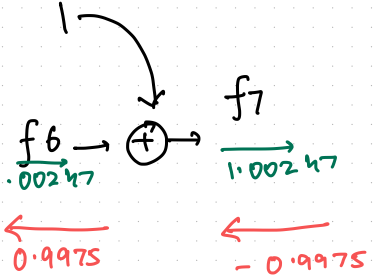


upstream grad. = 0.9975

local grad. = 1

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



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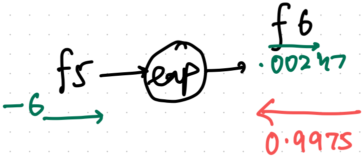
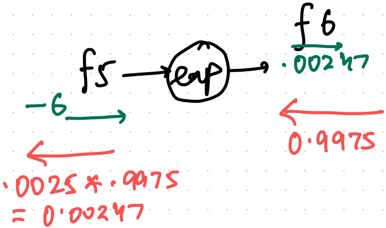


upstream grad. $= 0.9975$

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

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



upstream grad. = 0.9975

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

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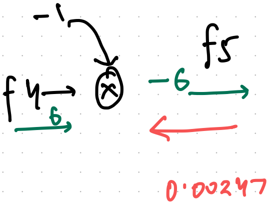
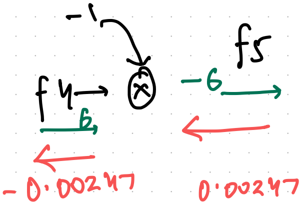


upstream grad. = 0.00247

local grad. = -1

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



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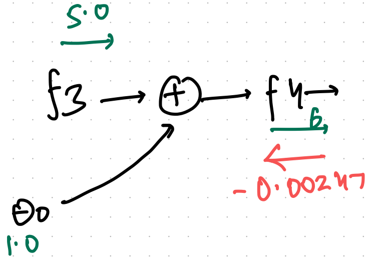
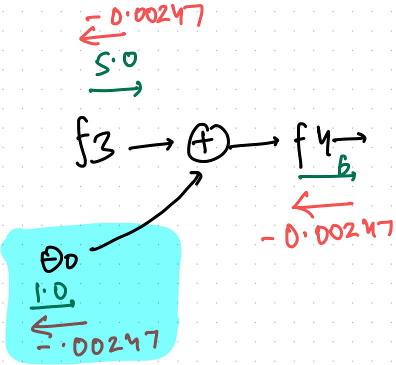


upstream grad. $= -0.00247$

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

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



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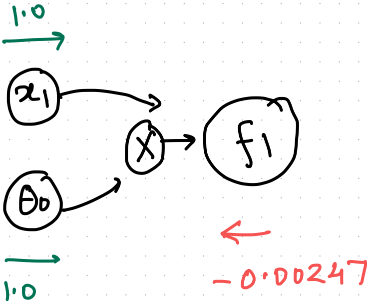

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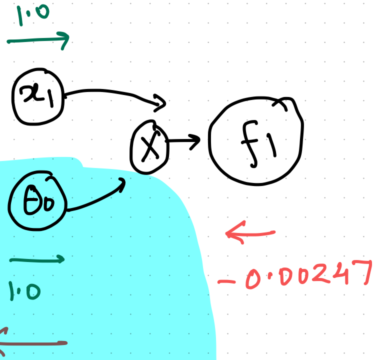

$-0.00247 * x_1$ (1.0)

$= -.00247$

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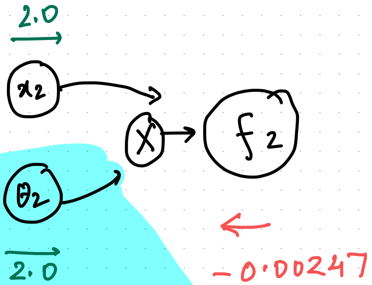


$$= -.00247 * \underset{(2.0)}{x_2}$$

$$= -.0049$$

What autodiff library needs to know

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

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

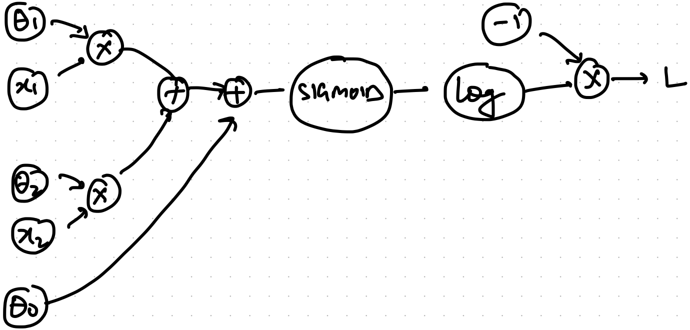
(iii) $f = e^a$; $\frac{\partial f}{\partial a} = e^a$

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

$\vdots$

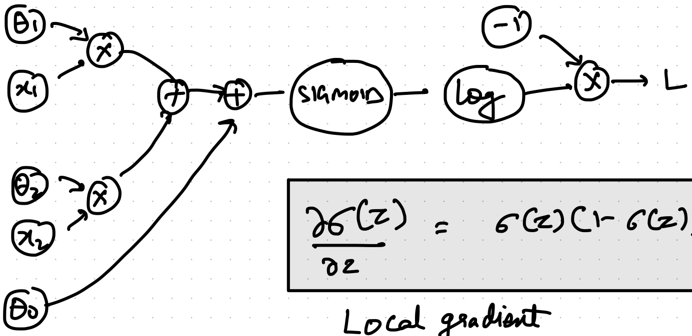
Simplifying computat^n graph

$$L = -1 * \log(\text{SIGMOID}(\theta_0+\theta_1 x_1+\theta_2 x))$$



* Simplifying computat^n graph

$$L = -1 * \log(\mathrm{SIGMOID}(\theta_0 + \theta_1 x_1 + \theta_2 x))$$



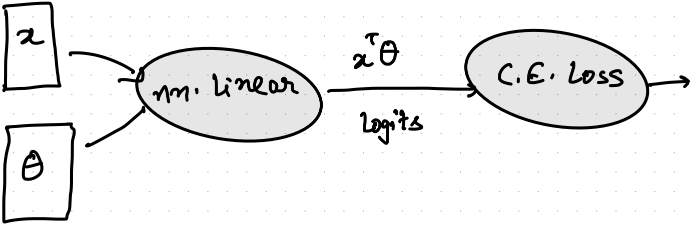
$$\boxed{\frac{\partial \sigma(z)}{\partial z} = \sigma(z)(1 - \sigma(z))}$$

Local gradient

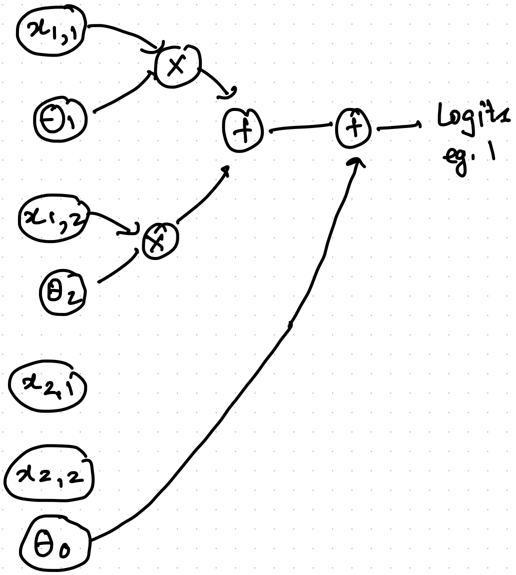
Exercise: show you get same answer as before

* Simplifying computat^n graph

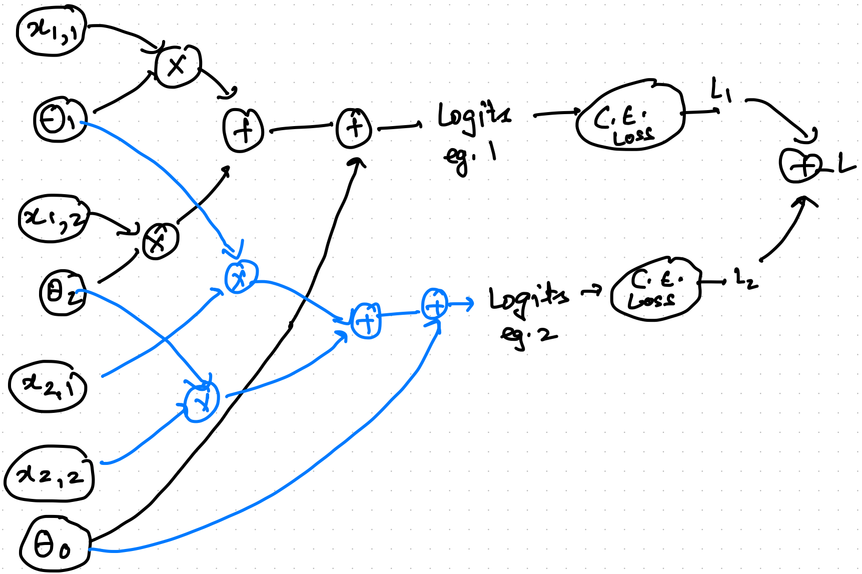
$$L = -1 * \log(\text{SIGMOID}(\theta_0 + \theta_1 x_1 + \theta_2 x))$$



* Training over N- examples



* Training over N-examples



* Training over N- examples

Chain Rule for One Independent Variable

Suppose that $x = g(t)$ and $y = h(t)$ are differentiable functions of t and $z = f(x, y)$ is a differentiable function of x and y. Then $z = f(x(t), y(t))$ is a differentiable function of t and

$$\frac{dz}{dt} = \frac{\partial z}{\partial x} \cdot \frac{dx}{dt} + \frac{\partial z}{\partial y} \cdot \frac{dy}{dt},$$

where the ordinary derivatives are evaluated at t and the partial derivatives are evaluated at (x, y).

* Training over N- examples

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$$L_1 = x_1 \theta$$

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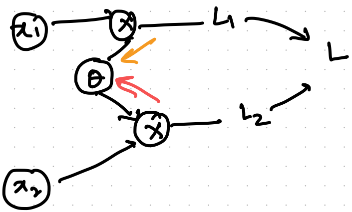

$$\frac{\partial L}{\partial \theta} = \rightarrow + \rightarrow$$

Addition of all incoming gradients