PROPAGAÇÃO RETRÓGRADA

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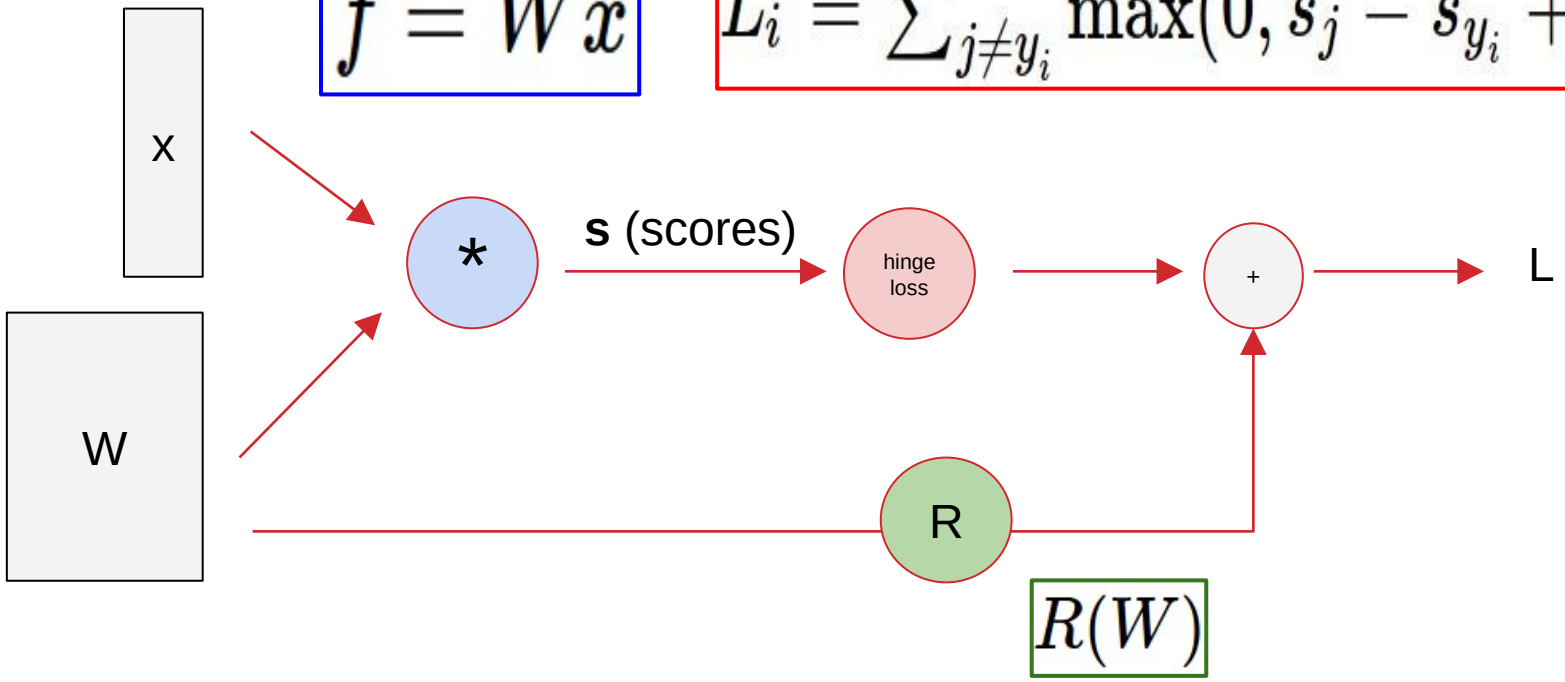
zenilton@pucminas.br

Grafo de Computação da Função de Perda

$$f = Wx$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

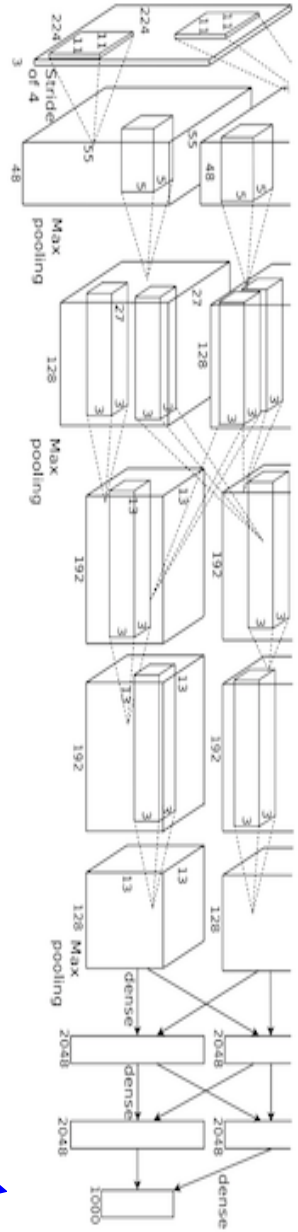


Rede Convolucional (AlexNet)

Imagem de entrada

Pesos

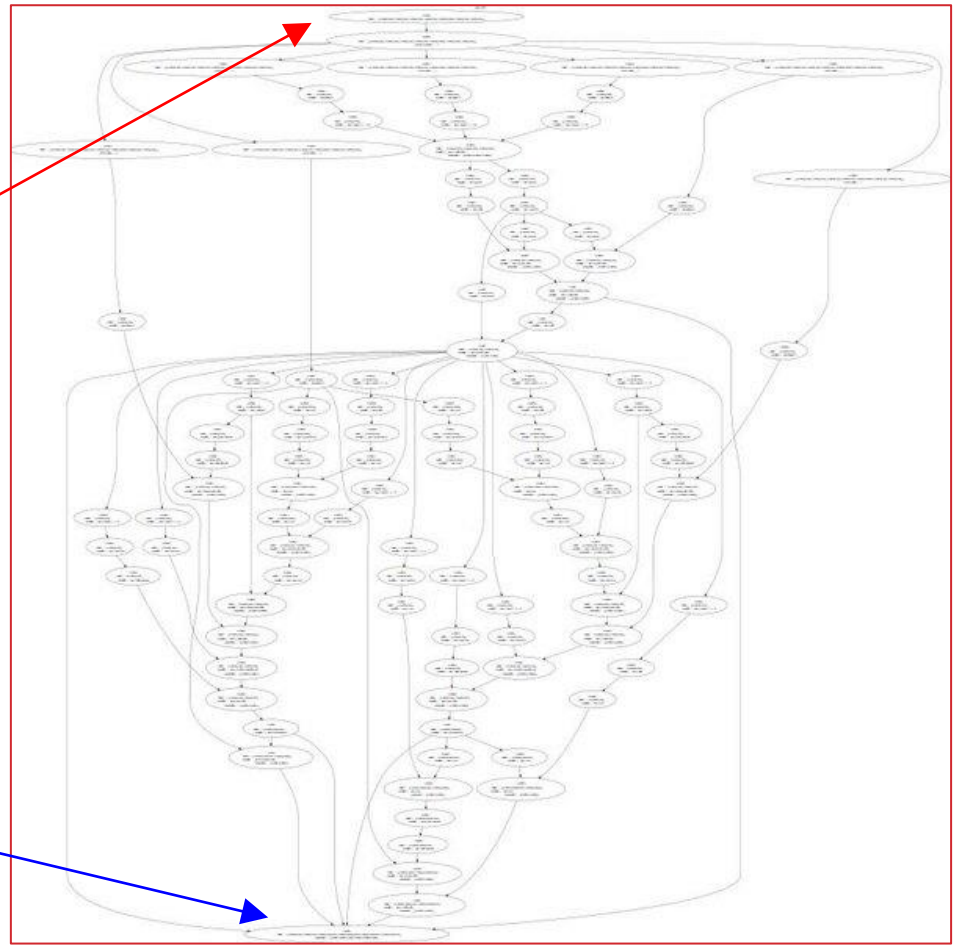
Perda



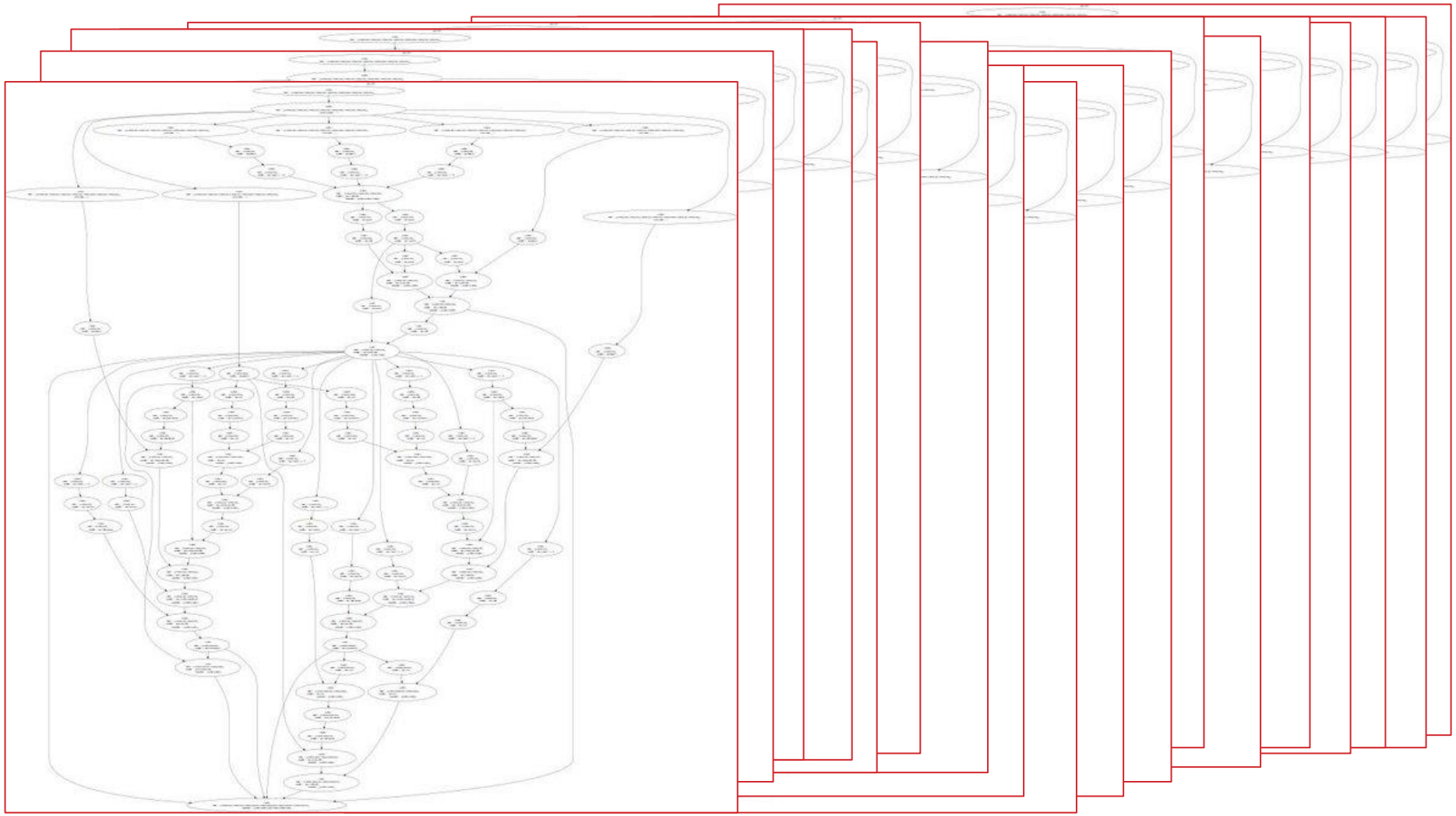
Máquina Neural de Turing

Fita de entrada

Perda

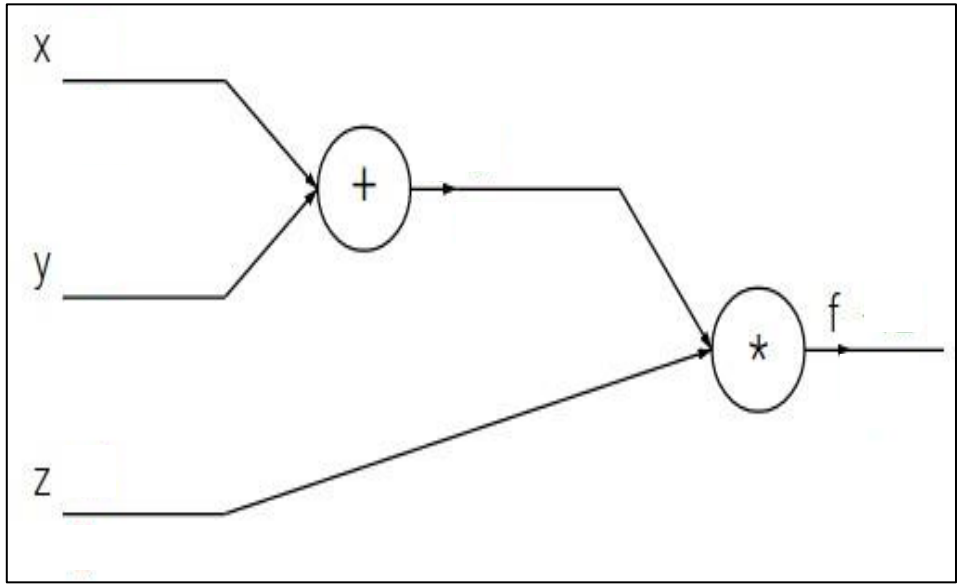


Neural Turing Machine



Diferenciação de um Grafo de Computação

Seja $f(x, y, z) = (x + y) \times z$



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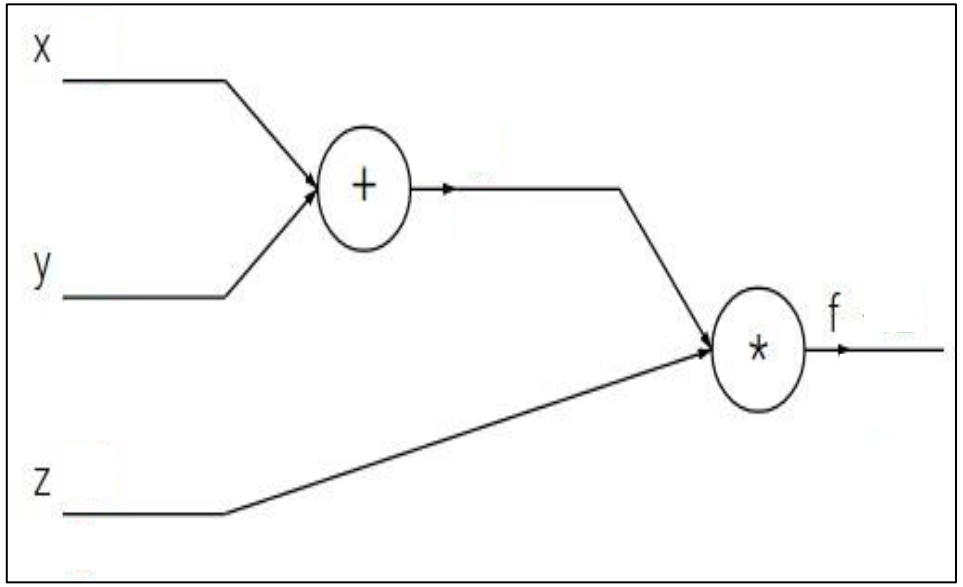

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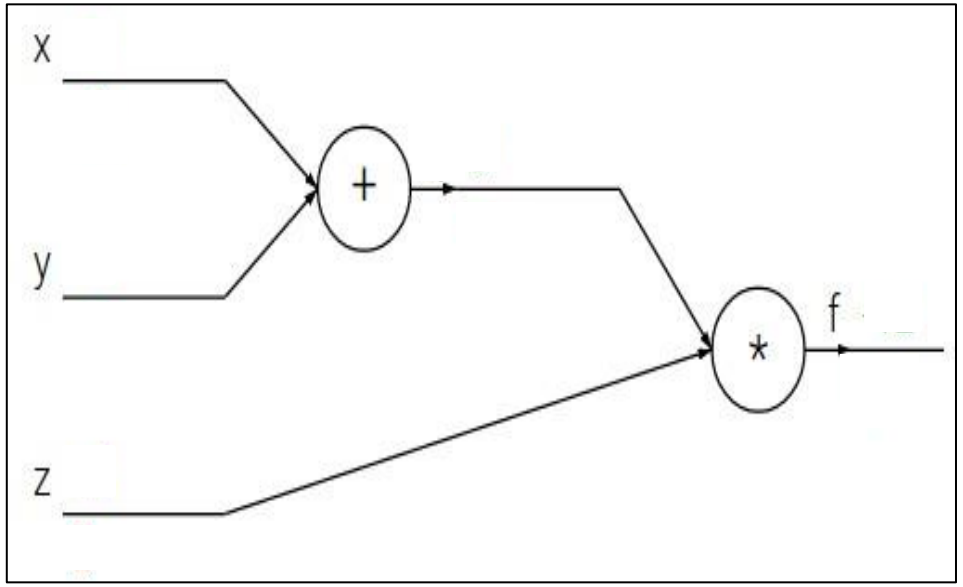

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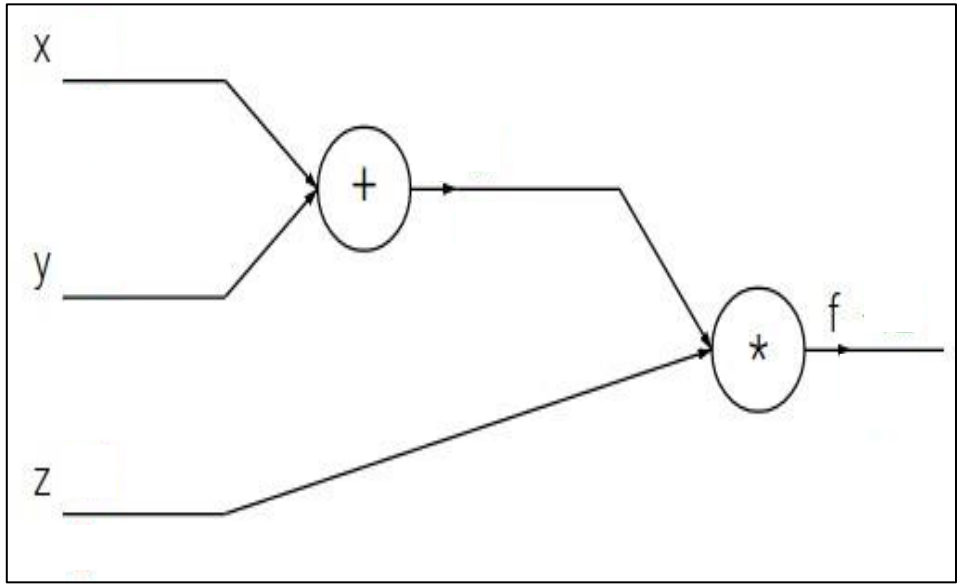

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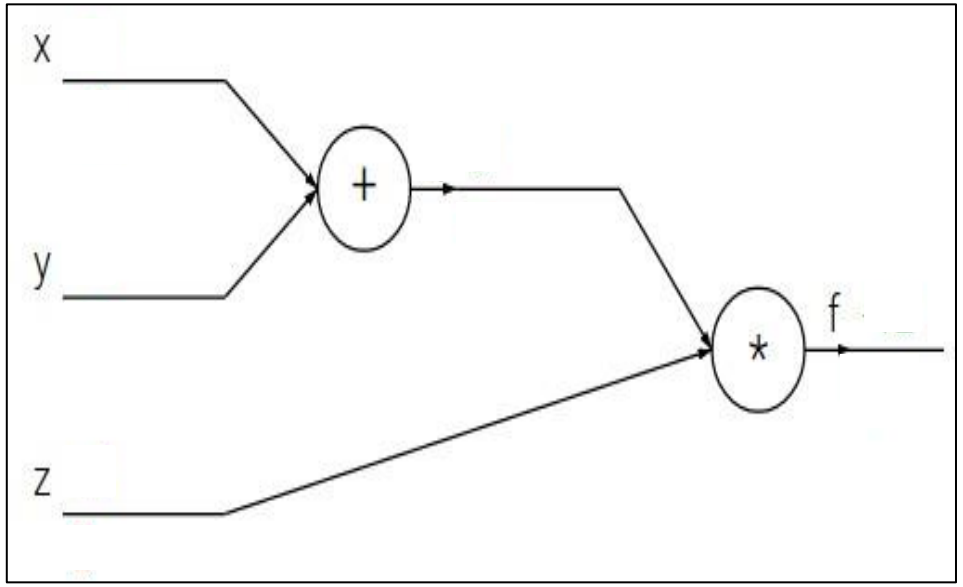

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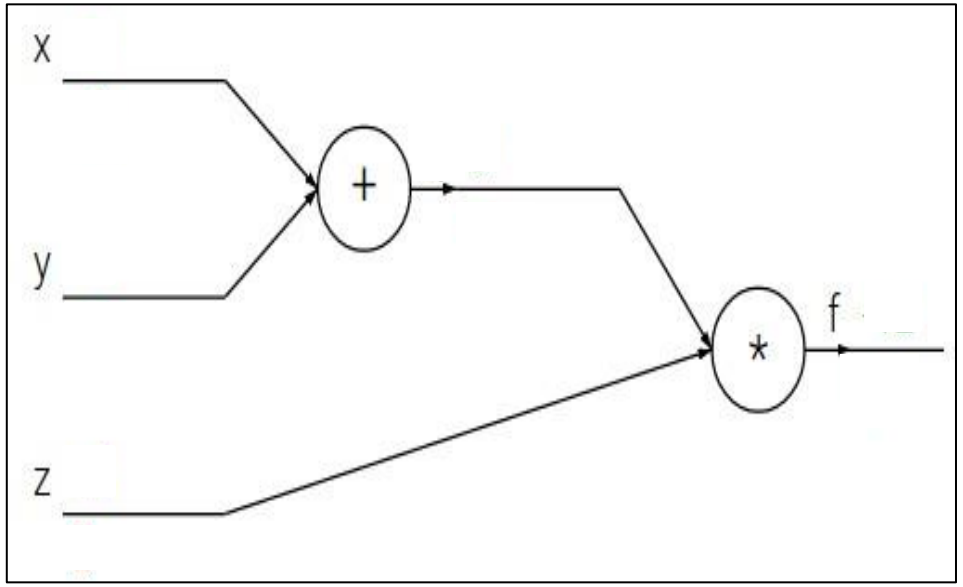

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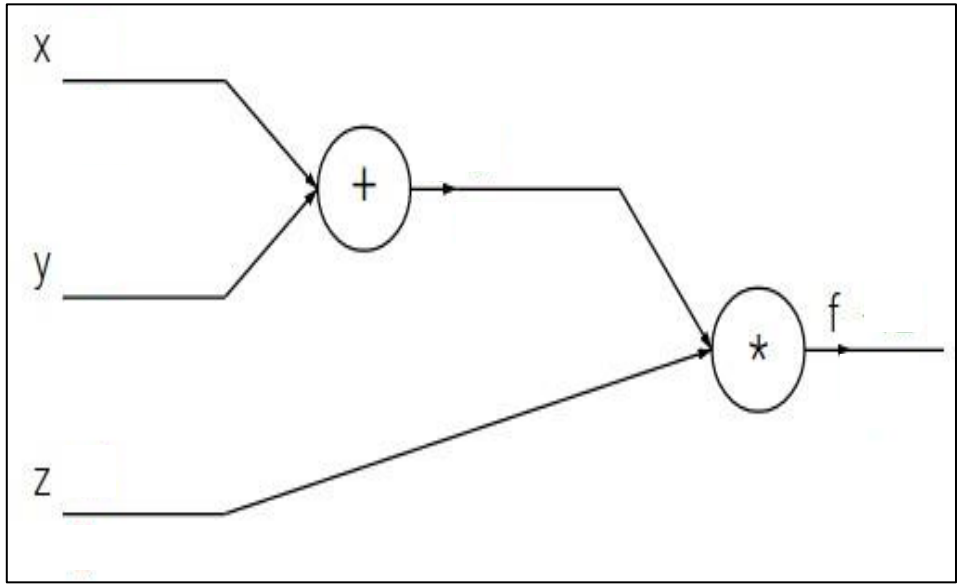

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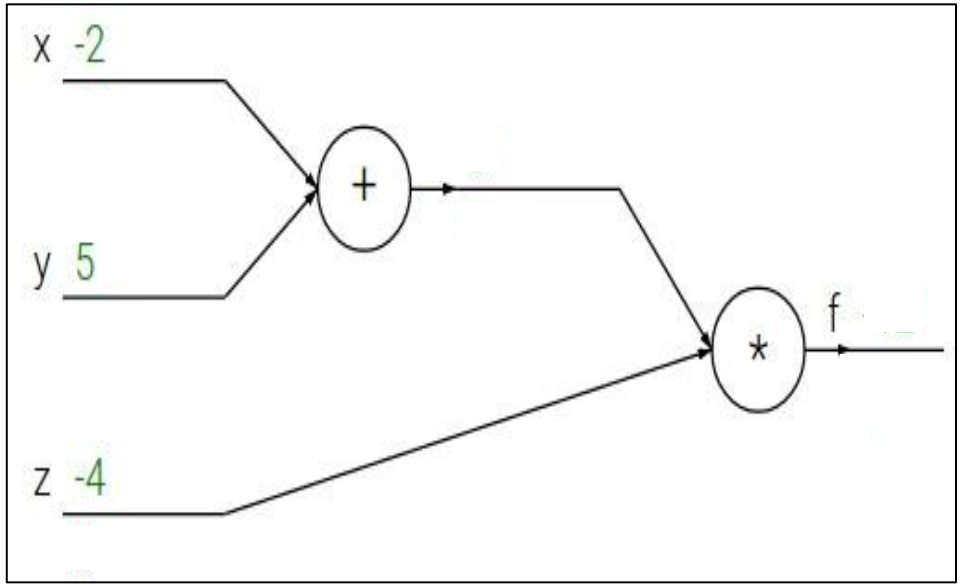

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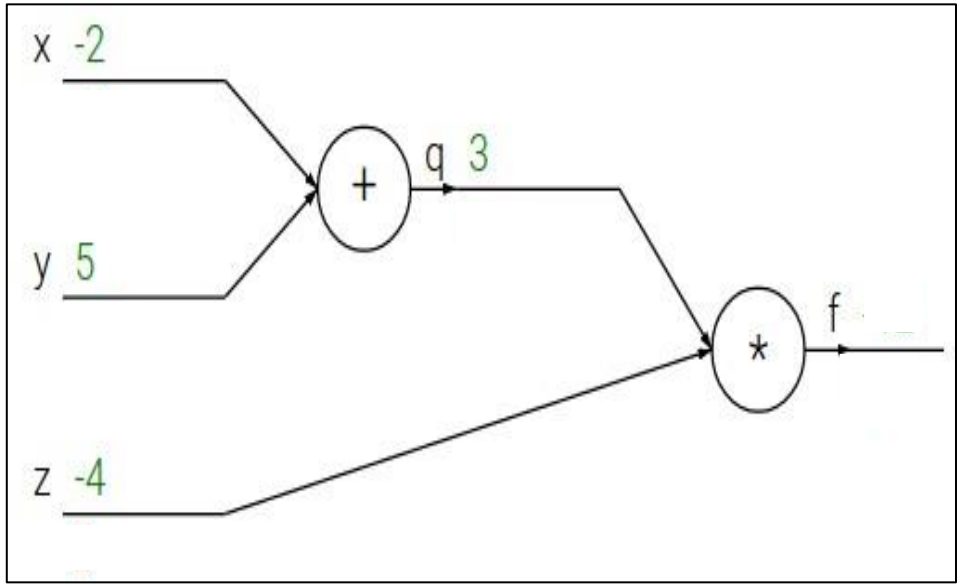

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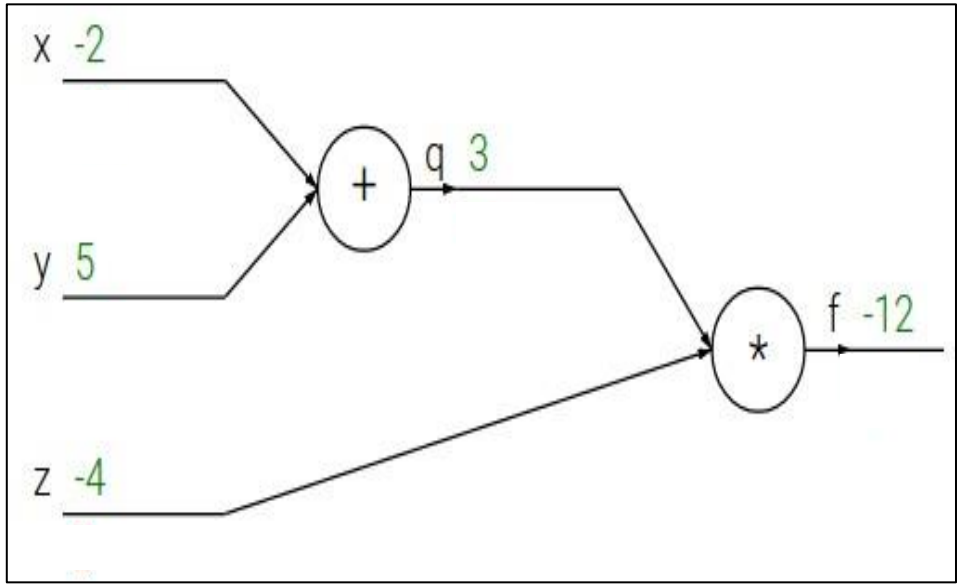

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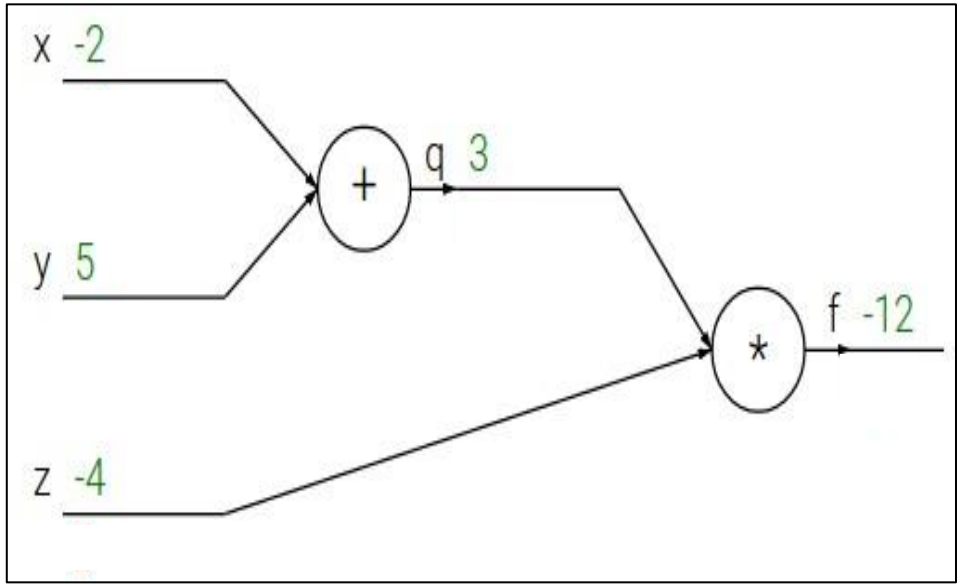

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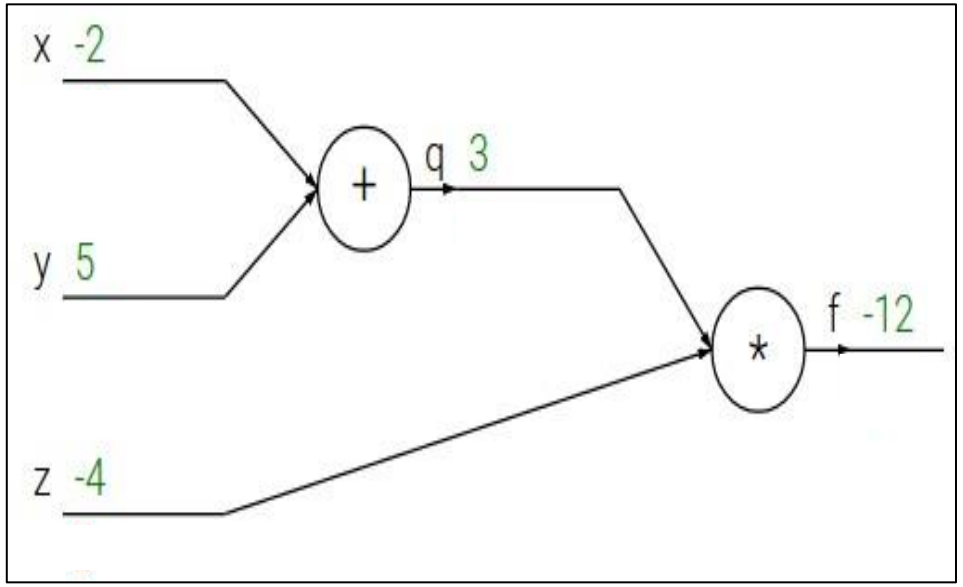

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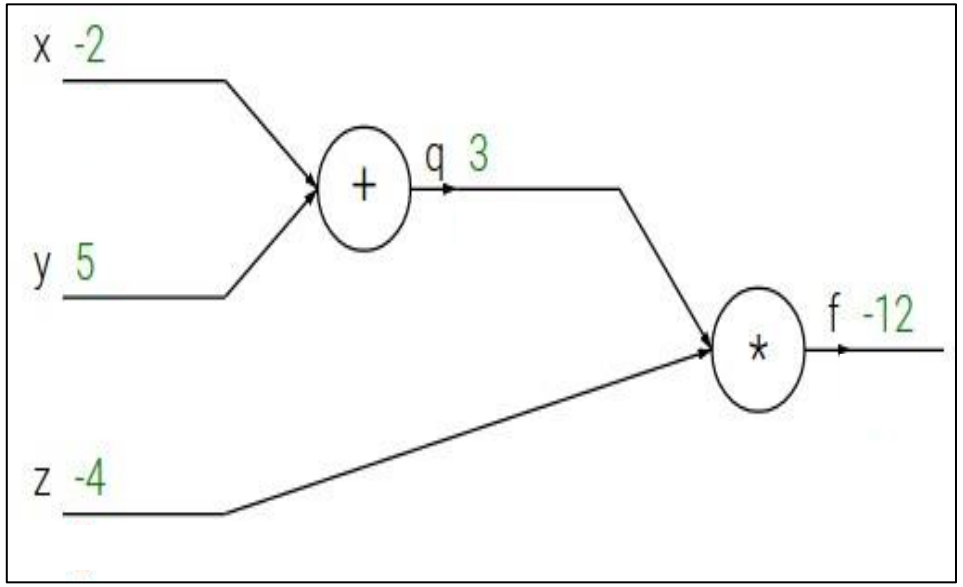

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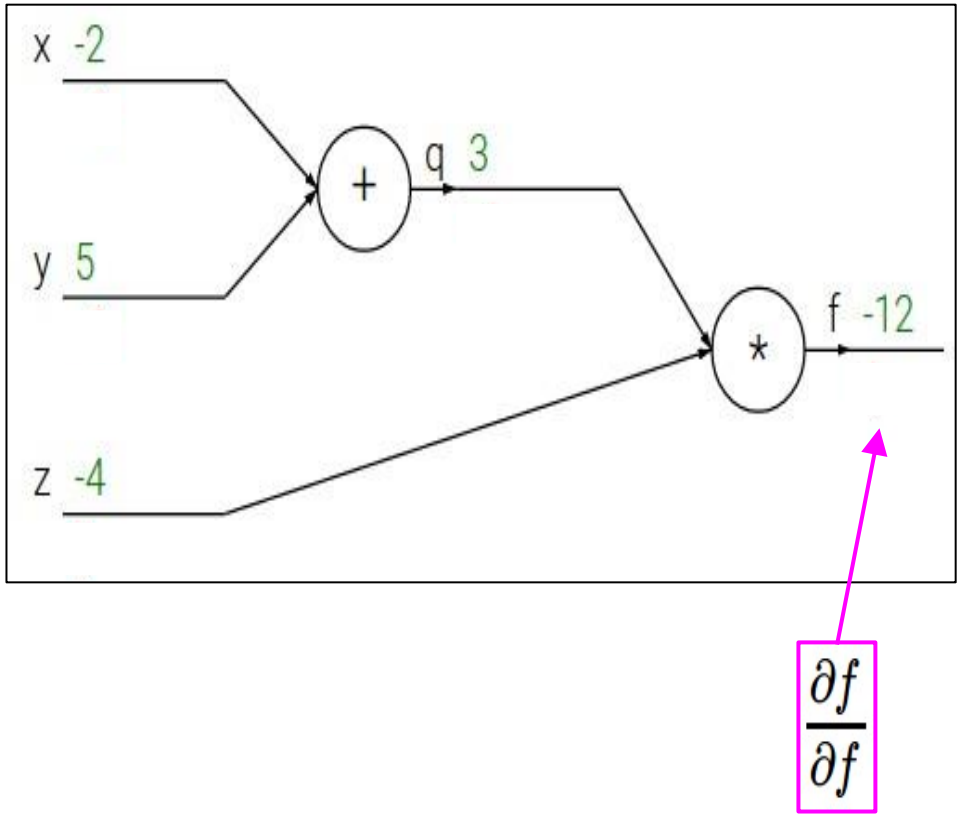

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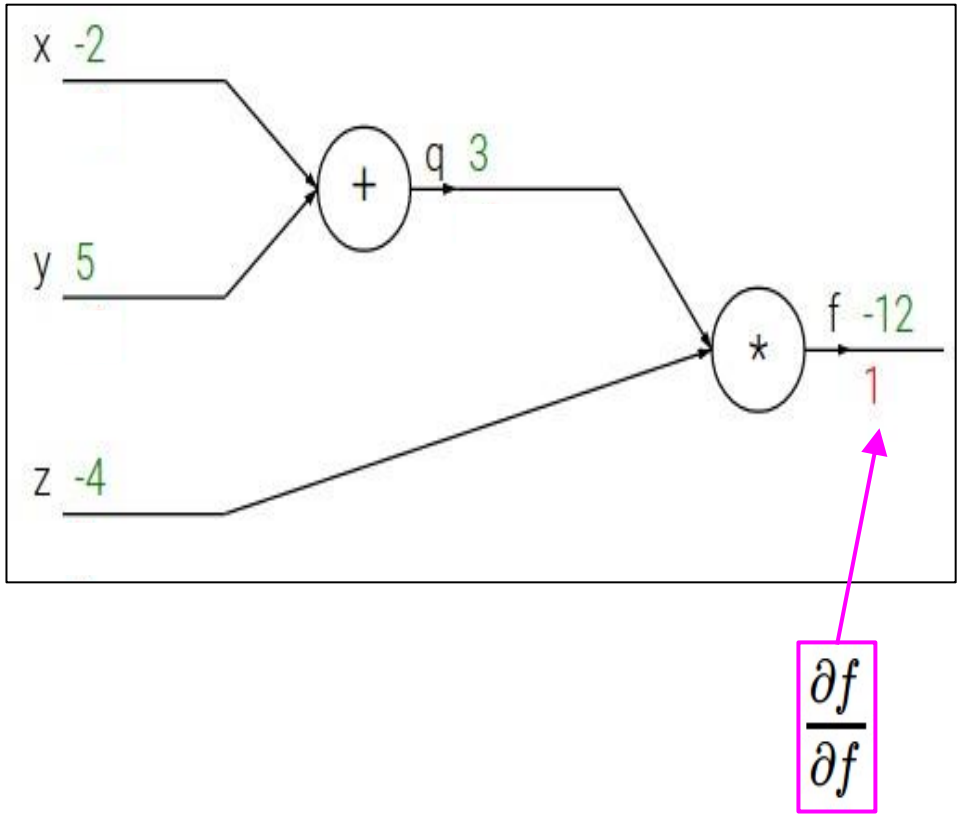

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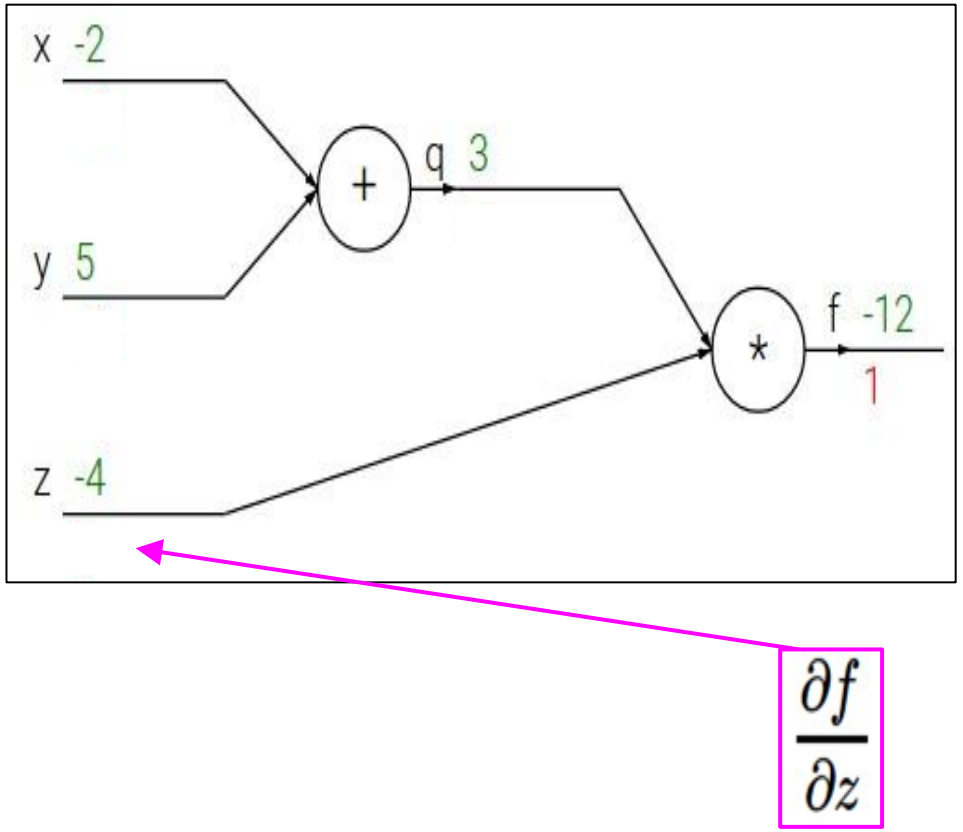

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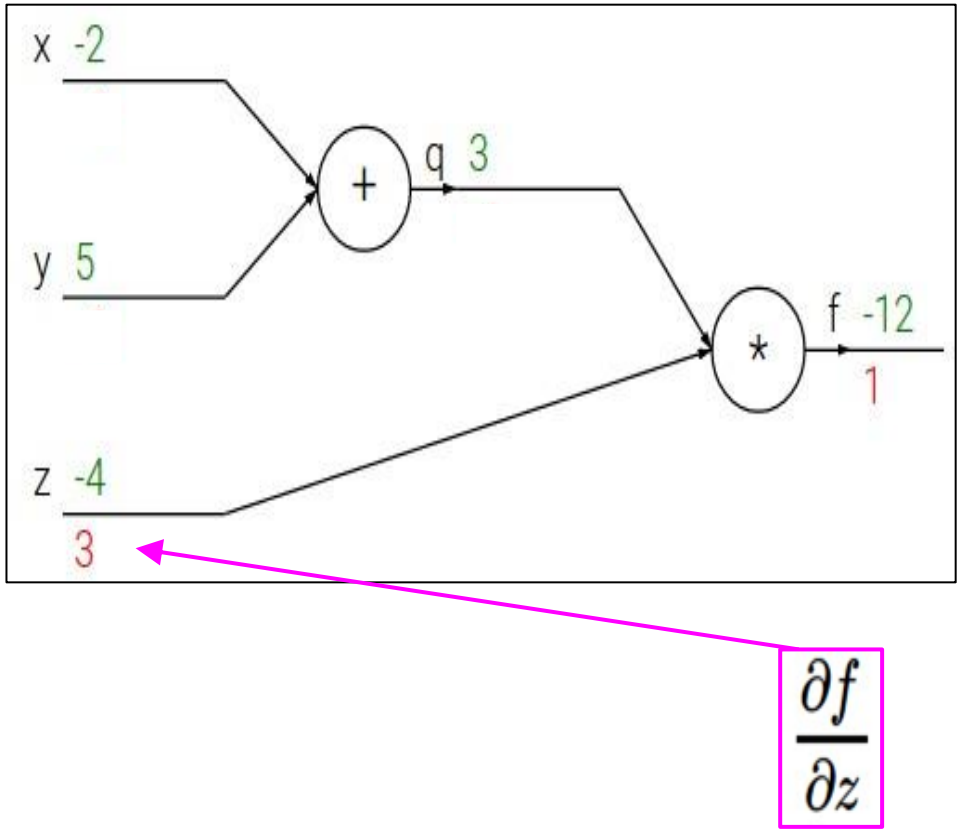

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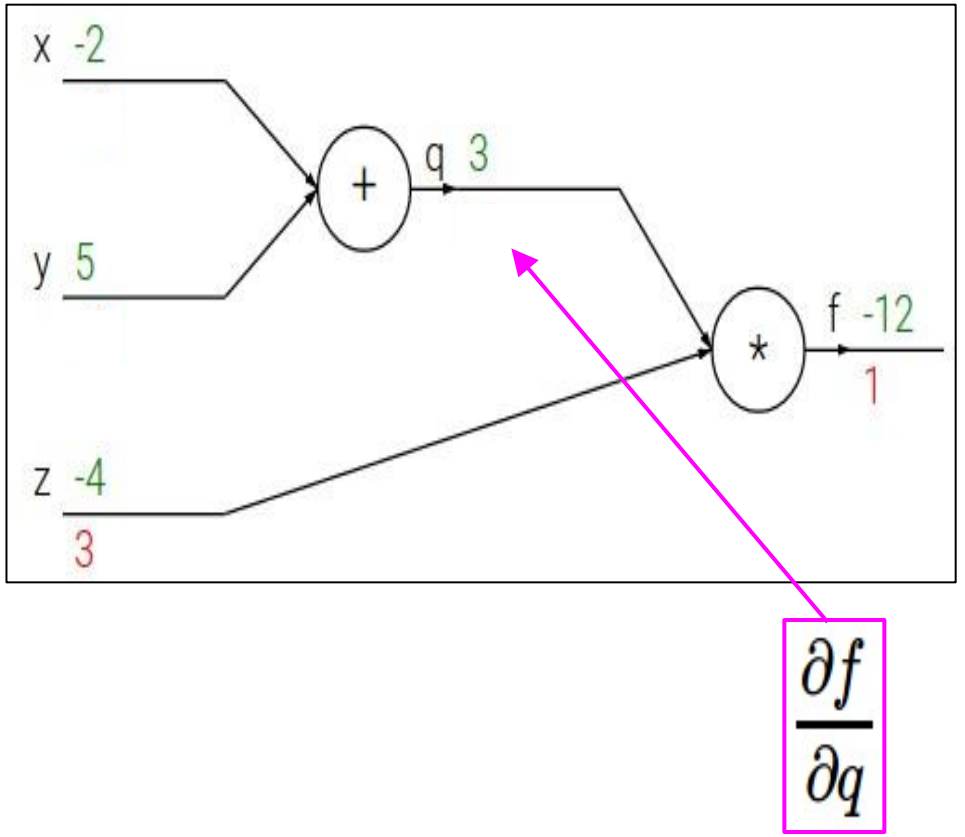

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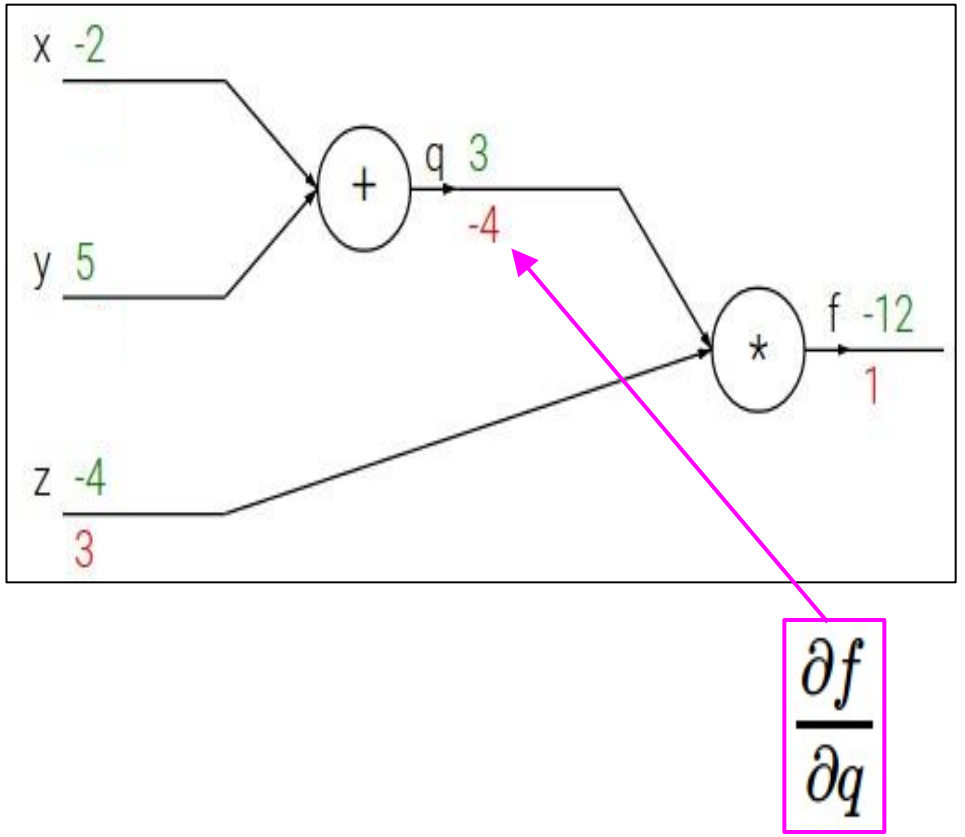

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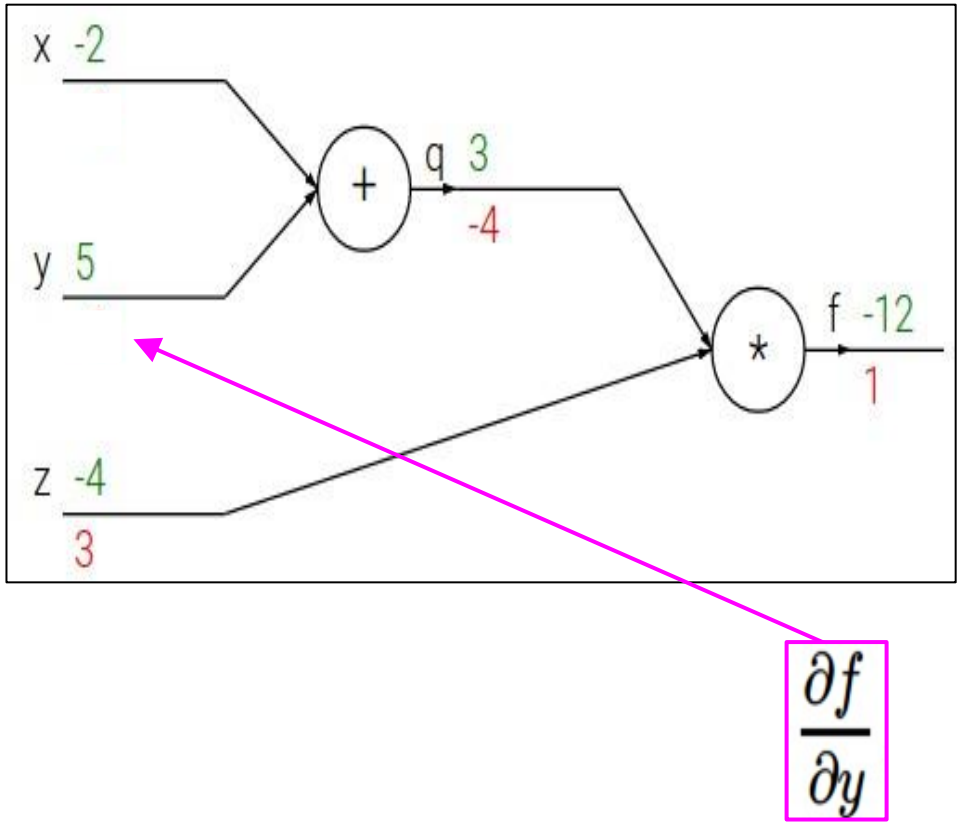

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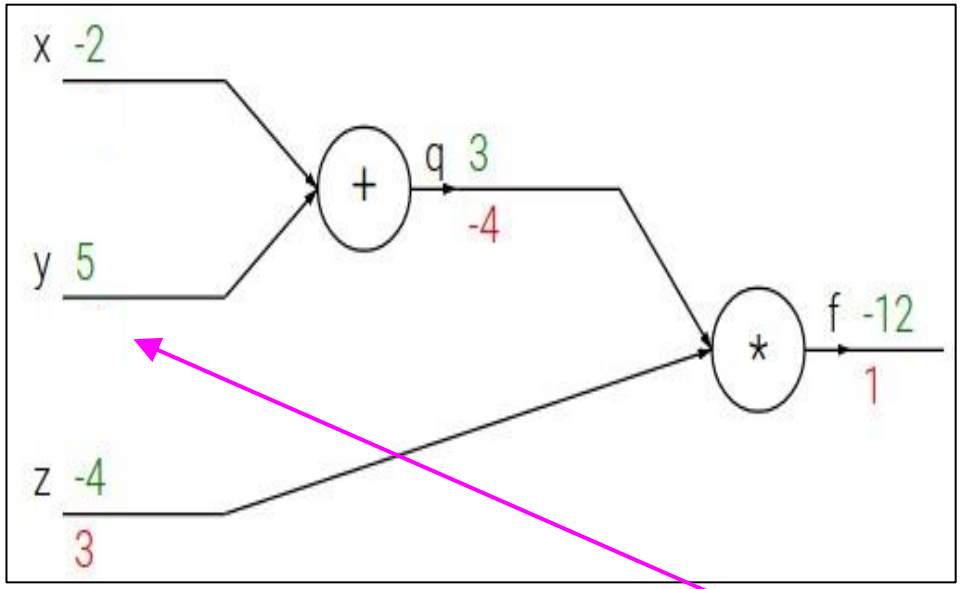

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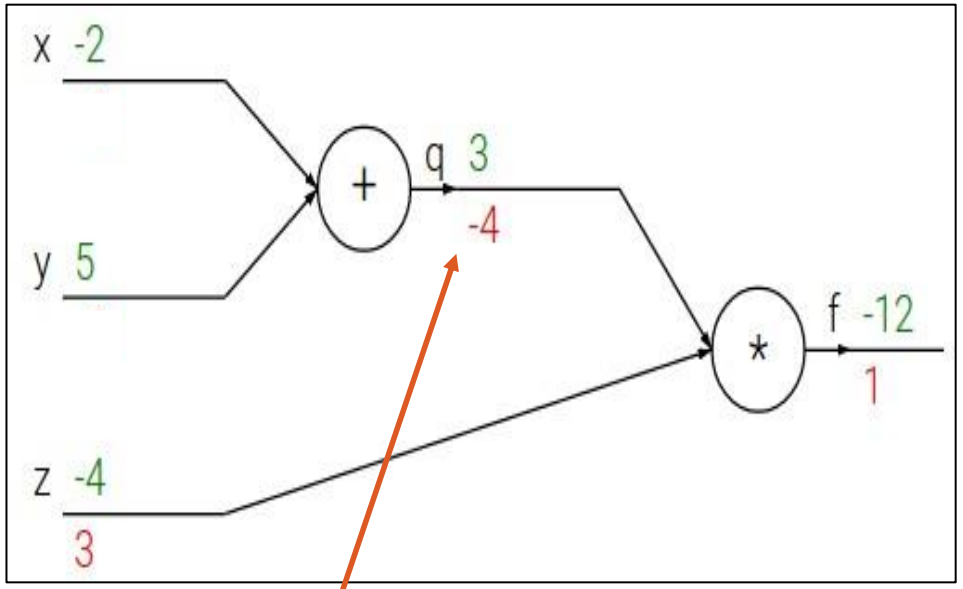

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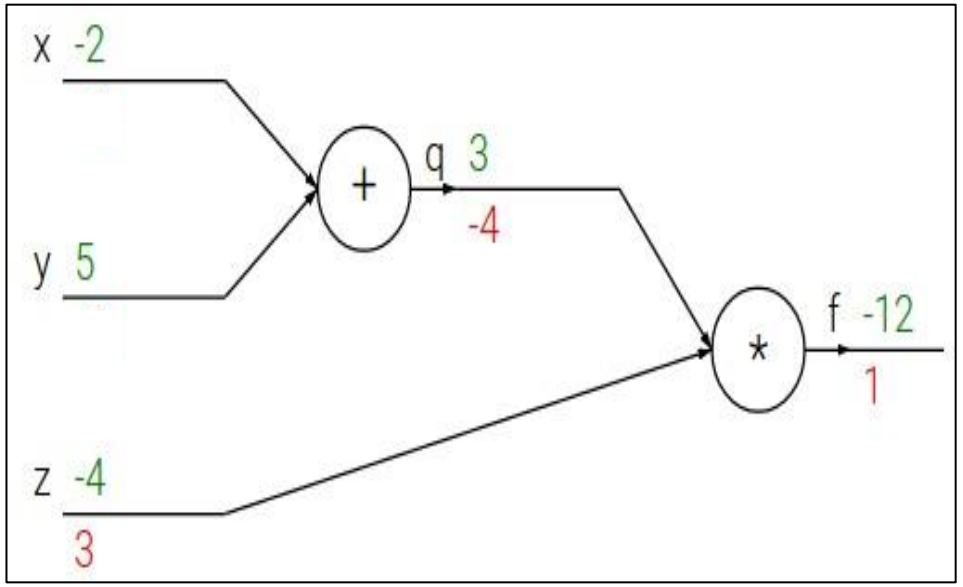

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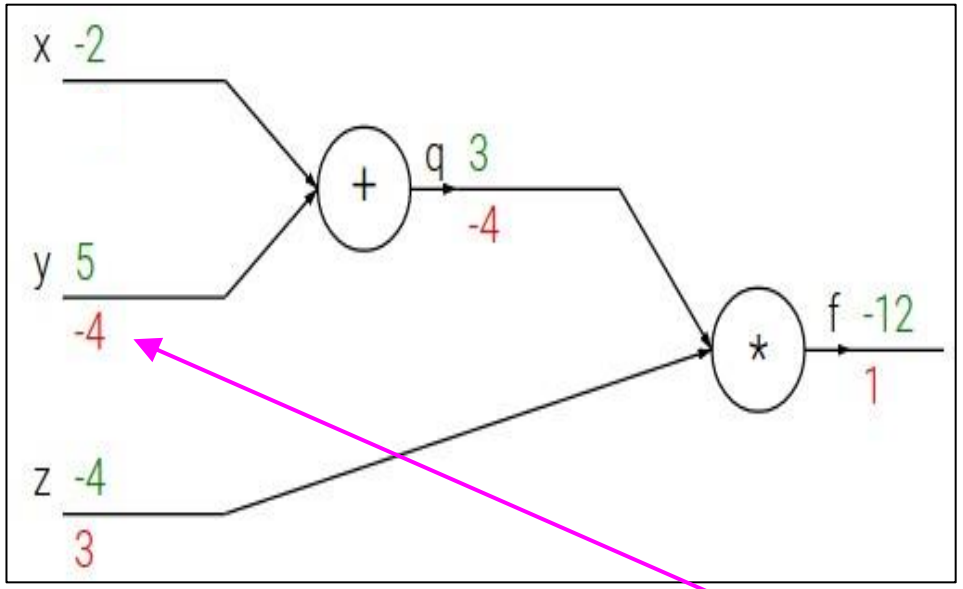

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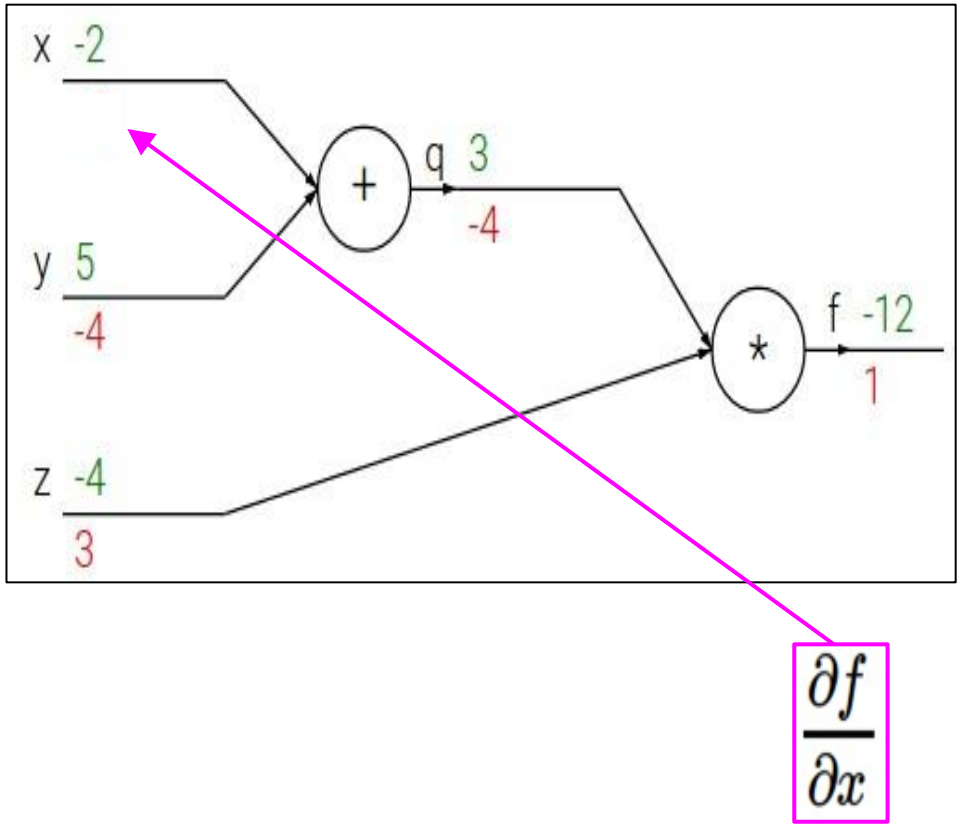

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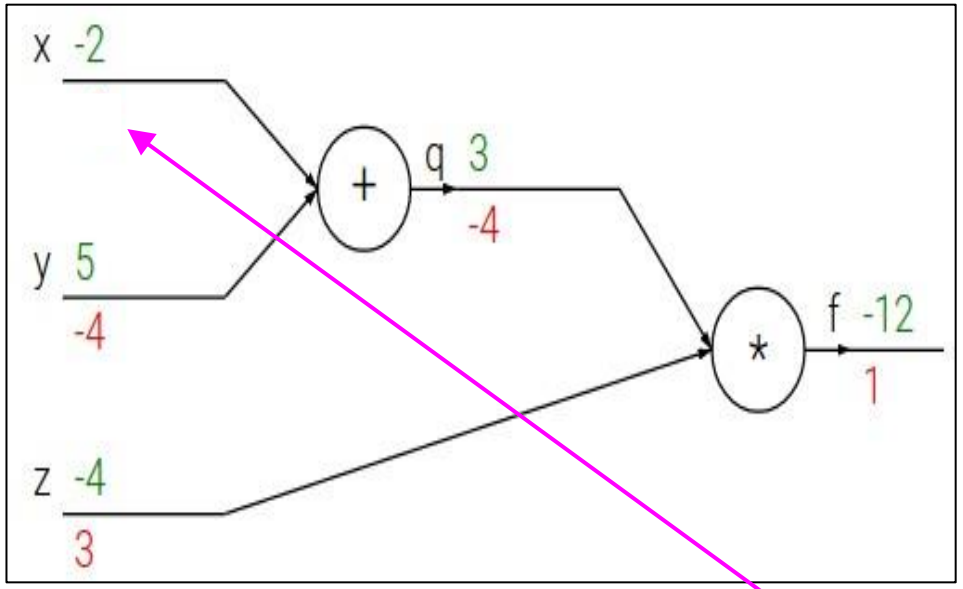

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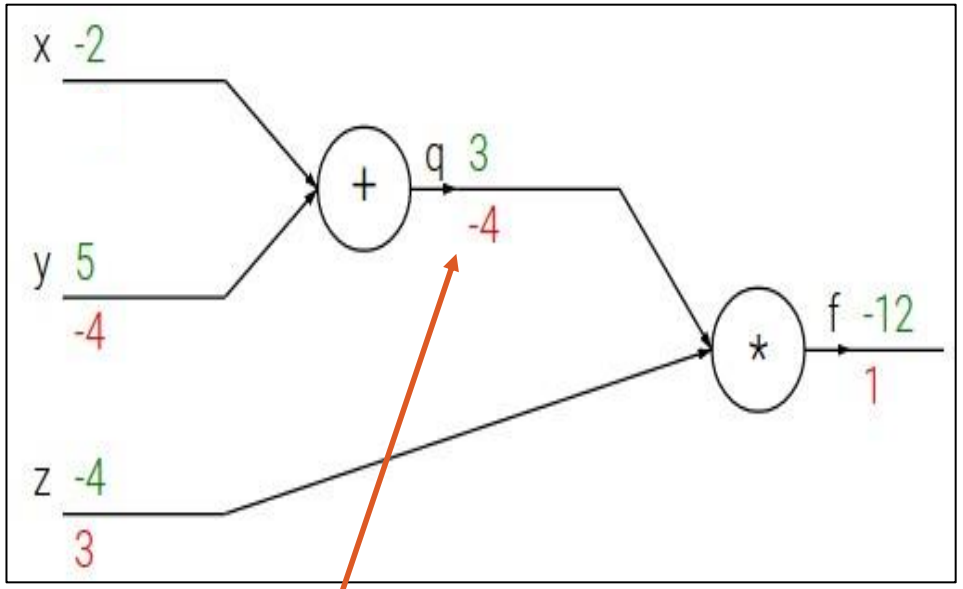

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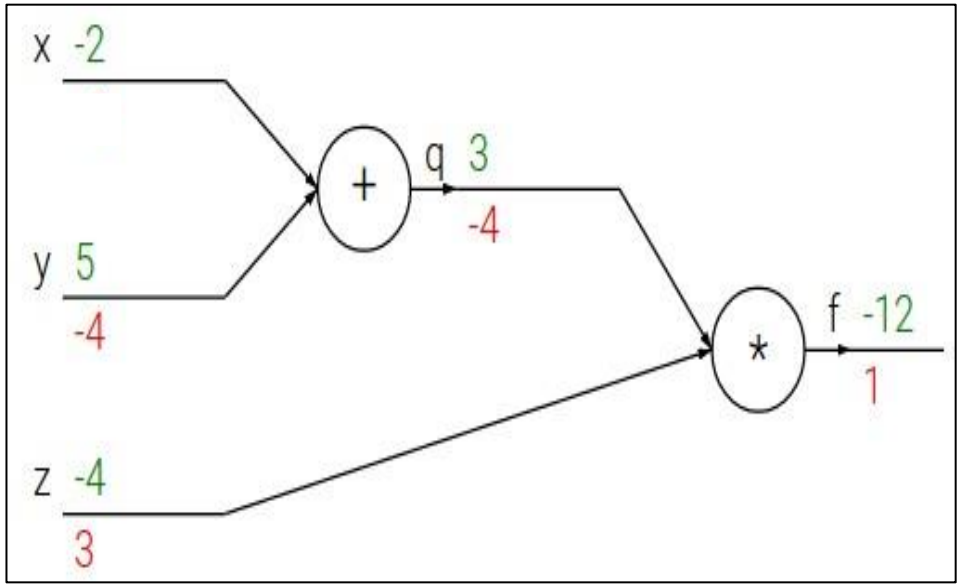


Regra da Cadeia:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

Diferenciação de um Grafo de Computação

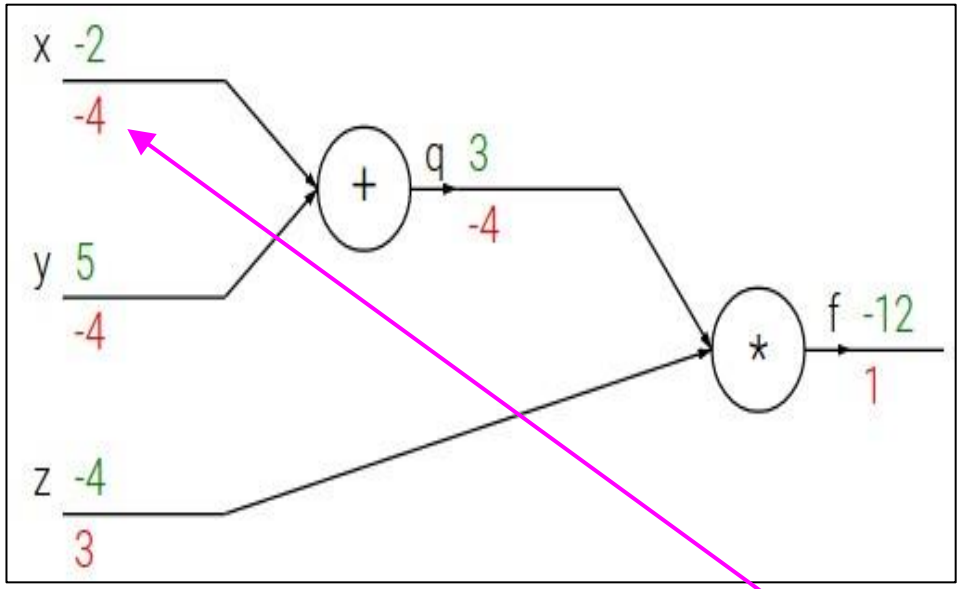
Seja $f(x, y, z) = (x + y) \times z$

Por exemplo: x = -2, y = 5, z = -4

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

Deseja-se: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

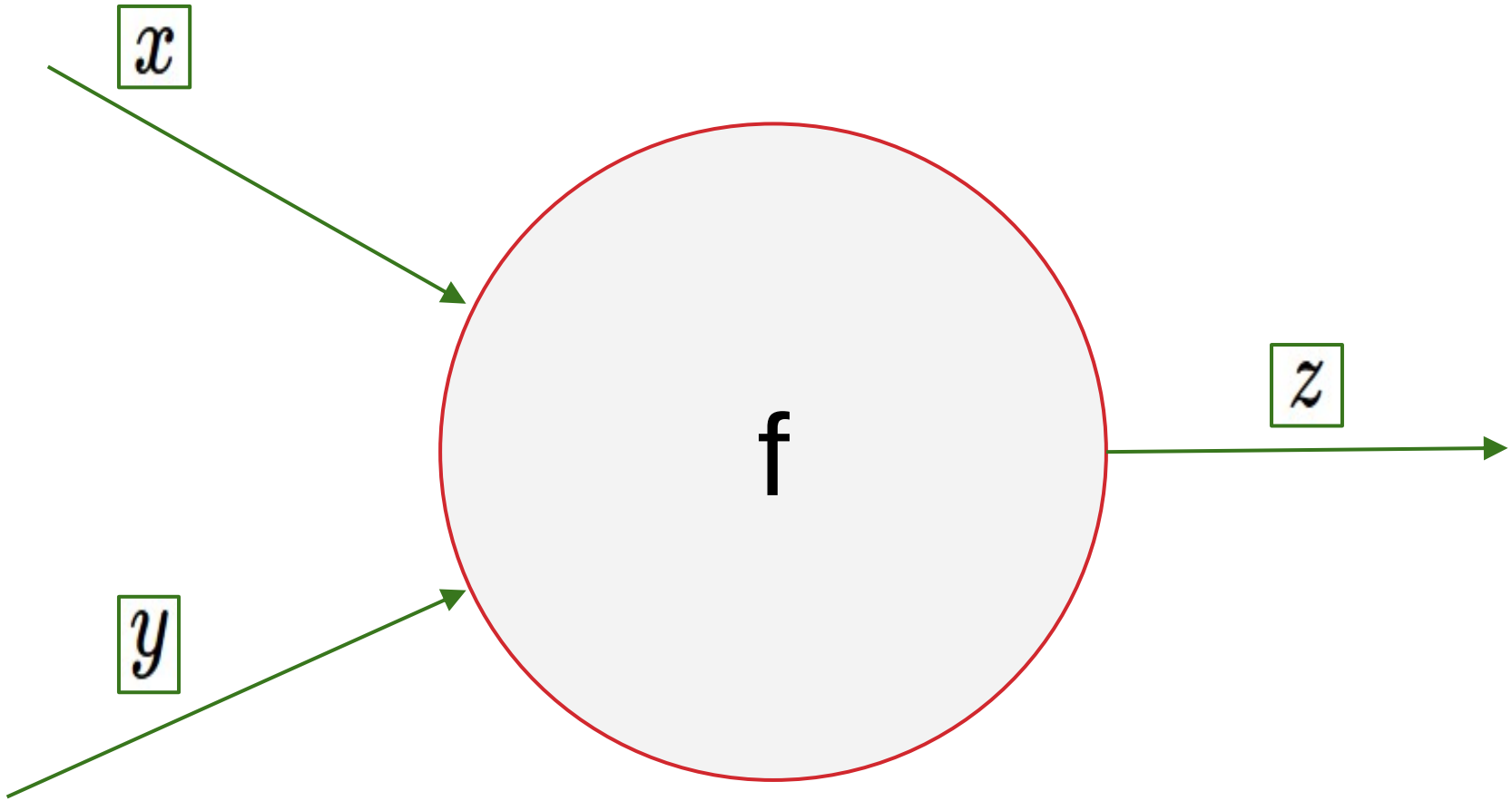


Regra da Cadeia:

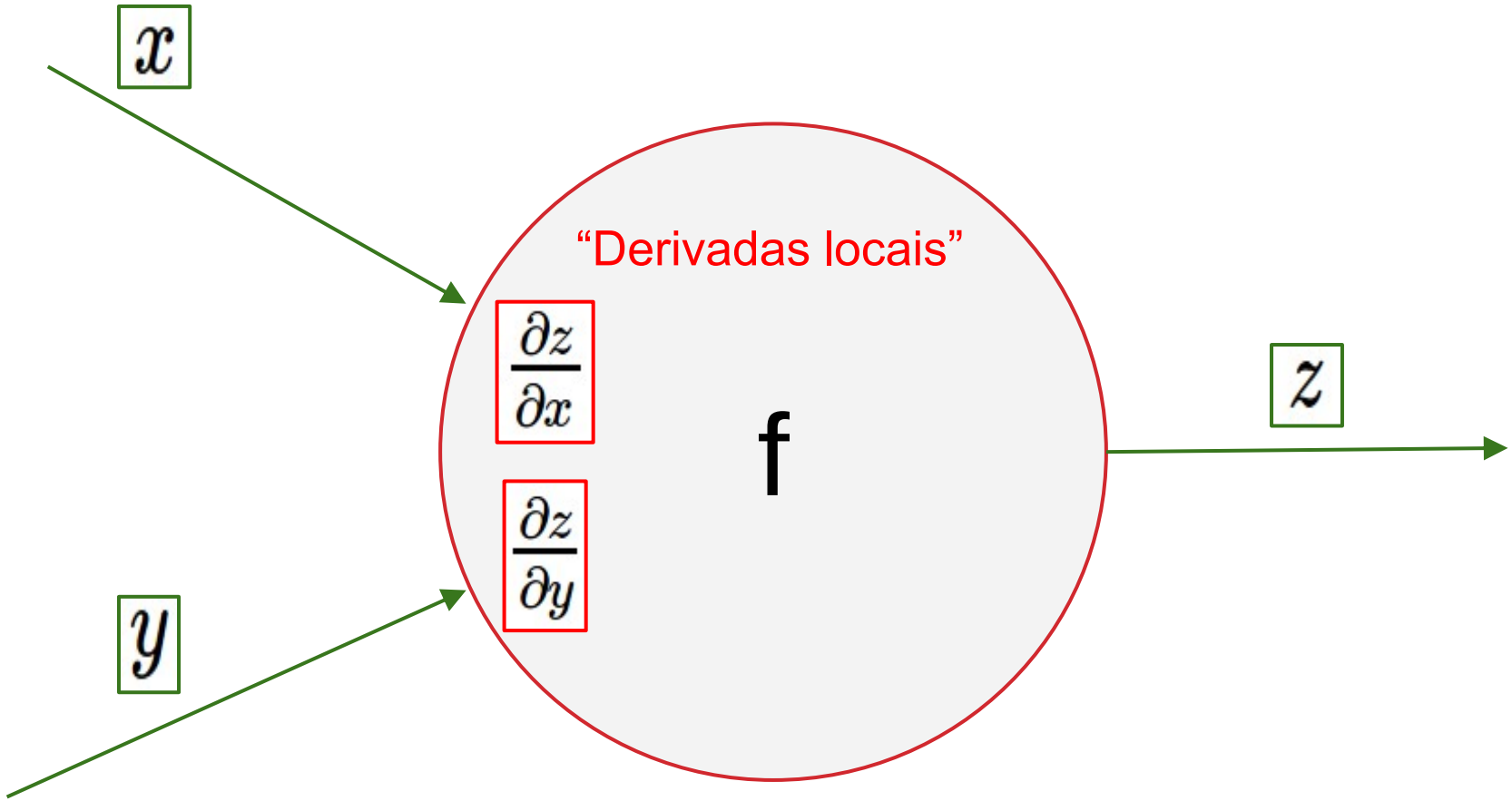
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

$\frac{\partial f}{\partial x}$

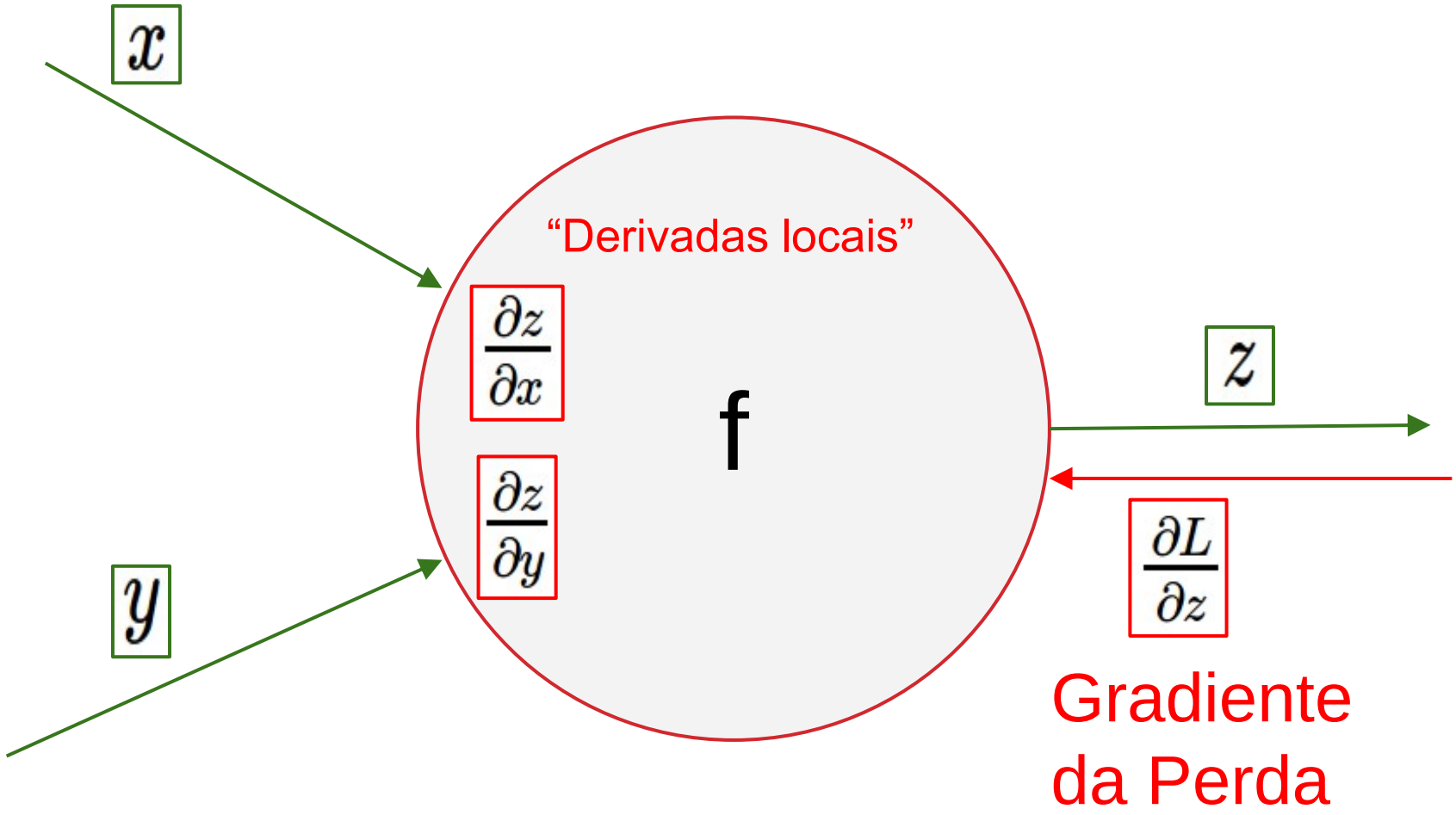
Passo Retrógrado (*Backward Pass*)



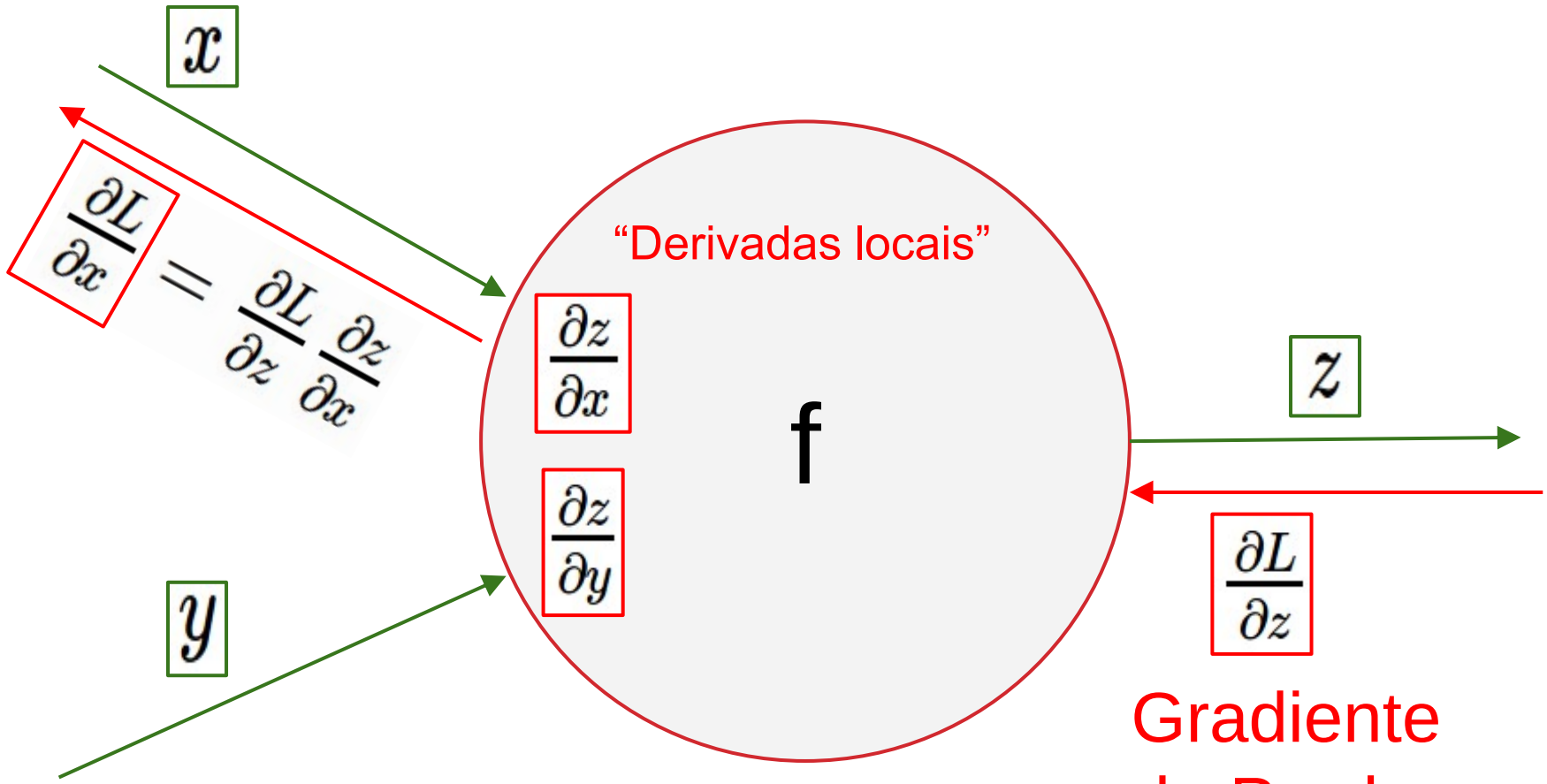
Passo Retrógrado (*Backward Pass*)



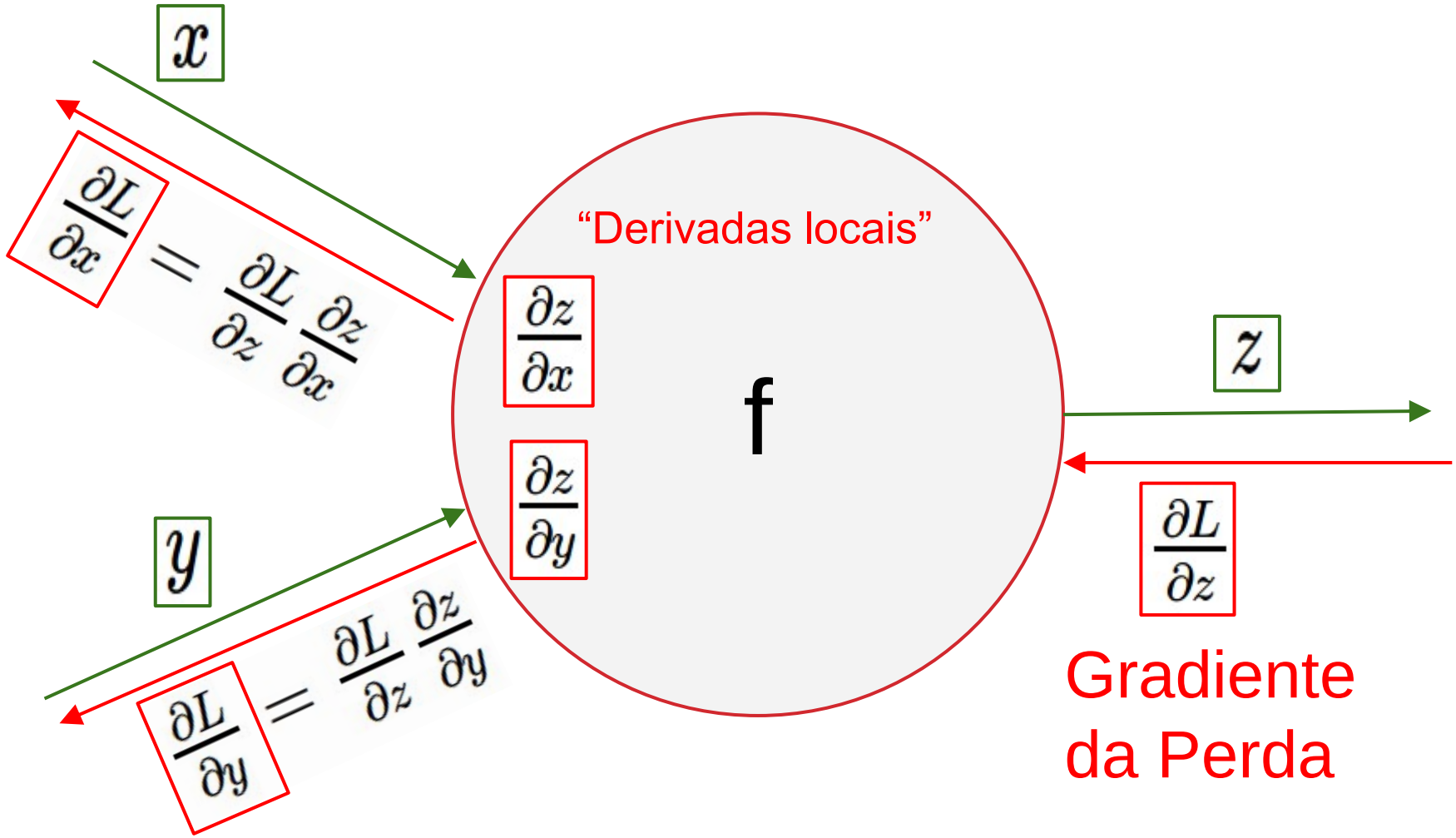
Passo Retrógrado (*Backward Pass*)



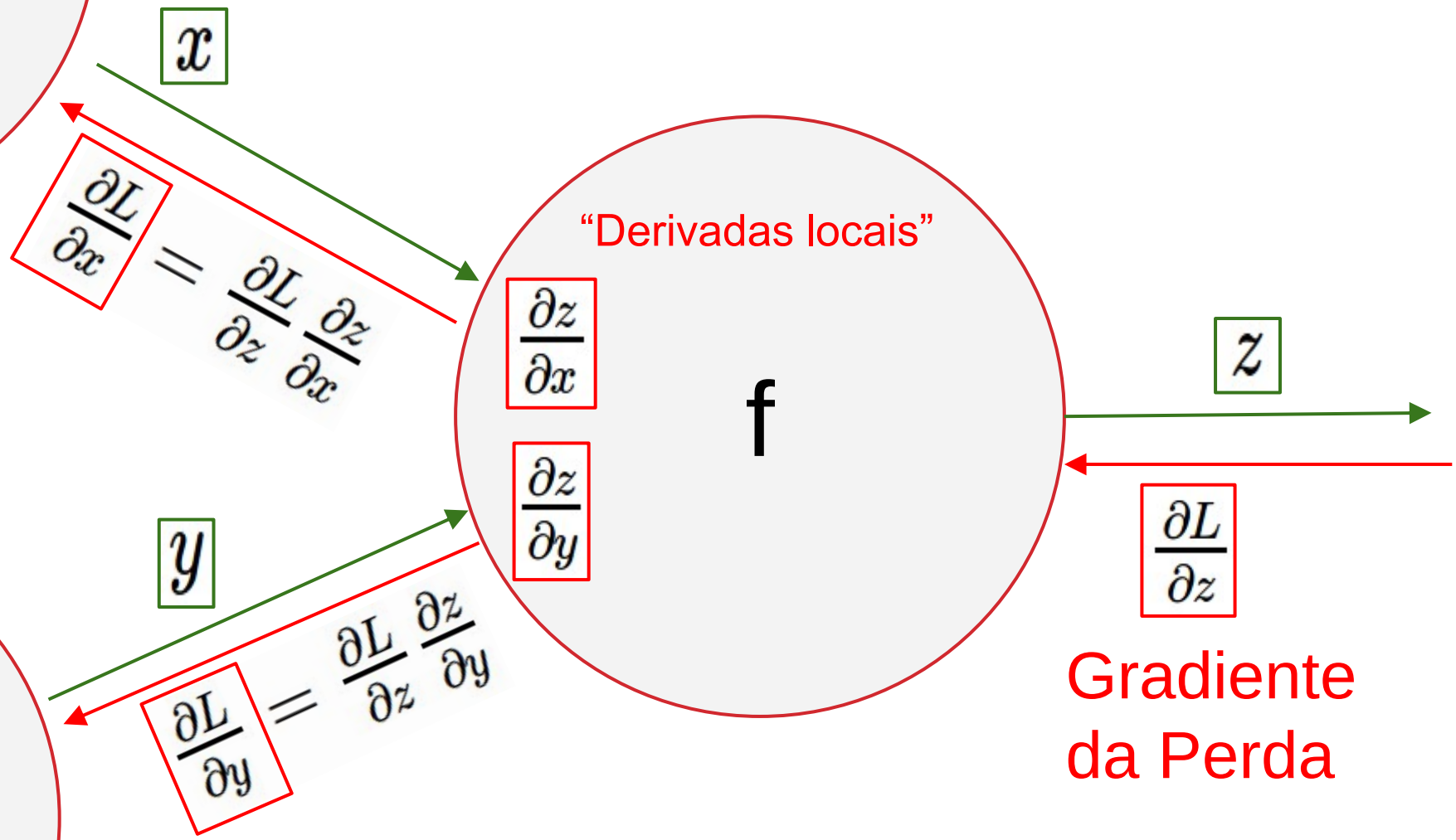
Passo Retrógrado (*Backward Pass*)



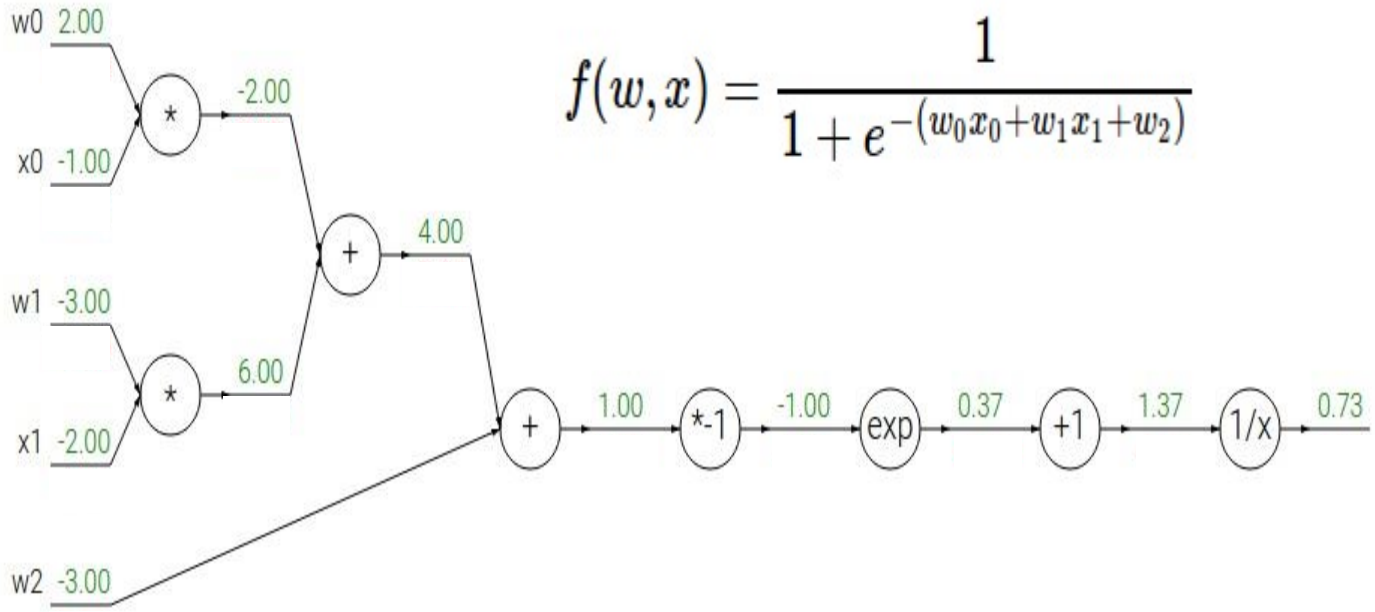
Passo Retrógrado (*Backward Pass*)



Passo Retrógrado (*Backward Pass*)

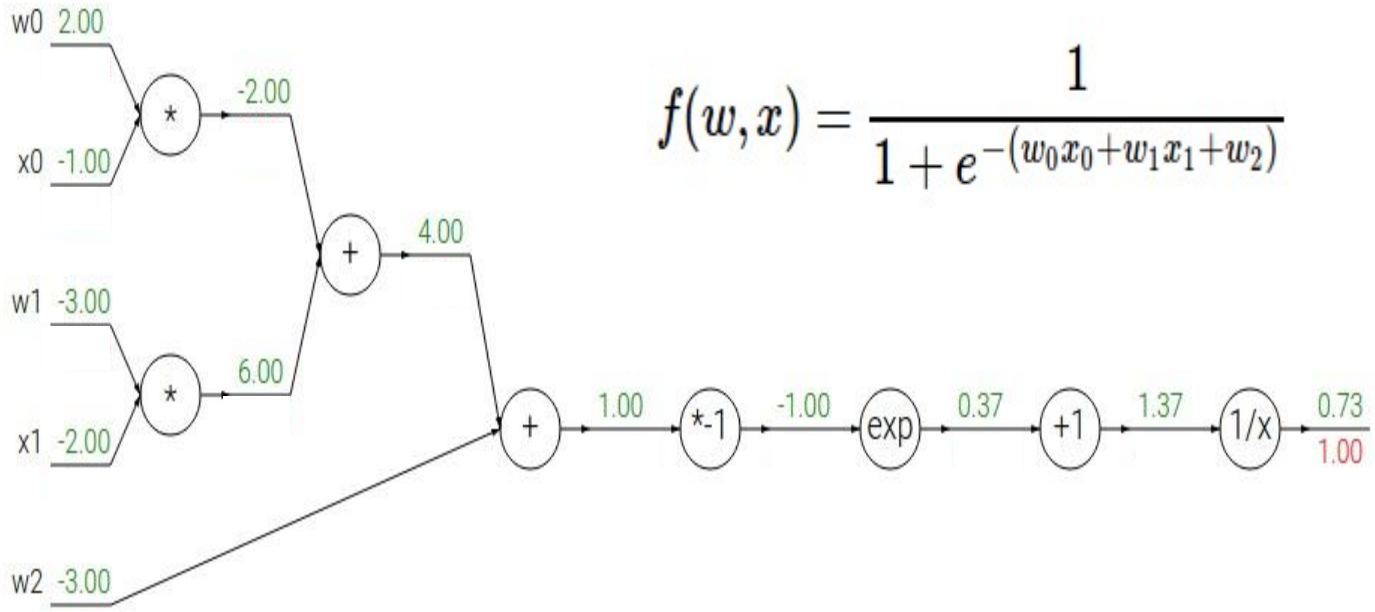


Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$

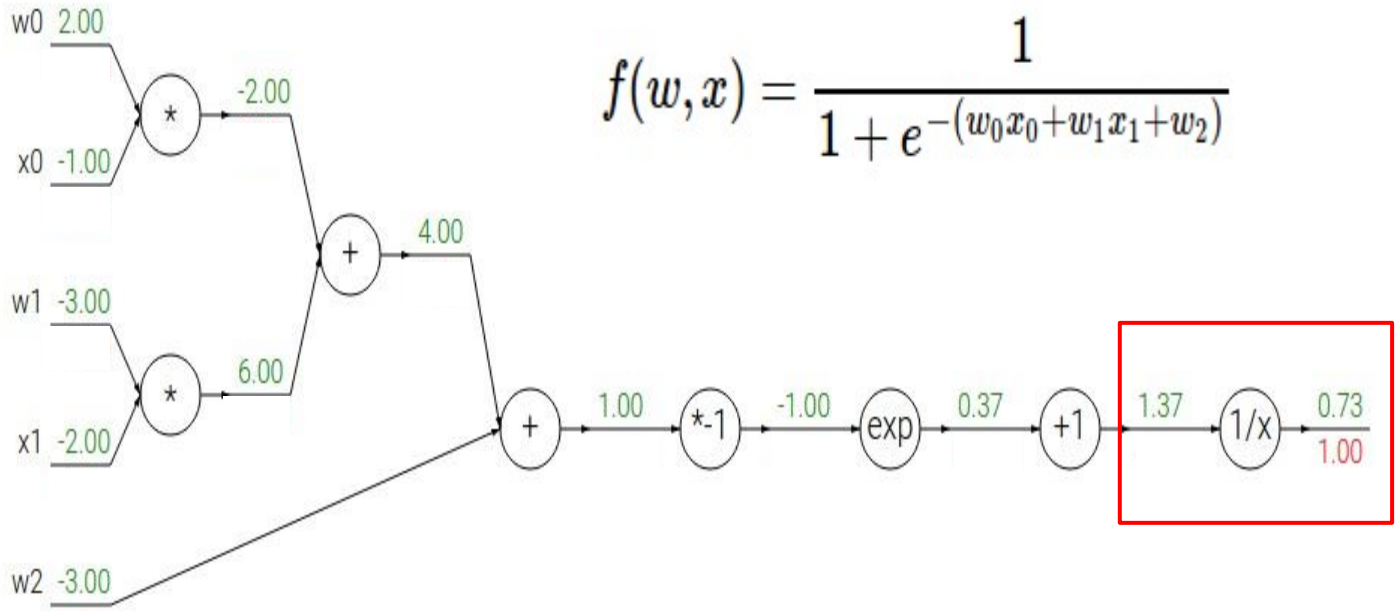
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

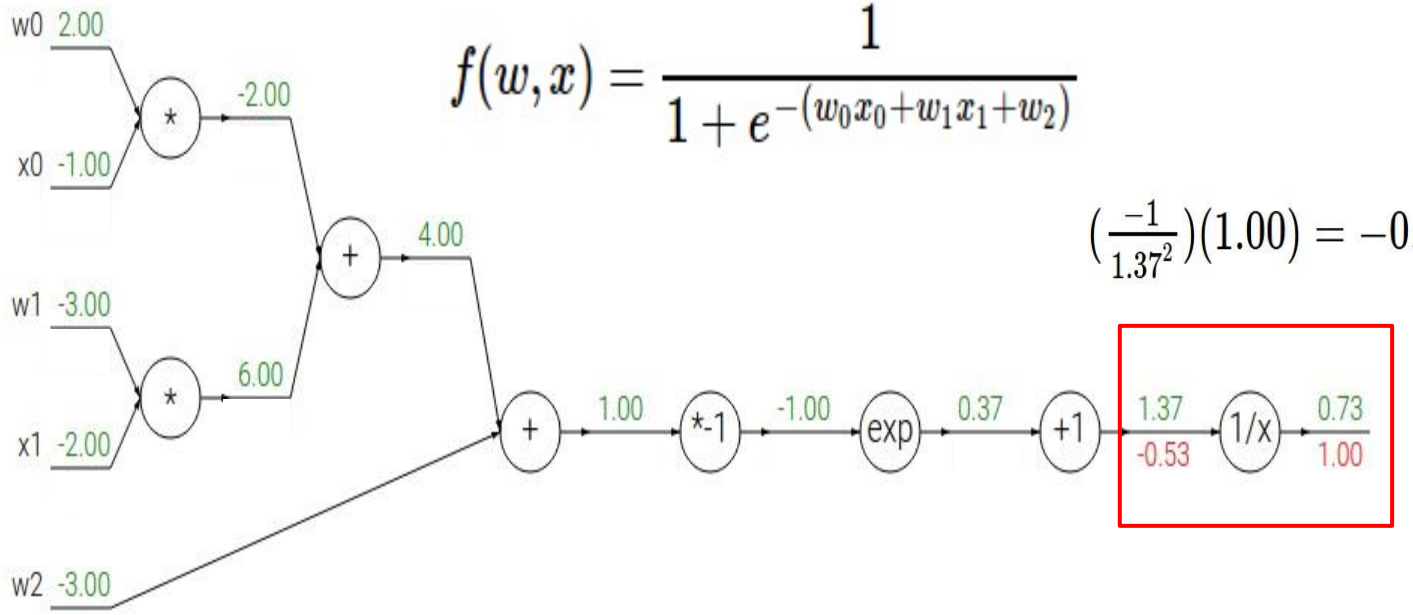
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$(\frac{-1}{1.37^2})(1.00) = -0.53$$

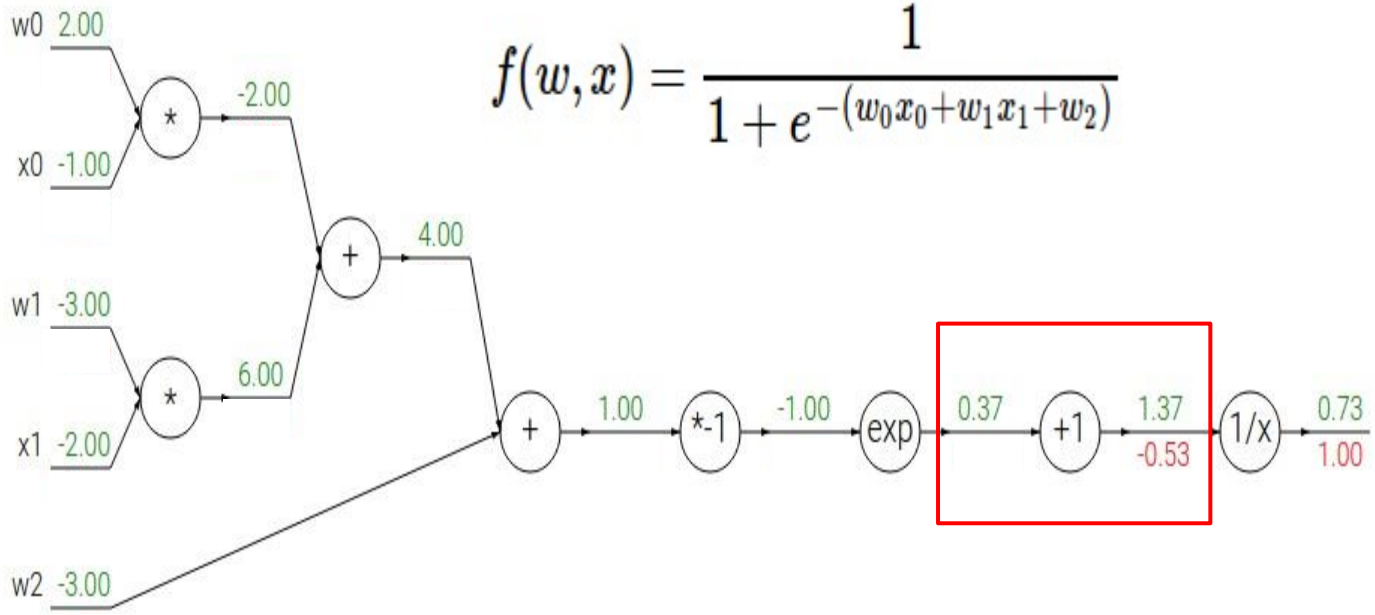
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

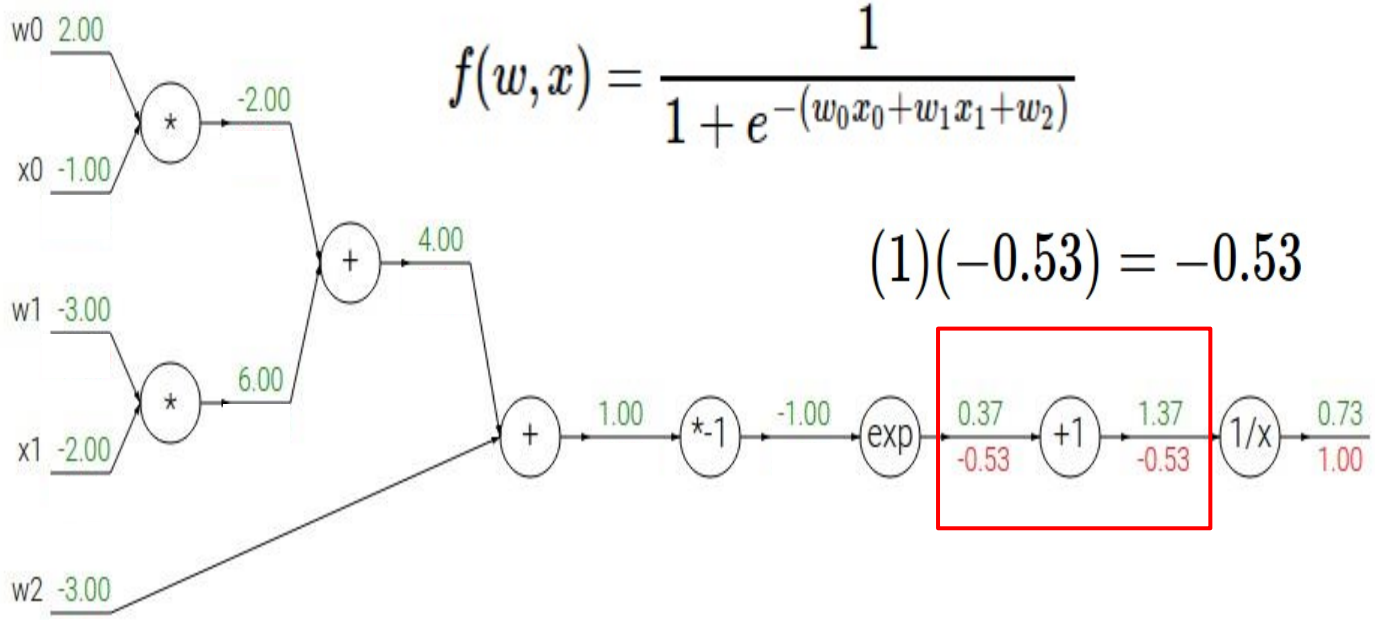
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado

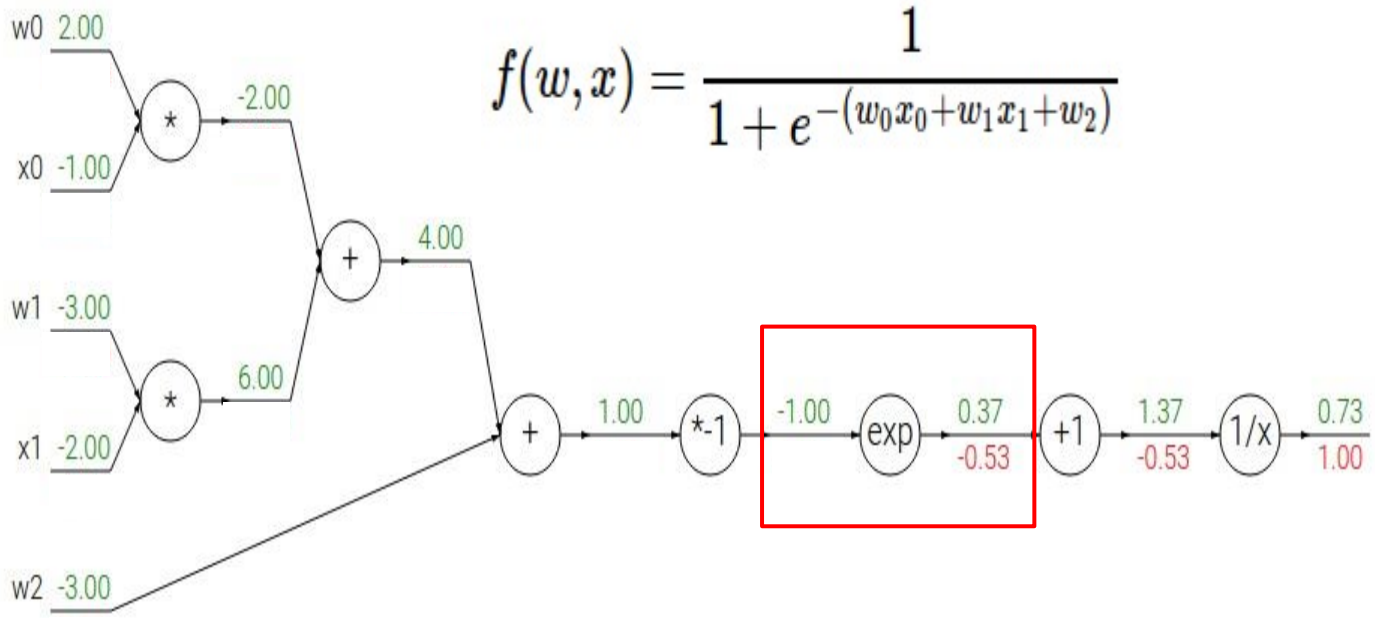


$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$(1)(-0.53) = -0.53$$

$f(x) = e^x$	$\rightarrow$	$\frac{df}{dx} = e^x$	$f(x) = \frac{1}{x}$	$\rightarrow$	$\frac{df}{dx} = -1/x^2$
$f_a(x) = ax$	$\rightarrow$	$\frac{df}{dx} = a$	$f_c(x) = c + x$	$\rightarrow$	$\frac{df}{dx} = 1$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

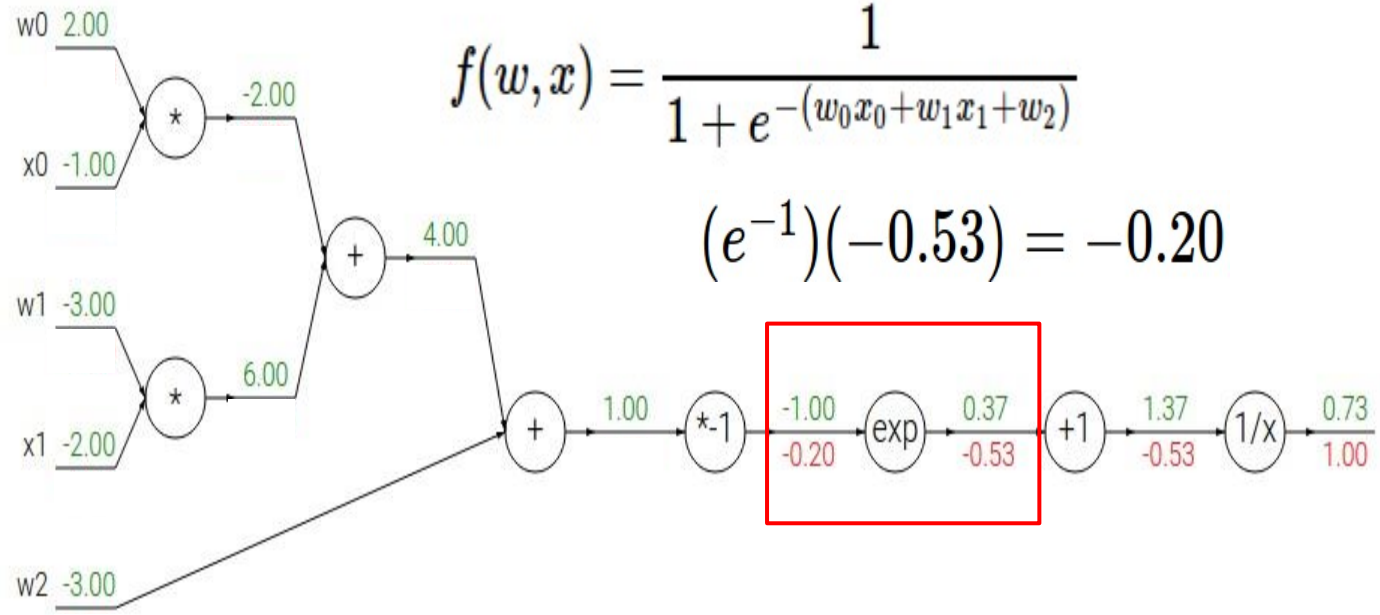
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$(e^{-1})(-0.53) = -0.20$$

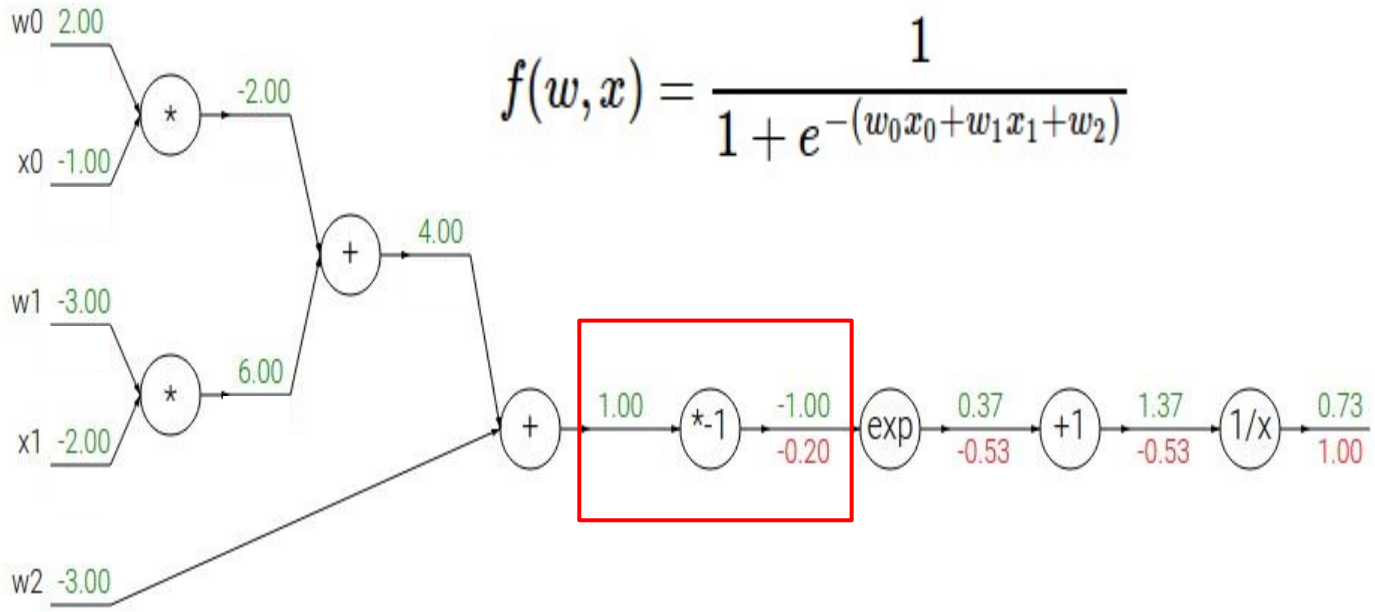
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

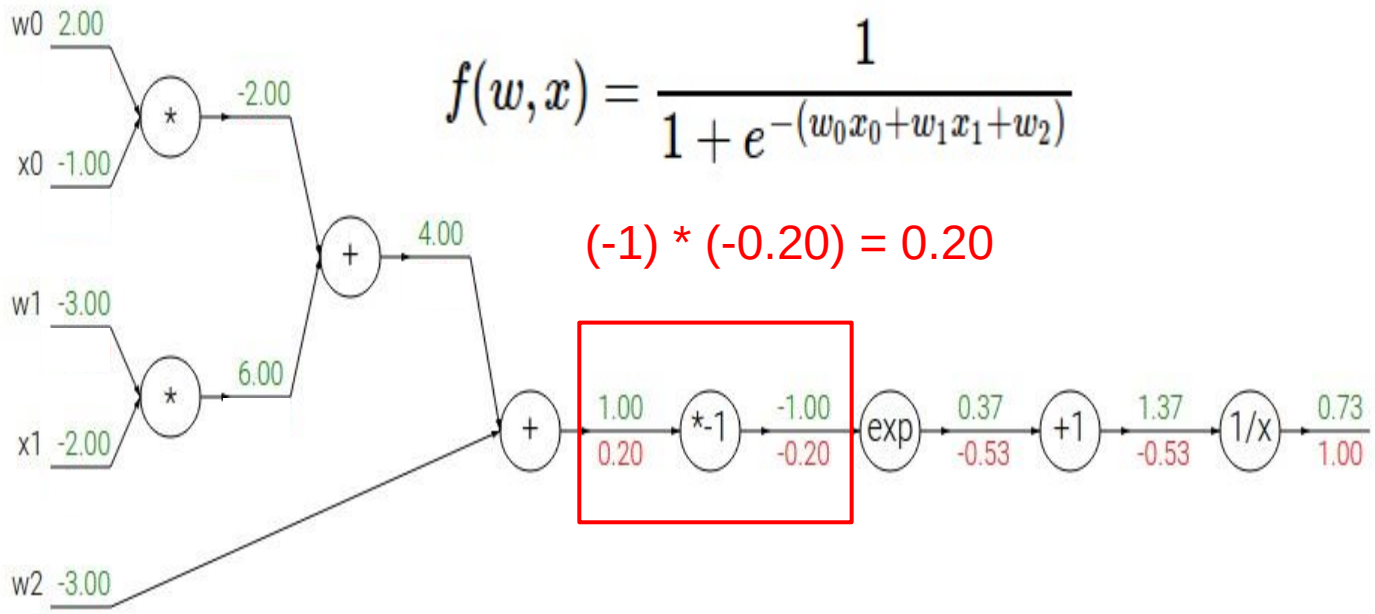
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

(-1) * (-0.20) = 0.20

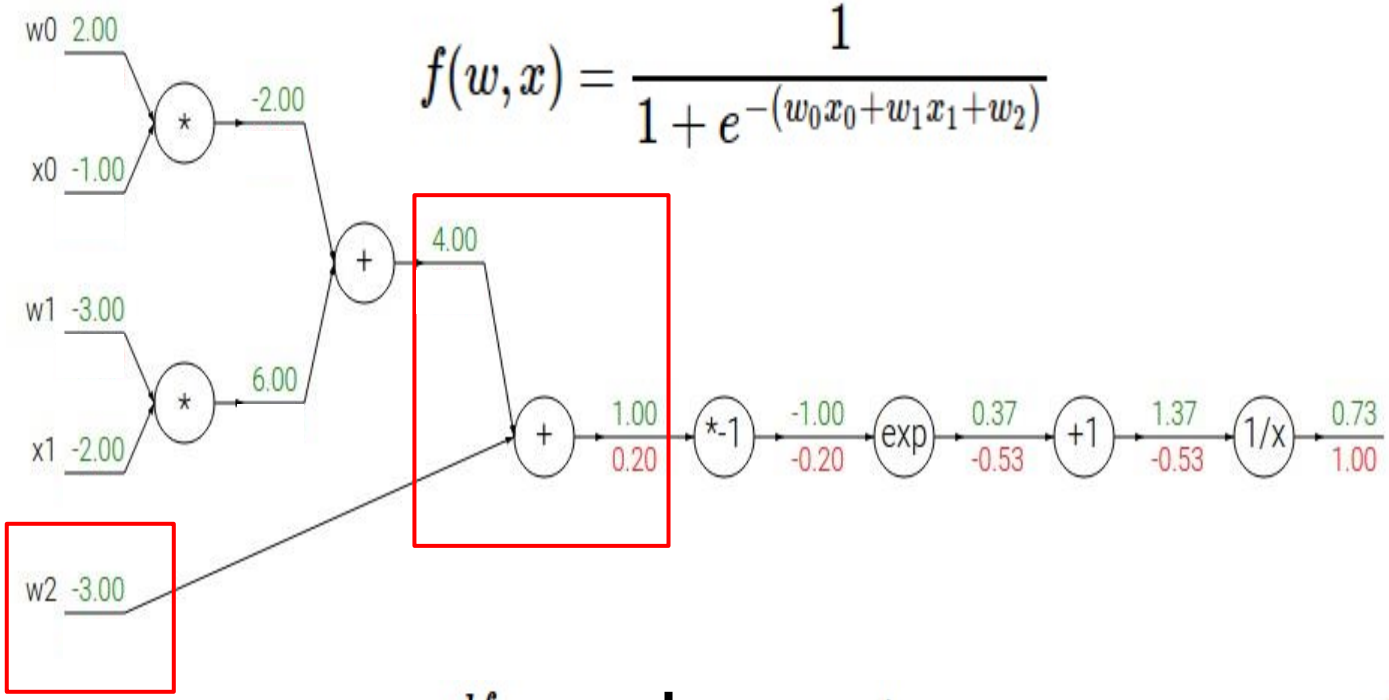
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

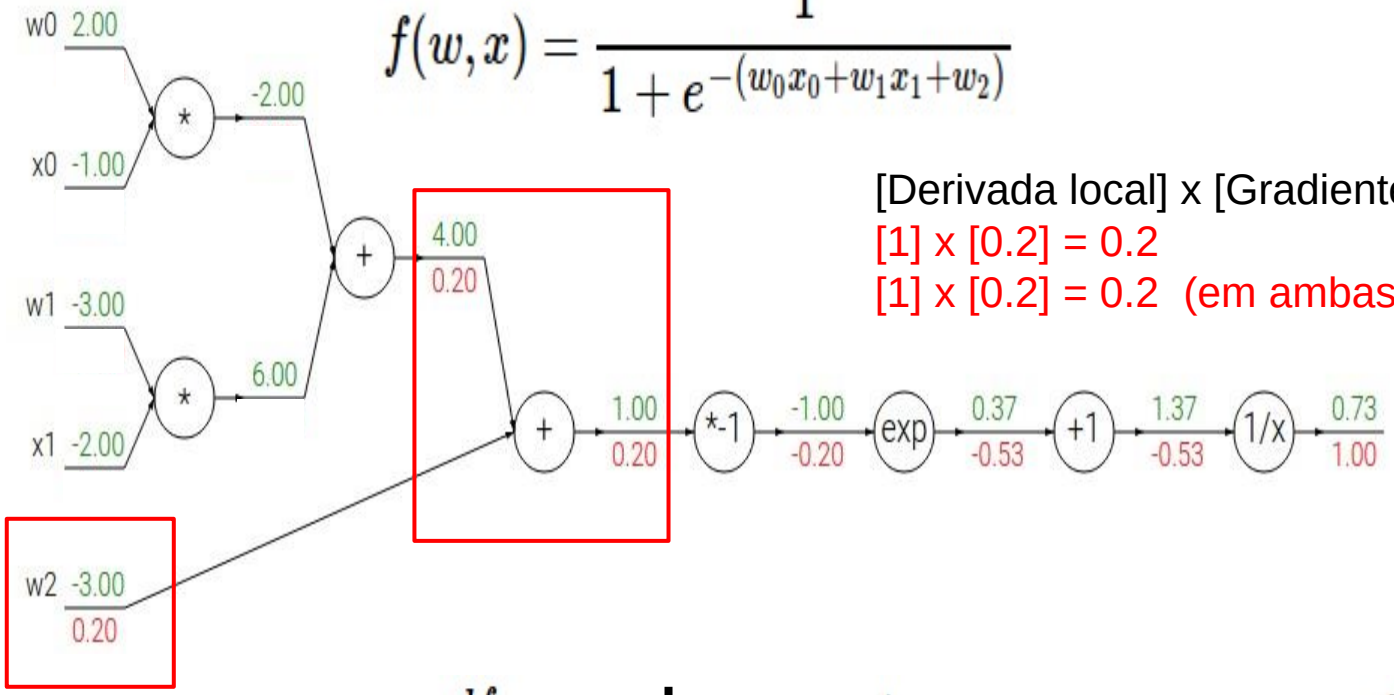
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

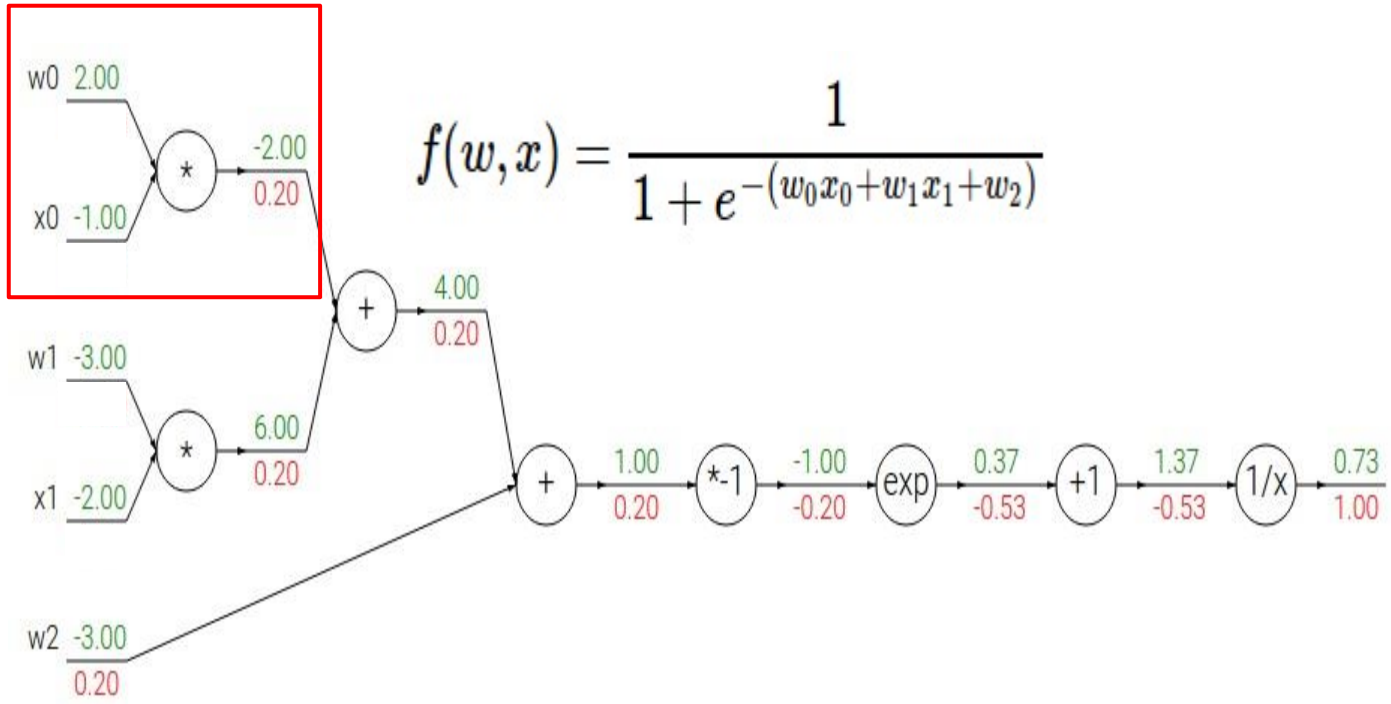


[Derivada local] x [Gradiente]
[1] x [0.2] = 0.2
[1] x [0.2] = 0.2 (em ambas entradas!)

$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x \qquad f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$$

$$f_a(x) = ax \rightarrow \frac{df}{dx} = a \qquad f_c(x) = c + x \rightarrow \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

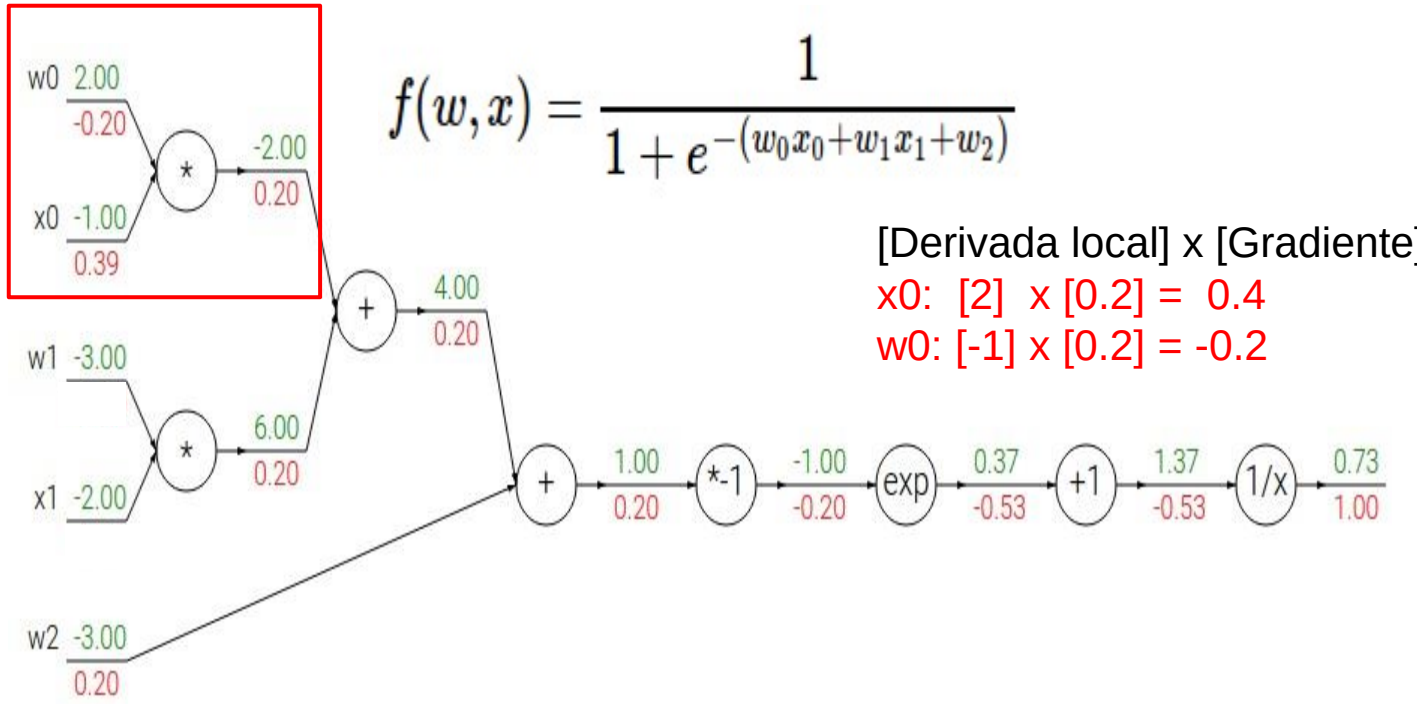
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado



$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

[Derivada local] x [Gradiente]

x0: [2] x [0.2] = 0.4

w0: [-1] x [0.2] = -0.2

$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \rightarrow \frac{df}{dx} = 1$$

Outro Exemplo – Passo Retrógrado

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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

Função sigmoide

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$

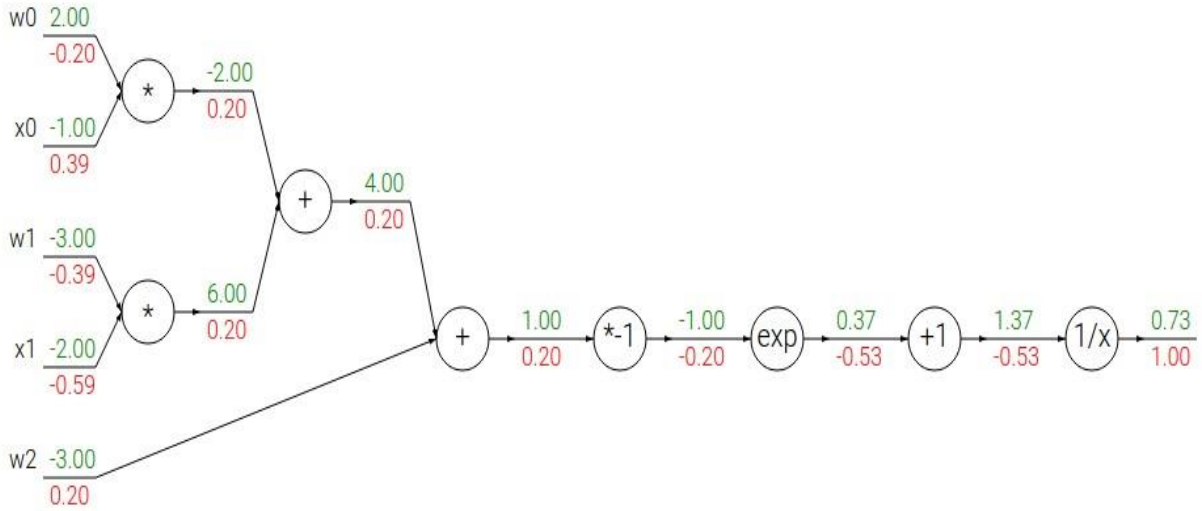
Outro Exemplo – Passo Retrógrado

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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

Função sigmoide

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



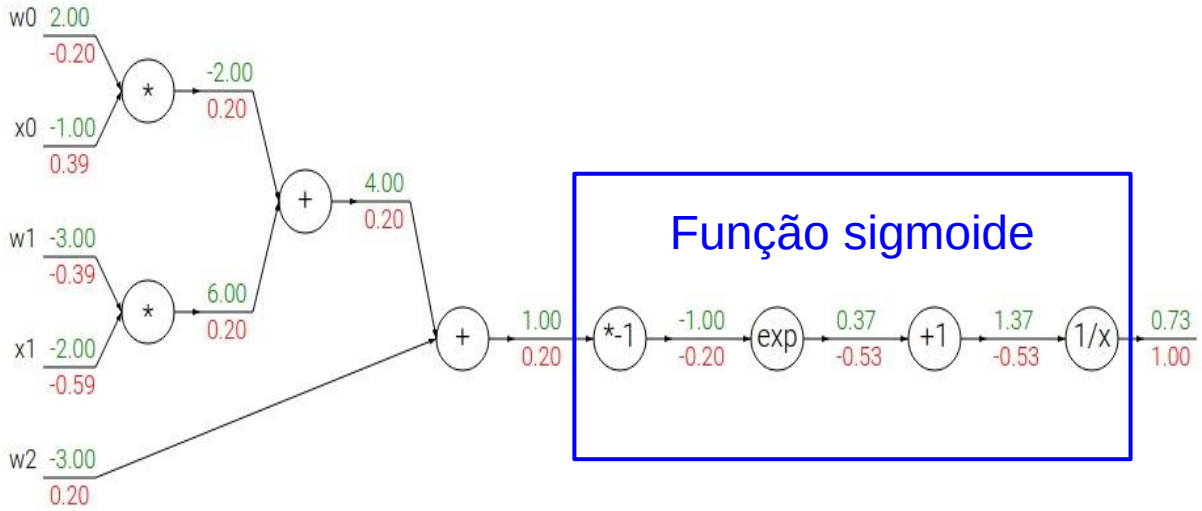
Outro Exemplo – Passo Retrógrado

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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

Função sigmoide

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



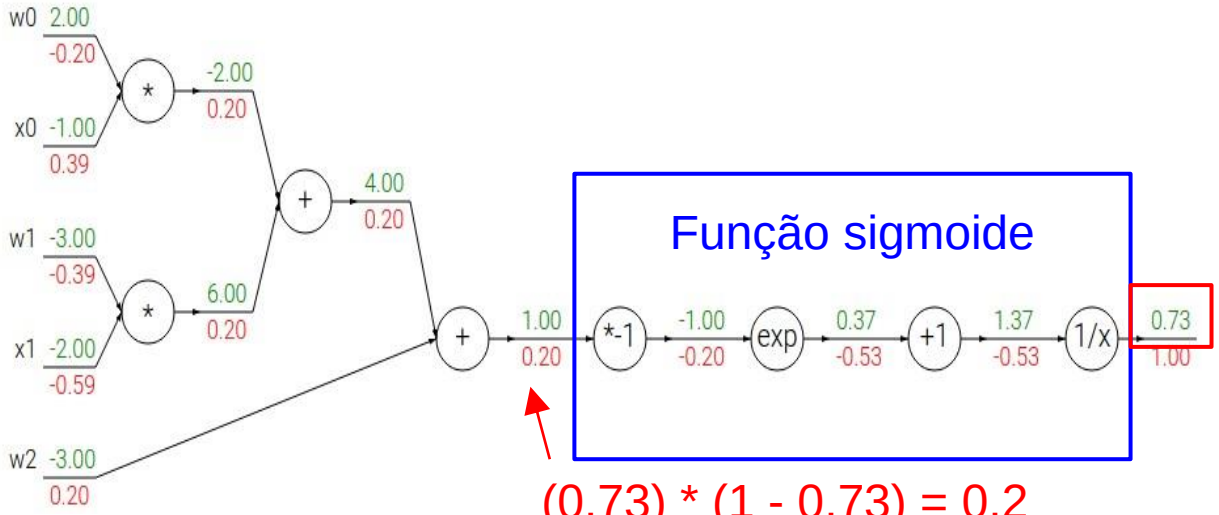
Outro Exemplo – Passo Retrógrado

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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

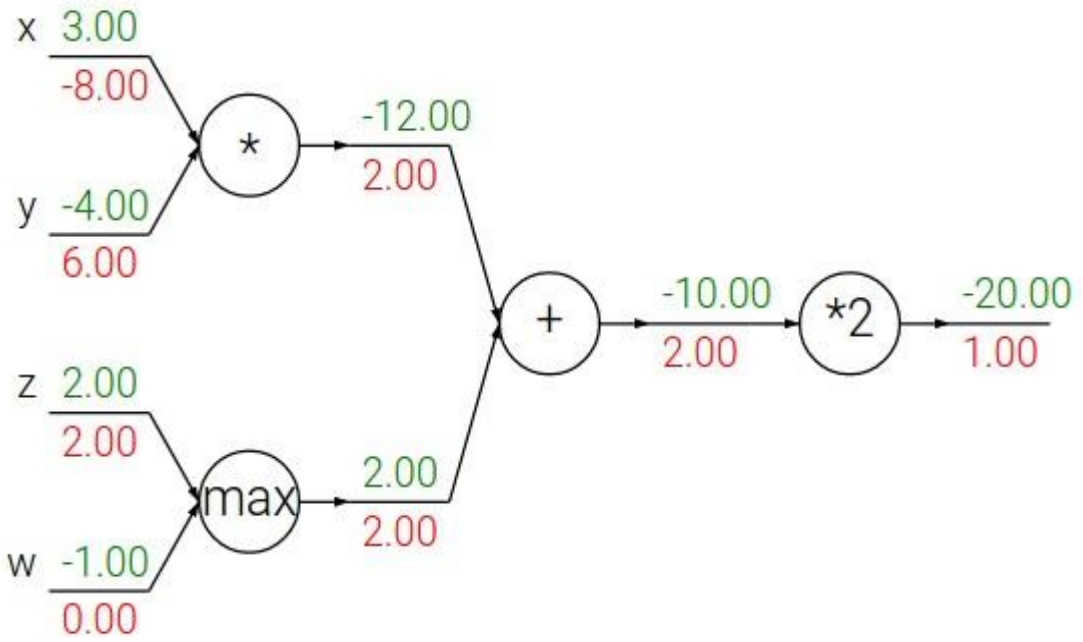
Função sigmoide

$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$



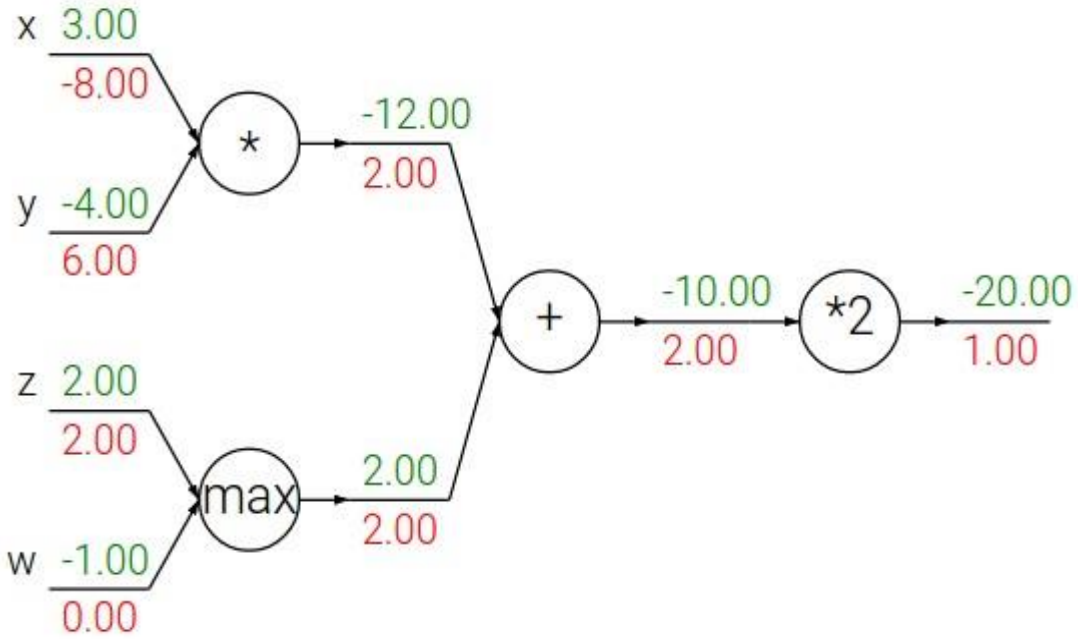
(0.73) * (1 - 0.73) = 0.2

Padrões no Fluxo Reverso



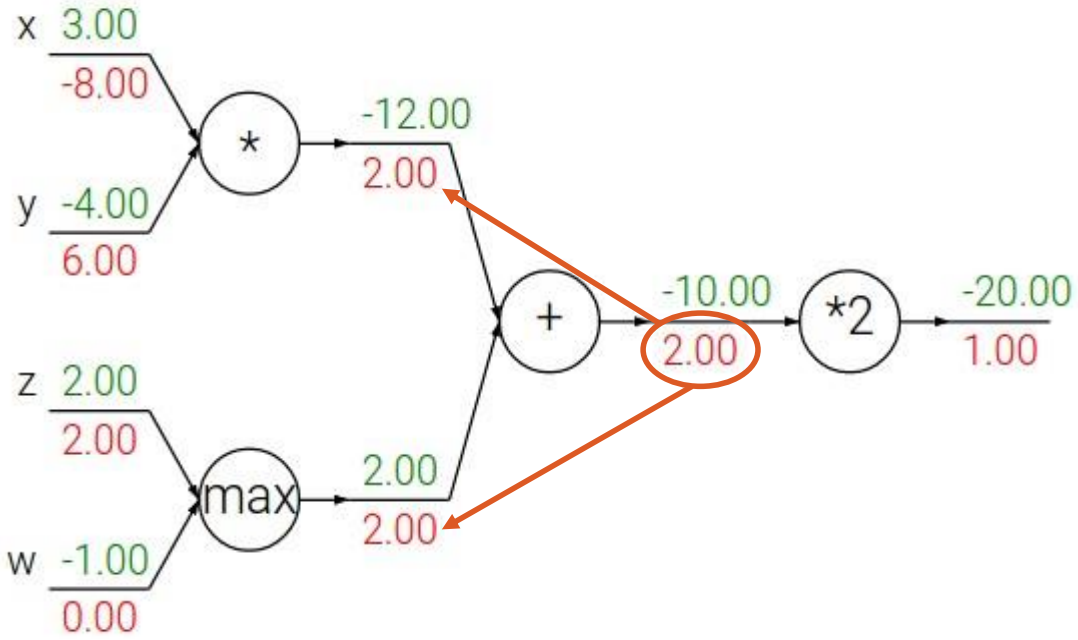
Padrões no Fluxo Reverso

Adição : distribuidor de gradiente



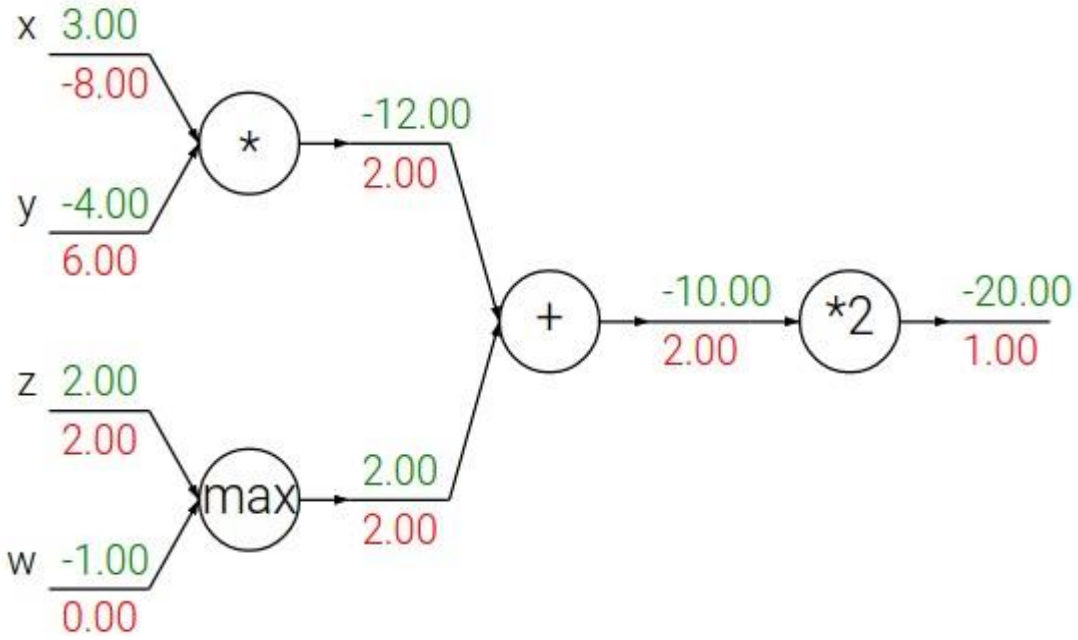
Padrões no Fluxo Reverso

Adição : distribuidor de gradiente



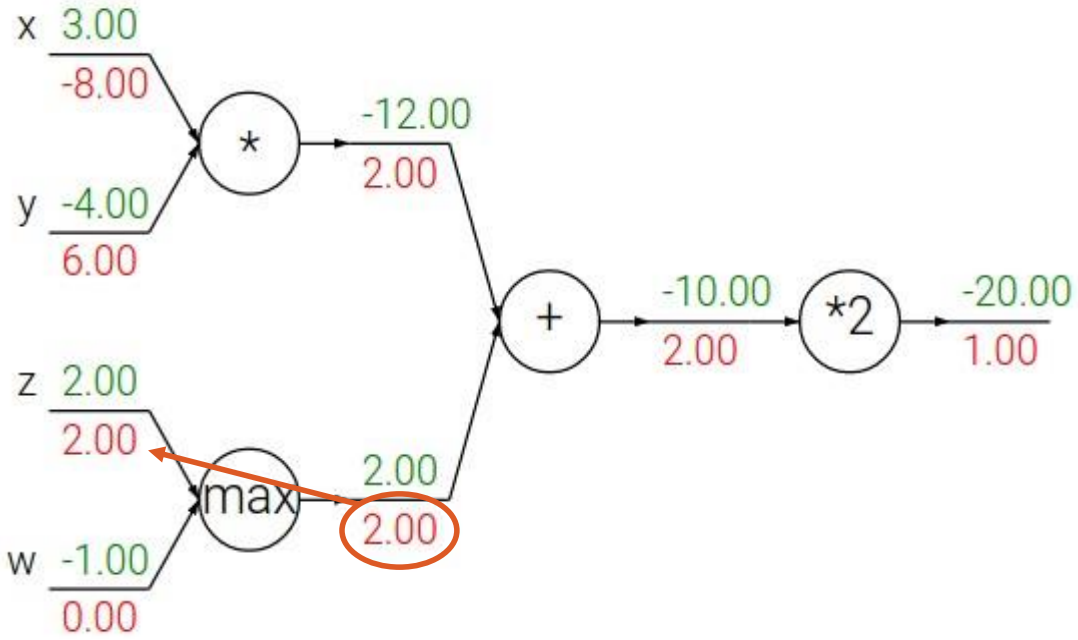
Padrões no Fluxo Reverso

Adição : distribuidor de gradiente
Max : direcionador de gradiente



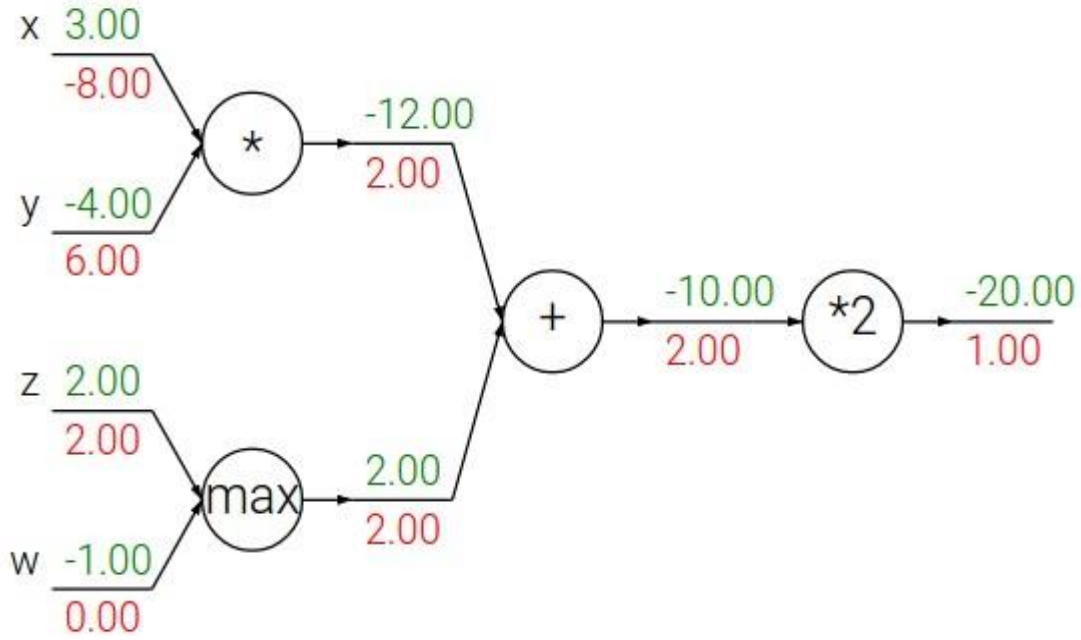
Padrões no Fluxo Reverso

Adição : distribuidor de gradiente
Max : direcionador de gradiente



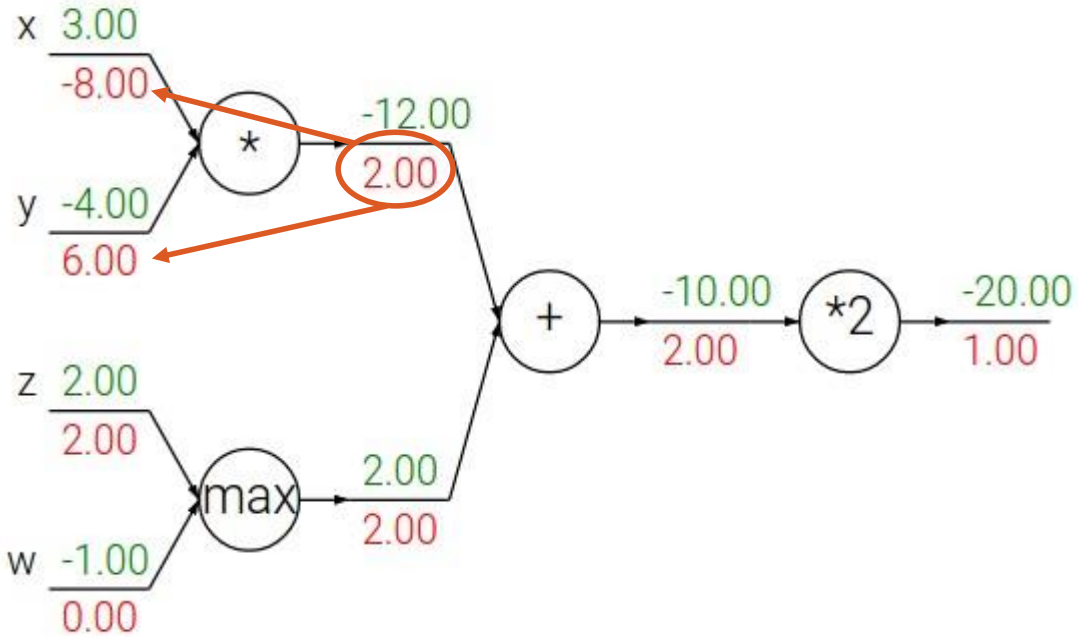
Padrões no Fluxo Reverso

Adição : distribuidor de gradiente
Max : direcionador de gradiente
Produto: “comutador” de gradiente



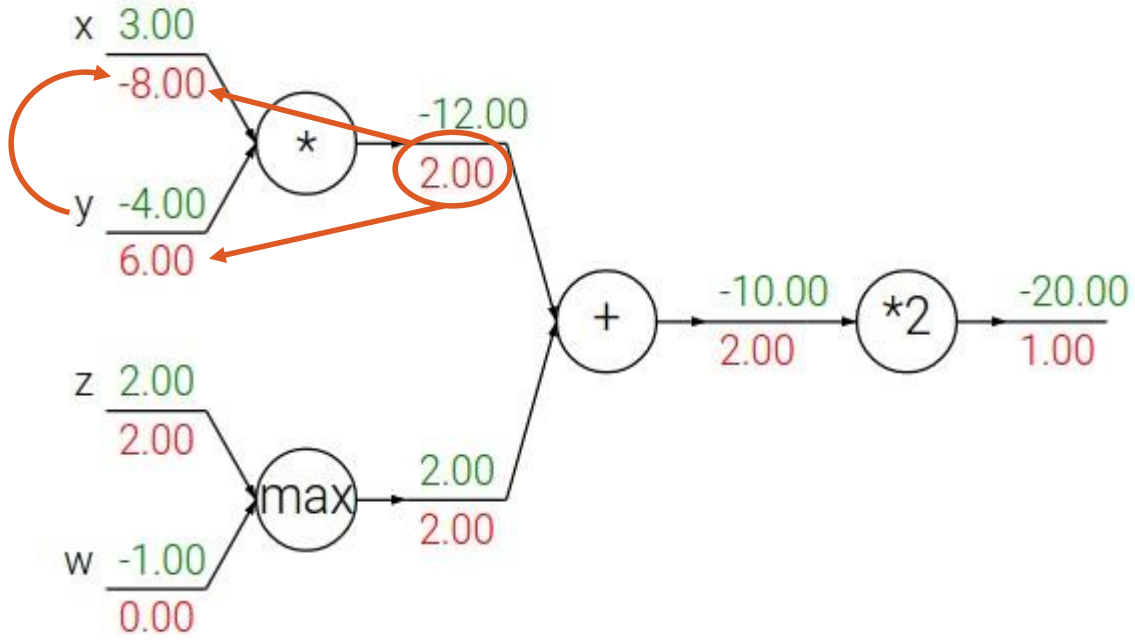
Padrões no Fluxo Reverso

Adição : distribuidor de gradiente
Max : direcionador de gradiente
Produto: “comutador” de gradiente



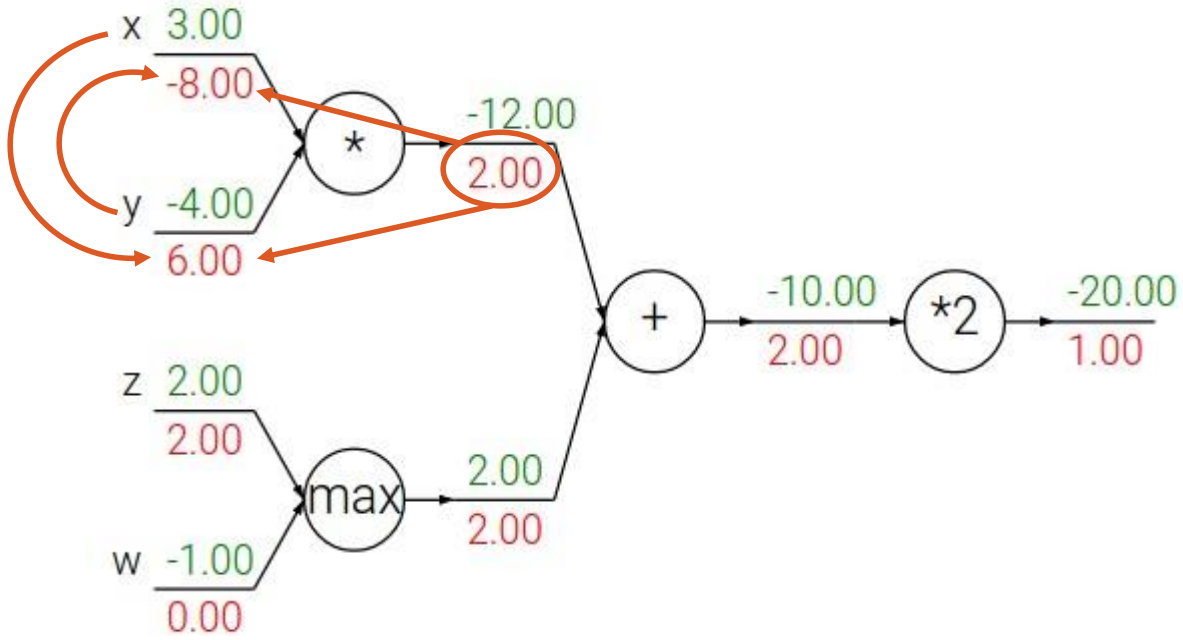
Padrões no Fluxo Reverso

Adição : distribuidor de gradiente
Max : direcionador de gradiente
Produto: “comutador” de gradiente

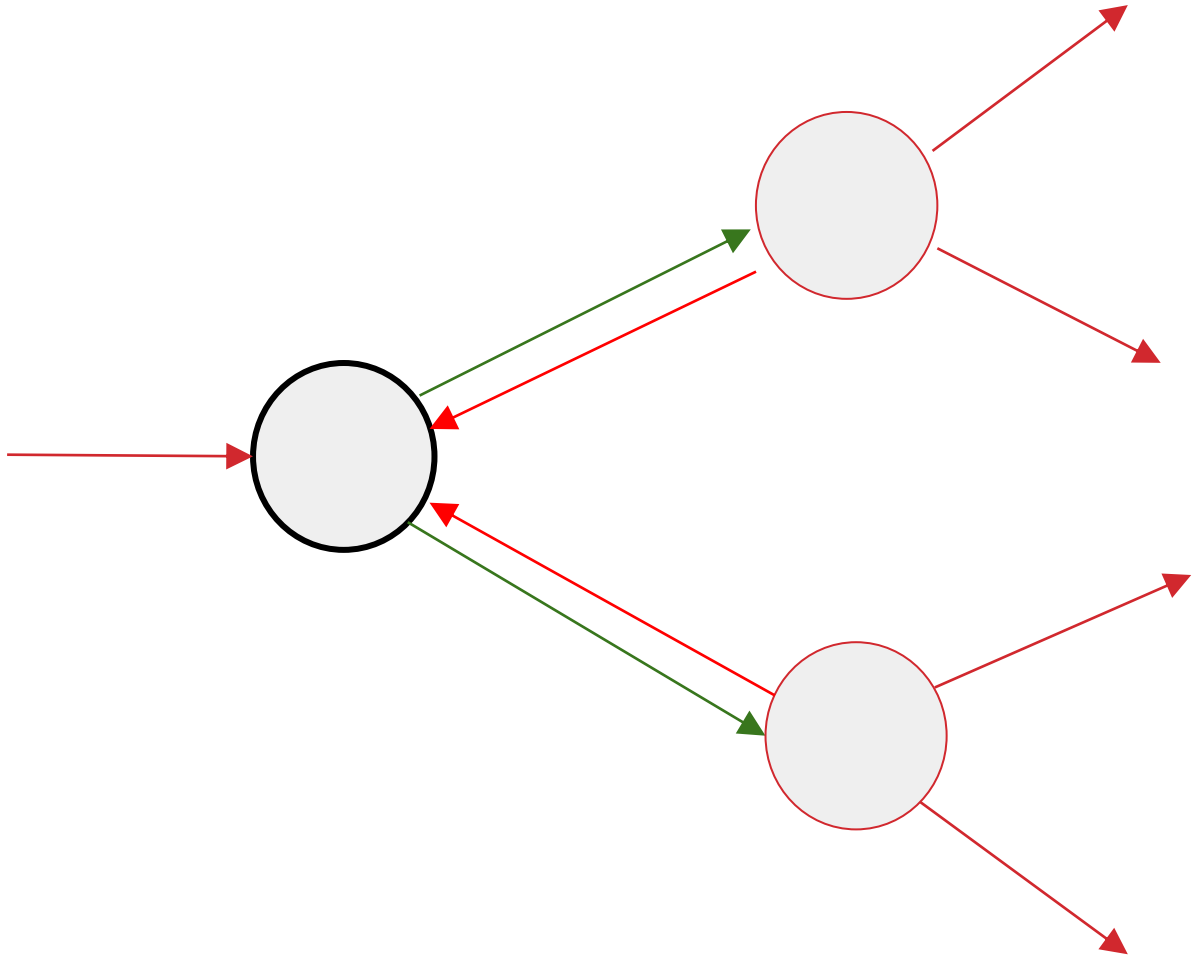


Padrões no Fluxo Reverso

Adição : distribuidor de gradiente
Max : direcionador de gradiente
Produto: “comutador” de gradiente



Gradientes nas Ramificações



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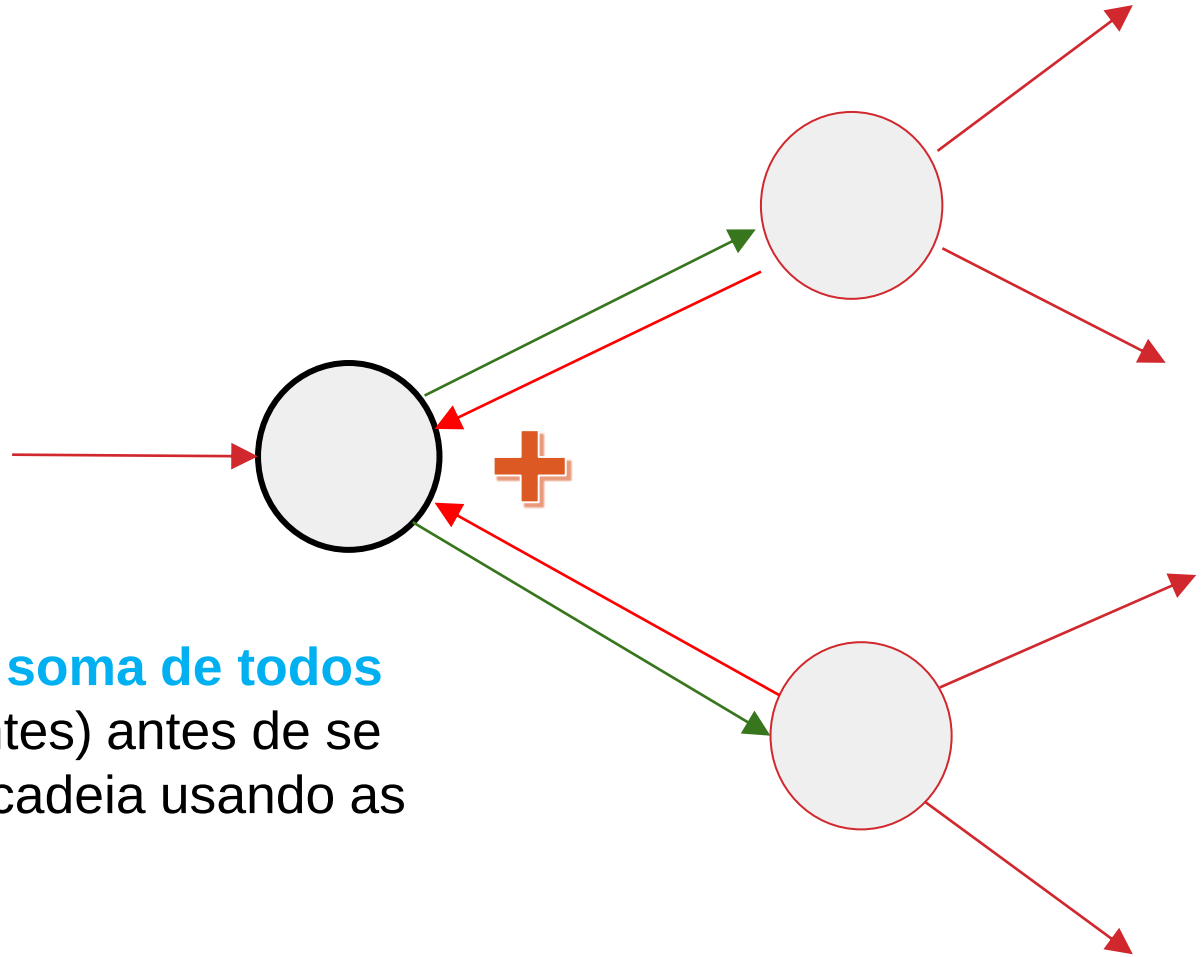
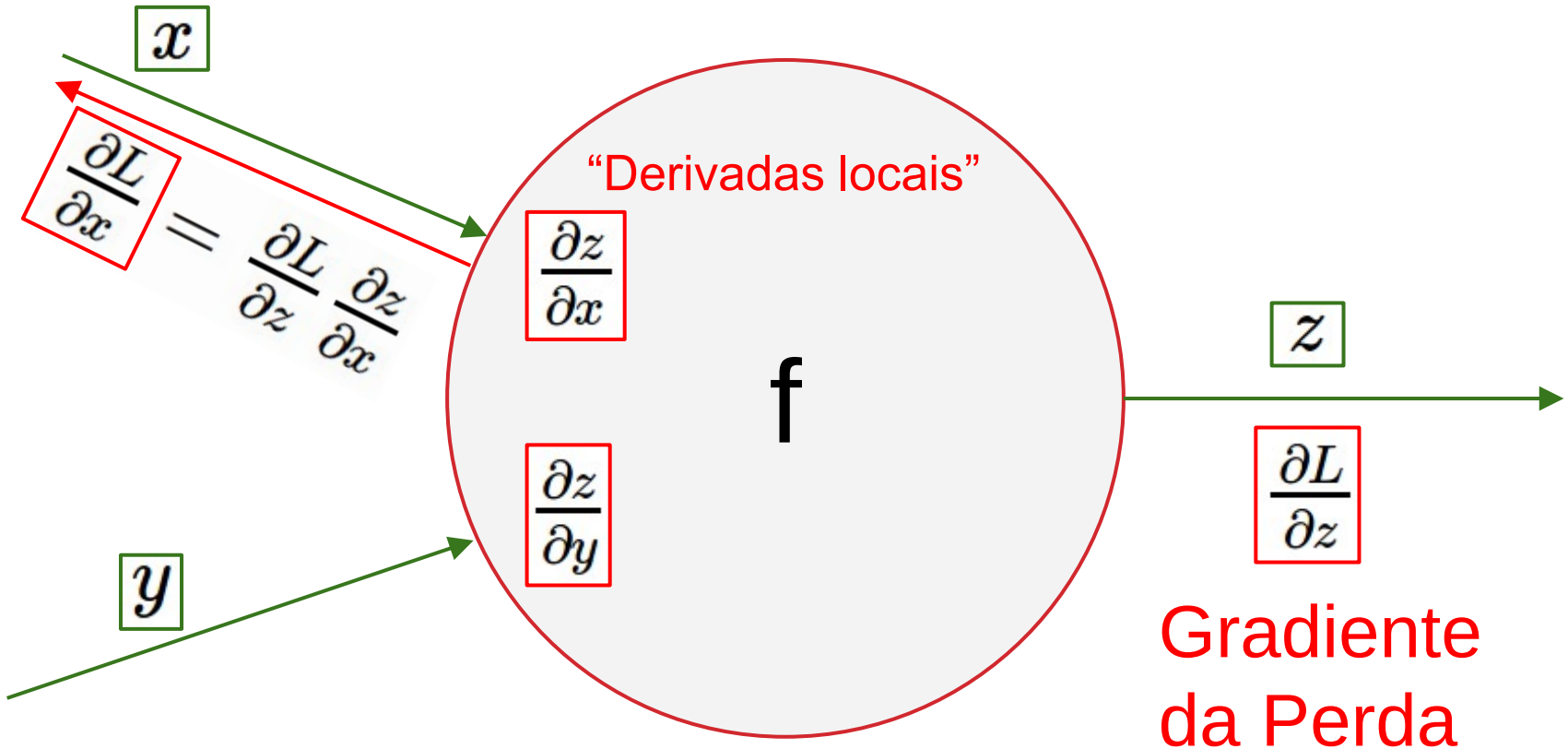
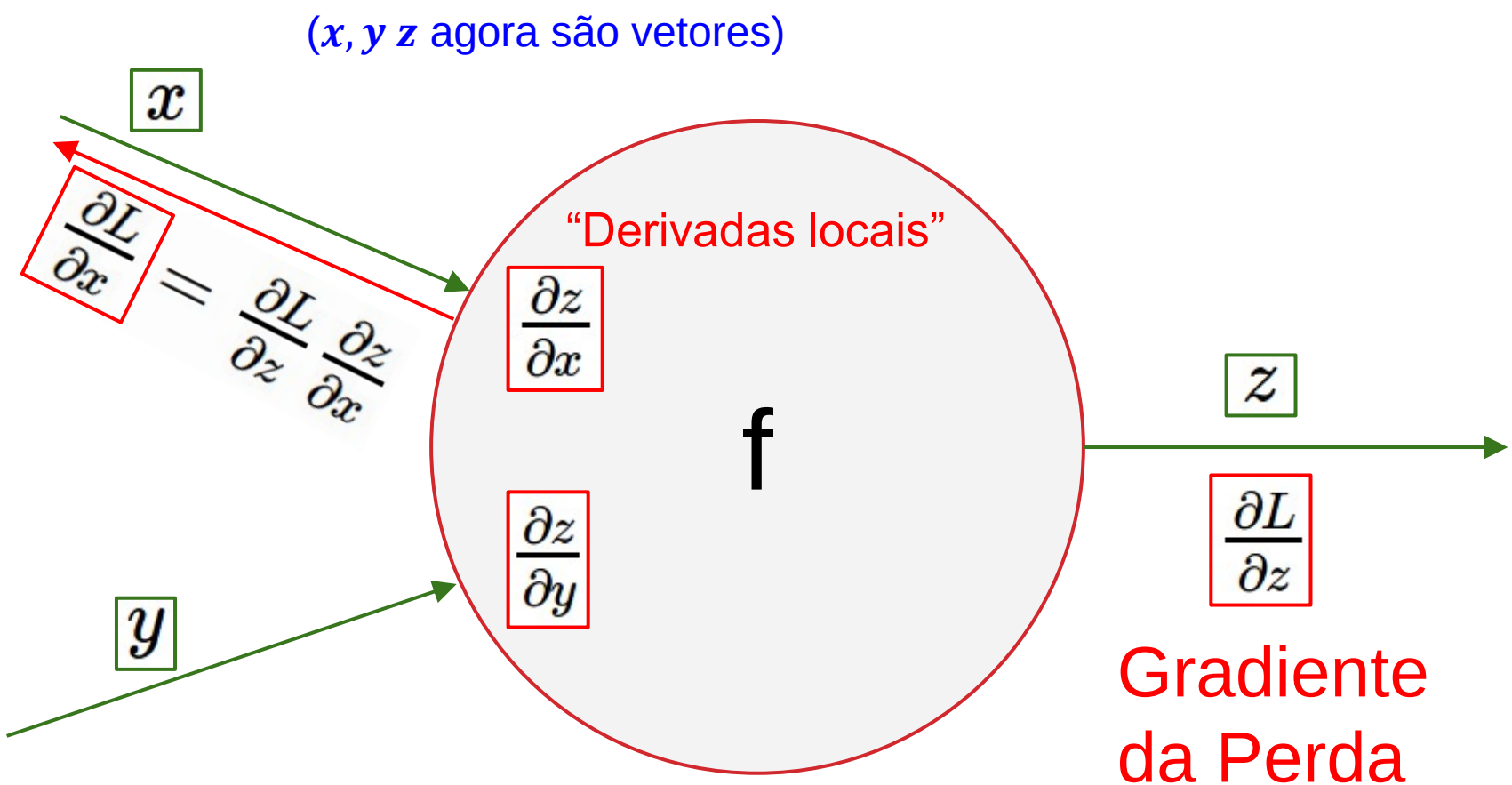


Deve-se realizar a **soma de todos os fluxos** (gradientes) antes de se aplicar a regra da cadeia usando as derivadas locais

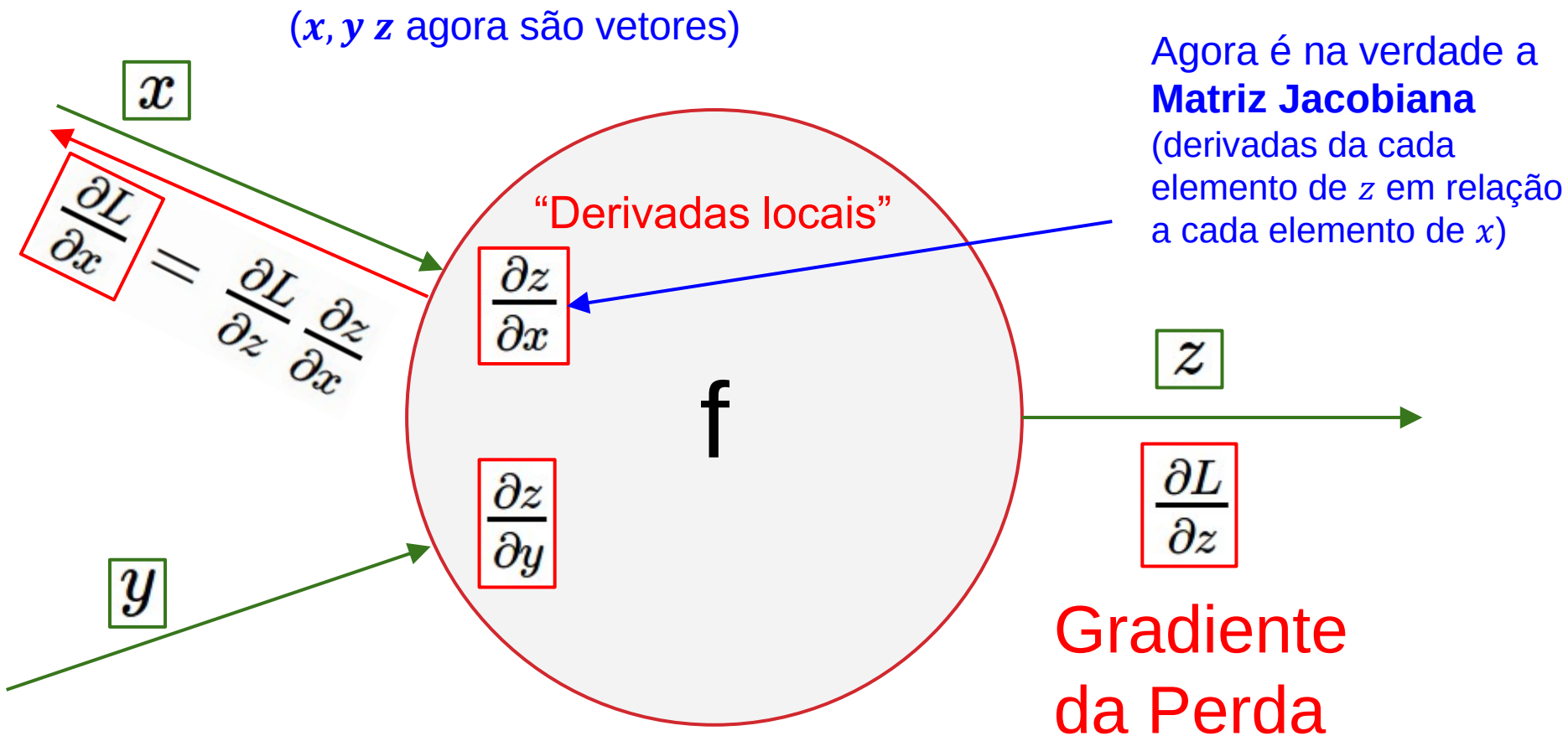
Gradientes para Dados Multidimensionais



Gradientes para Dados Multidimensionais



Gradientes para Dados Multidimensionais



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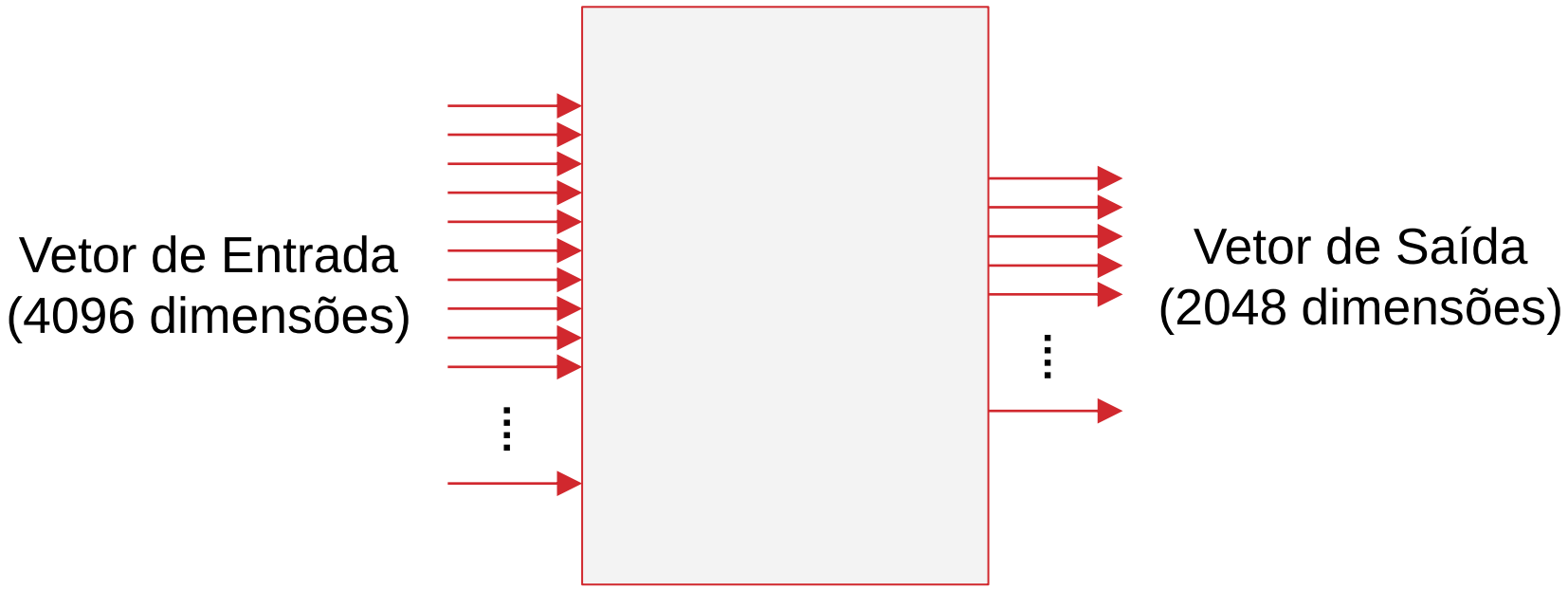
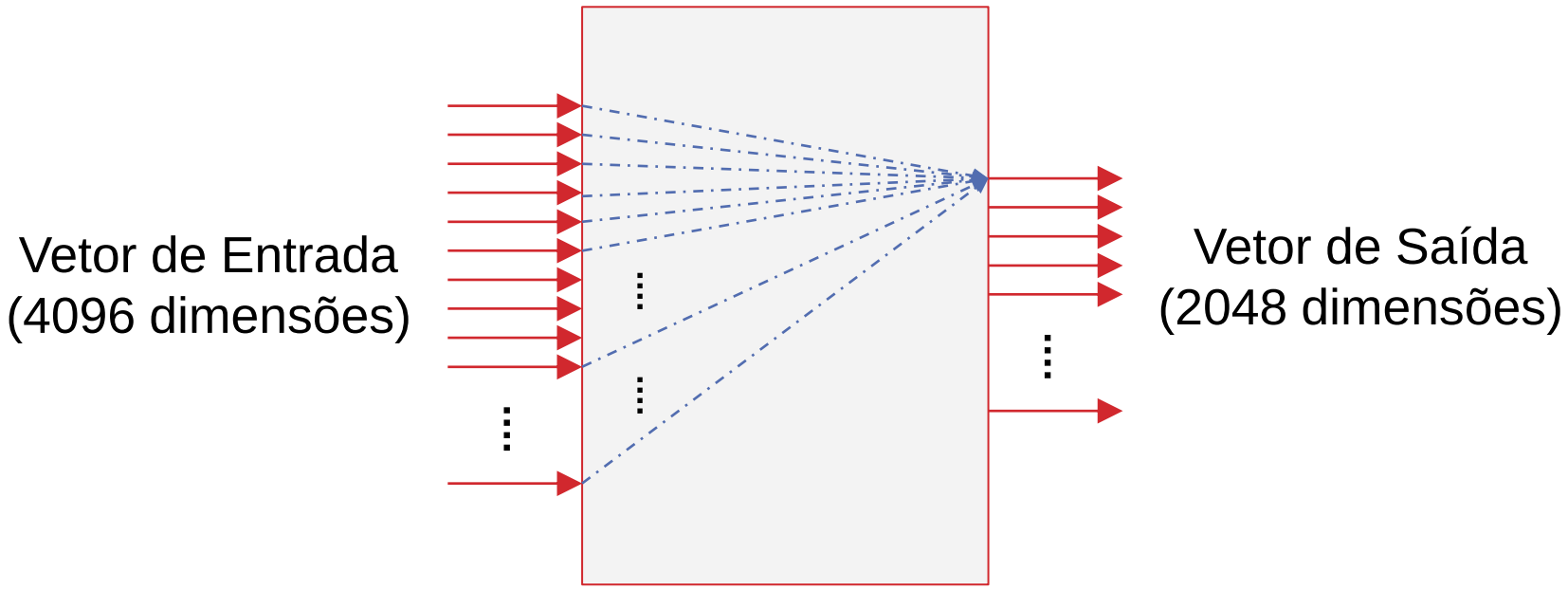


Gradientes para Dados Multidimensionais

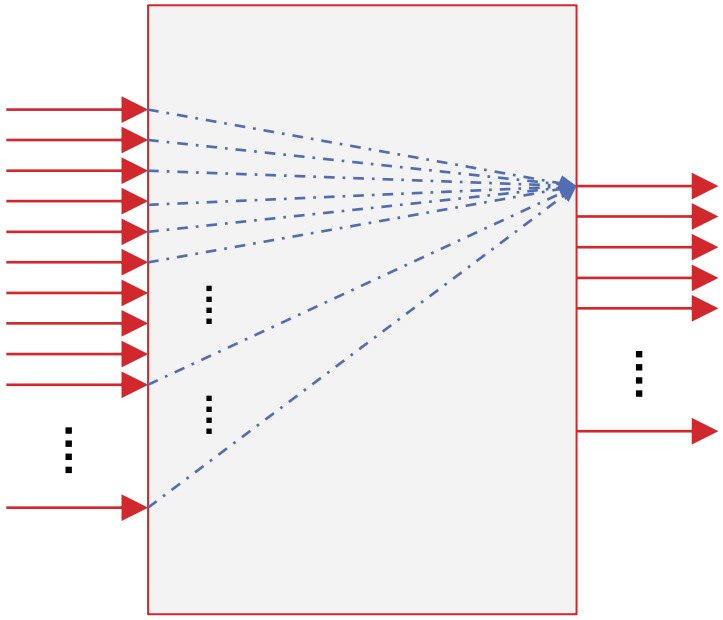


Gradientes para Dados Multidimensionais

$$\frac{\partial L}{\partial x} = \boxed{\frac{\partial f}{\partial x}} \frac{\partial L}{\partial f}$$

Matriz Jacobiana

Vetor de Entrada
(4096 dimensões)



Vetor de Saída
(2048 dimensões)

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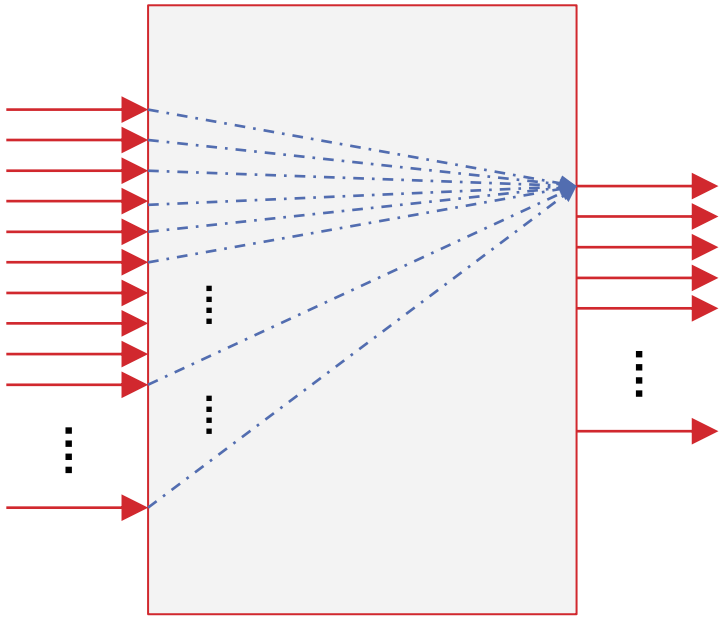

Vetor de Saída
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P1: qual o tamanho
da matriz Jacobiana?

Gradientes para Dados Multidimensionais

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Matriz Jacobiana

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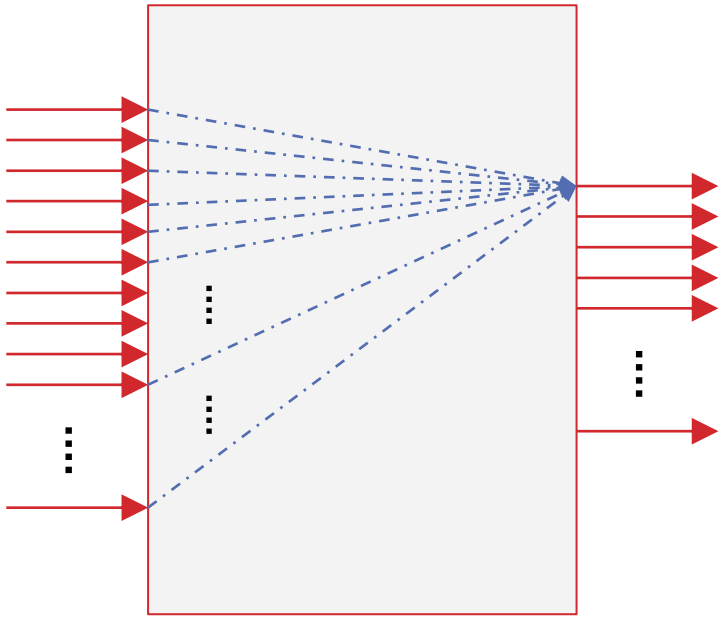

Vetor de Saída
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P1: qual o tamanho
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$\Rightarrow$ 2048 × 4096 !

Gradientes para Dados Multidimensionais

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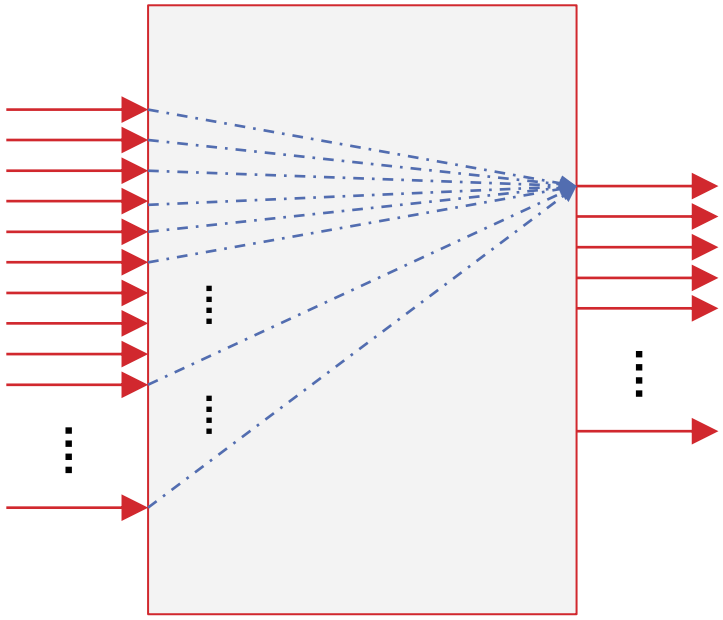

Vetor de Saída
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P1: qual o tamanho
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$\Rightarrow$ 2048 × 4096 !

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dessa matriz?

Gradientes para Dados Multidimensionais

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Matriz Jacobiana

Vetor de Entrada
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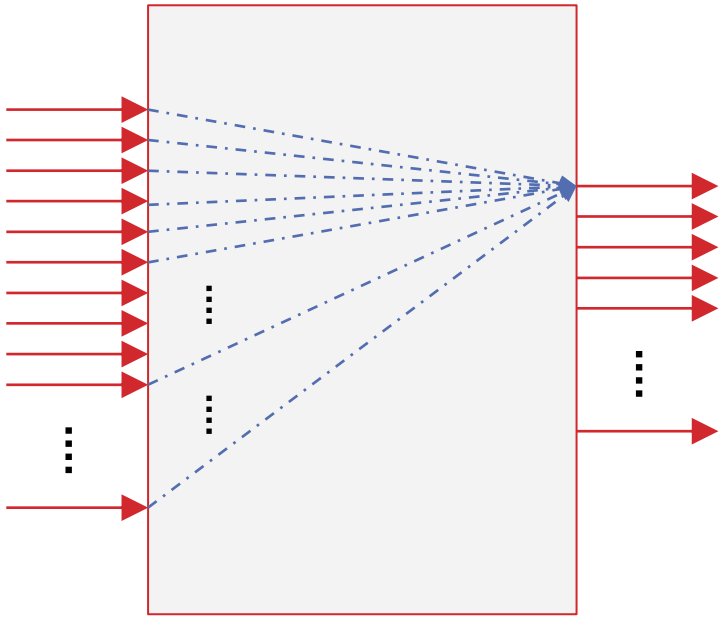

Vetor de Saída
(2048 dimensões)

P1: qual o tamanho
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$\Rightarrow$ 2048 × 4096 !

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dessa matriz?

$$\begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_m} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_k}{\partial x_1} & \frac{\partial f_k}{\partial x_2} & \cdots & \frac{\partial f_k}{\partial x_m} \end{bmatrix}$$

Gradientes para Dados Multidimensionais

$$\frac{\partial L}{\partial x} = \boxed{\frac{\partial f}{\partial x}} \frac{\partial L}{\partial f}$$

Matriz Jacobiana

Vetor de Entrada
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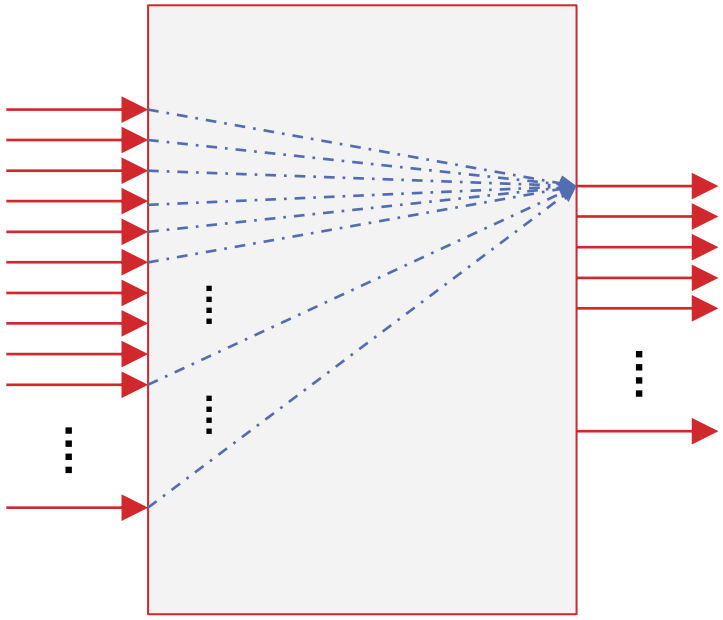

Vetor de Saída
(2048 dimensões)

Na prática, processa-se todo um lote ou "*minibatch*" (p.ex. 100 amostras) de uma só vez

Gradientes para Dados Multidimensionais

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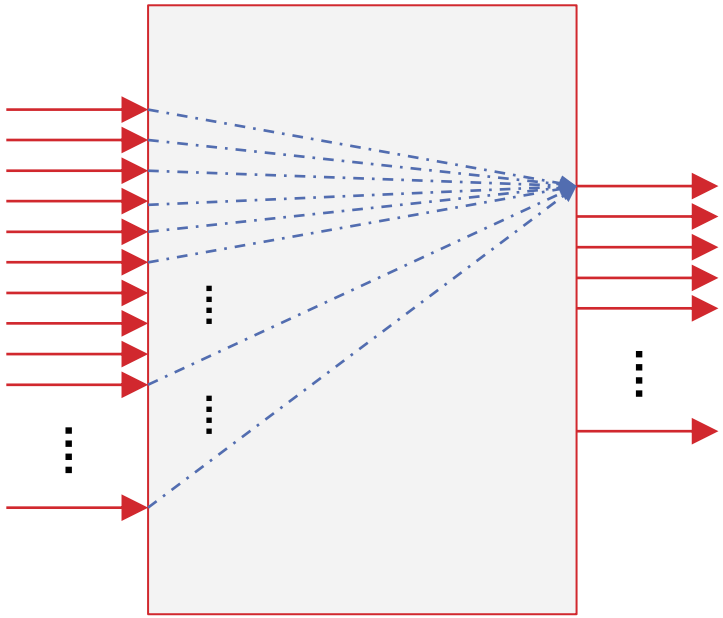
Matriz Jacobiana

Vetor de Entrada
(4096 dimensões)



Vetor de Saída
(2048 dimensões)

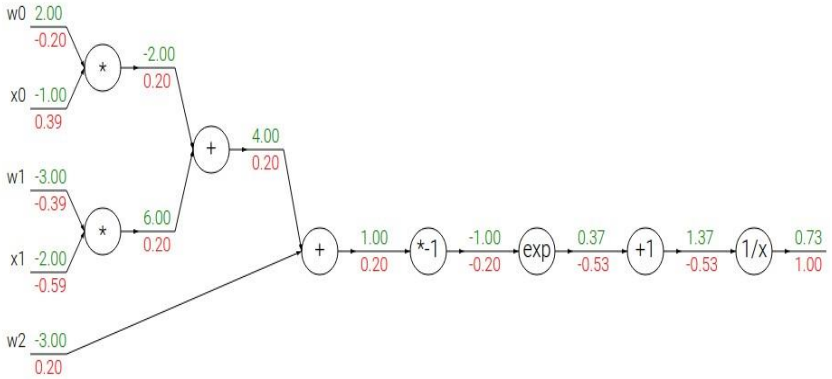
Na prática, processa-se todo um lote ou "*minibatch*" (p.ex. 100 amostras) de uma só vez

Assim, as dimensões da matriz Jacobiana desse exemplo seriam

2.048 × 4.096 × 100

≈ 839 milhões de pesos :(

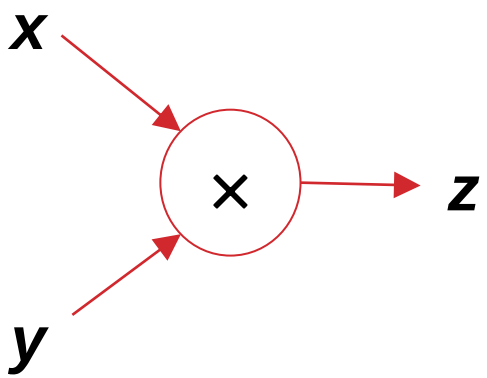
Implementação – Forward / Backward API



Para um grafo ou rede (*pseudocódigo*)

```
class ComputationalGraph(object):
    #...
    def forward(inputs):
        # 1. [pass inputs to input gates...]
        # 2. forward the computational graph:
        for gate in self.graph.nodes_topologically_sorted():
            gate.forward()
        return loss # the final gate in the graph outputs the loss
    def backward():
        for gate in reversed(self.graph.nodes_topologically_sorted()):
            gate.backward() # little piece of backprop (chain rule applied)
        return inputs_gradients
```

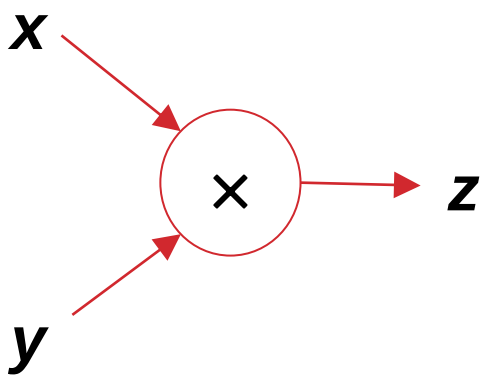
Implementação – Forward / Backward API



(*x*, *y*, *z* escalares)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        return z
    def backward(dz):
        # dx = ... #todo
        # dy = ... #todo
        return [dx, dy]
```

Implementação – Forward / Backward API



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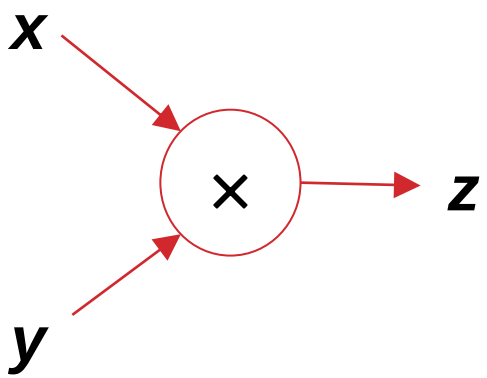

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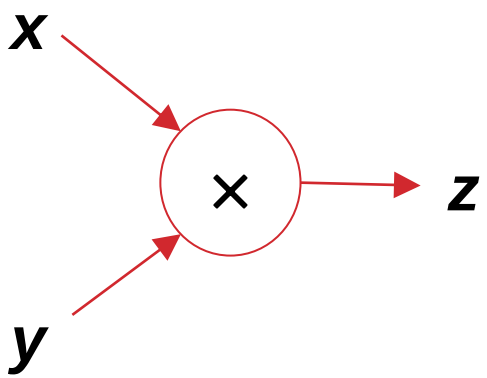
$\frac{\partial L}{\partial z}$

$\frac{\partial L}{\partial x}$

Implementação – Forward / Backward API



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class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
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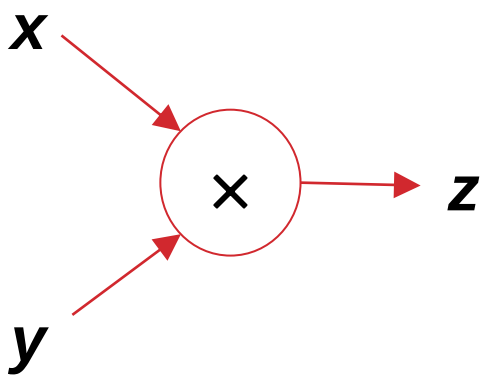
Implementação – Forward / Backward API



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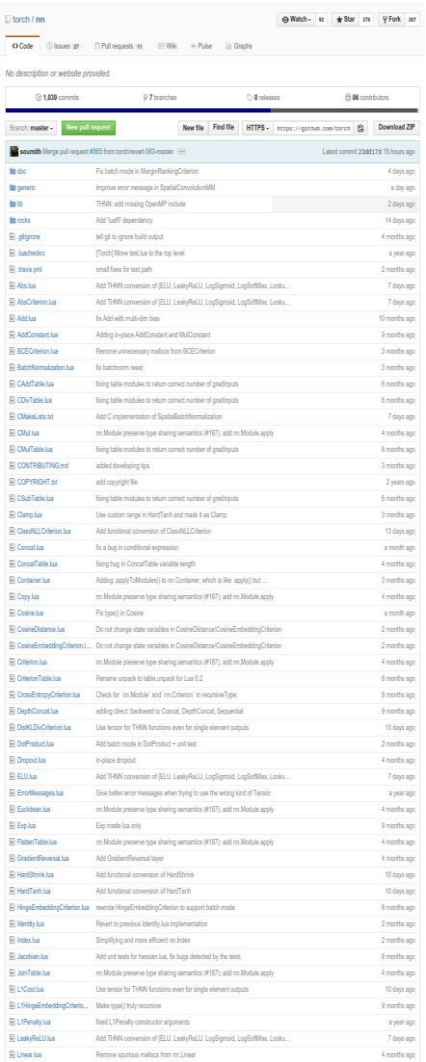
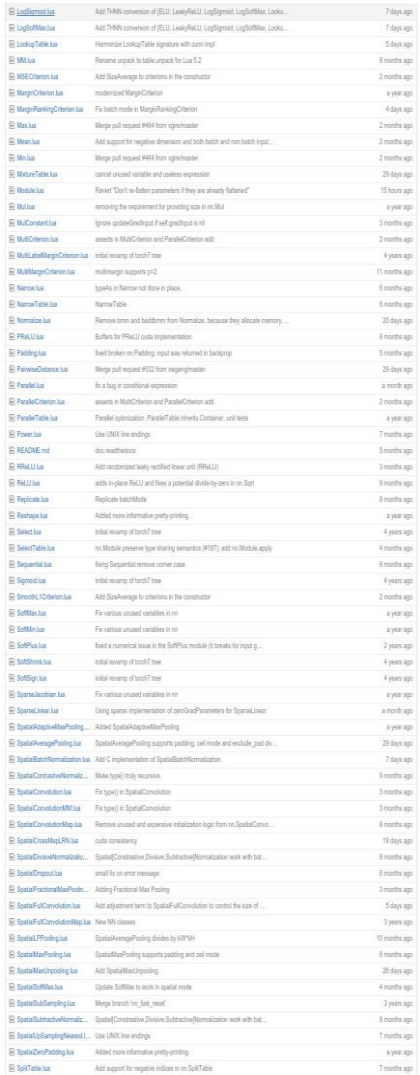
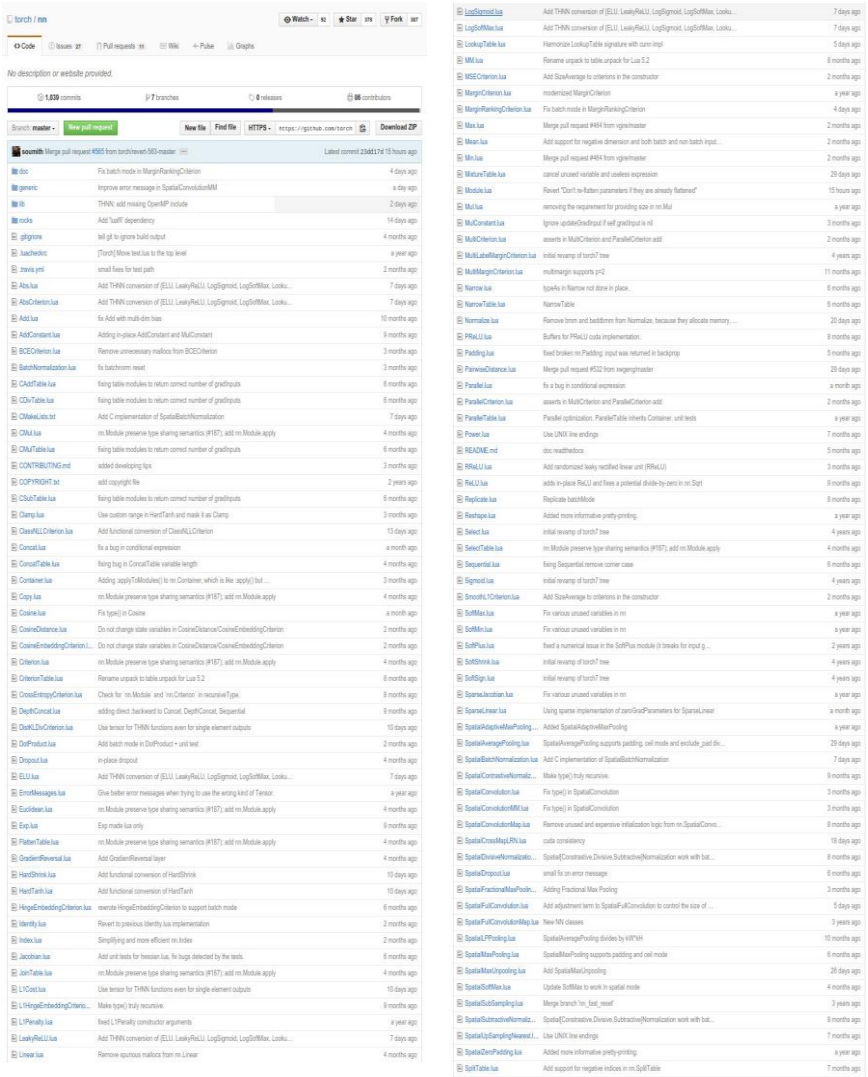
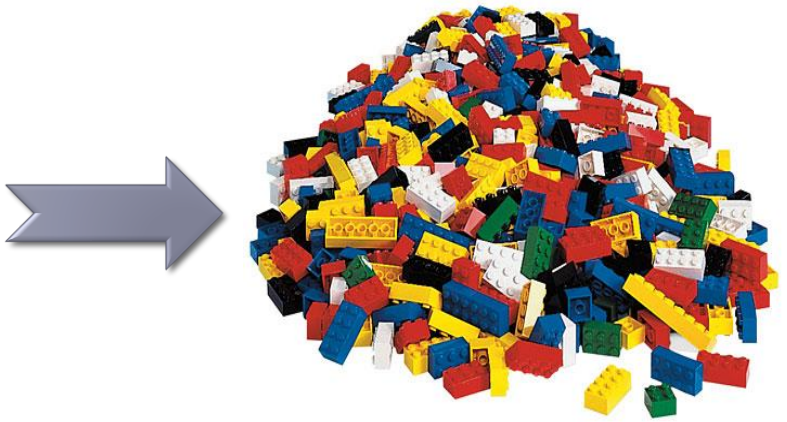
Biblioteca de Componentes / Camadas





Biblioteca de Componentes / Camadas





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