

Backpropagation and Neural Networks

Slides adapted from: <http://cs231n.stanford.edu/syllabus.html>

Gerard Pons-Moll

Where we are...

$$s = f(x; W) = Wx$$

scores function

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

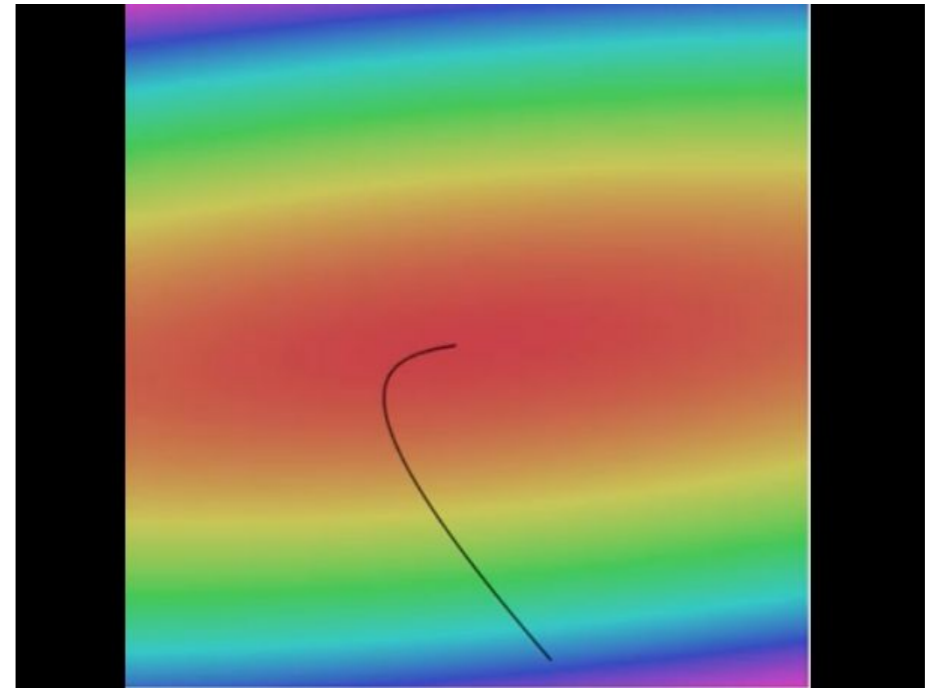
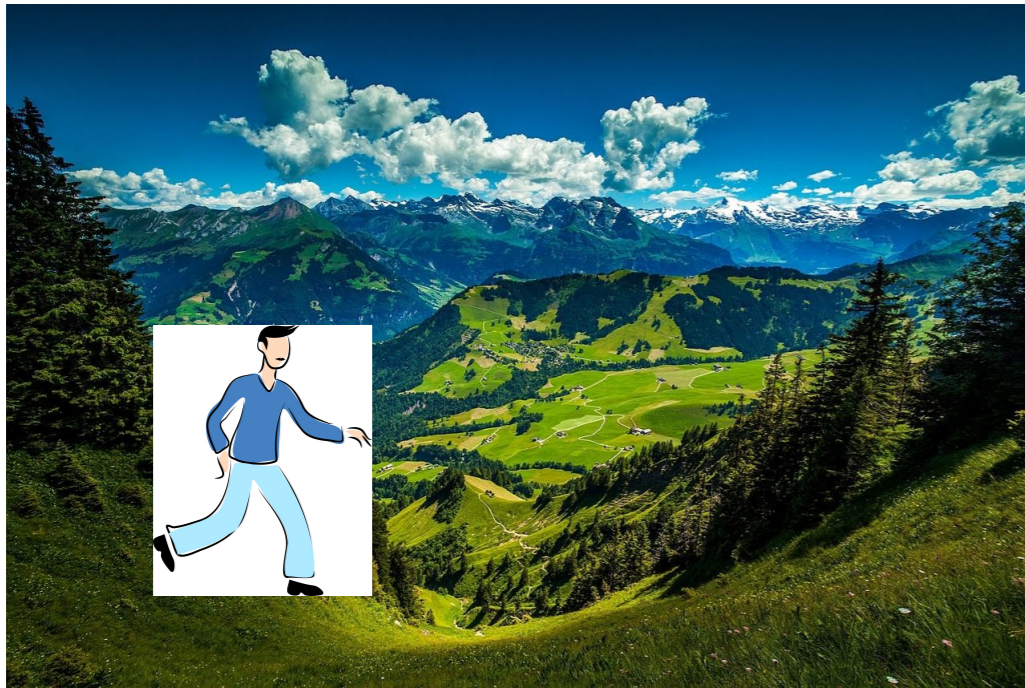
SVM loss

$$L = \frac{1}{N} \sum_{i=1}^N L_i + \sum_k W_k^2$$

data loss + regularization

want $\nabla_W L$

Optimization



```
# Vanilla Gradient Descent

while True:
    weights_grad = evaluate_gradient(loss_fun, data, weights)
    weights += - step_size * weights_grad # perform parameter update
```

[Landscape image](#) is [CC0 1.0](#) public domain
[Walking man image](#) is [CC0 1.0](#) public domain

Gradient descent

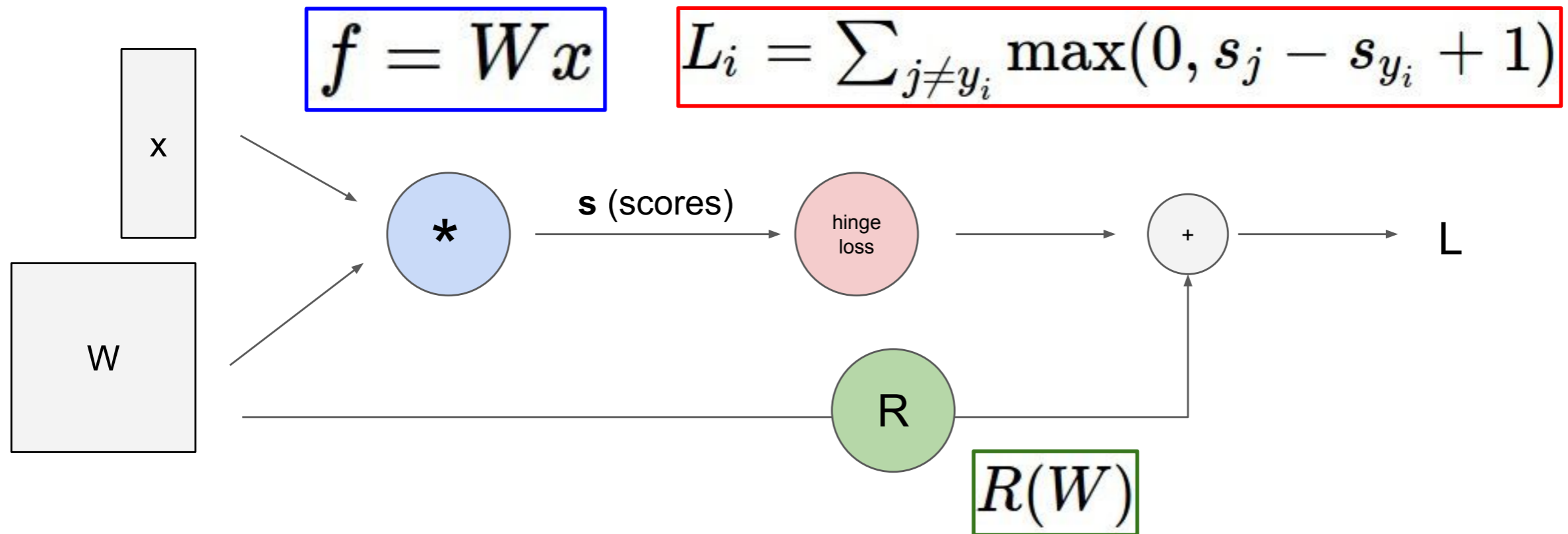
$$\frac{df(x)}{dx} = \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}$$

Numerical gradient: slow :(, approximate :(, easy to write :)

Analytic gradient: fast :), exact :), error-prone :(

In practice: Derive analytic gradient, check your implementation with numerical gradient

Computational graphs



Convolutional network (AlexNet)

input image

weights

loss

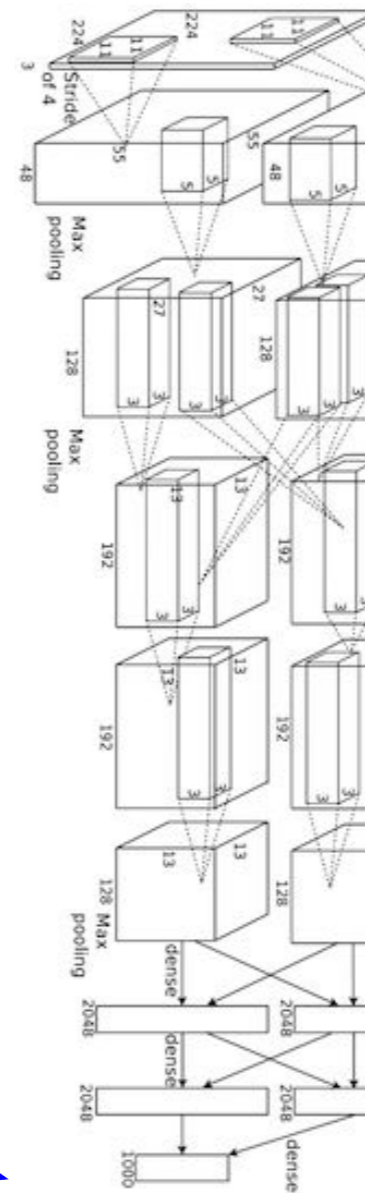


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

Neural Turing Machine

input image

loss

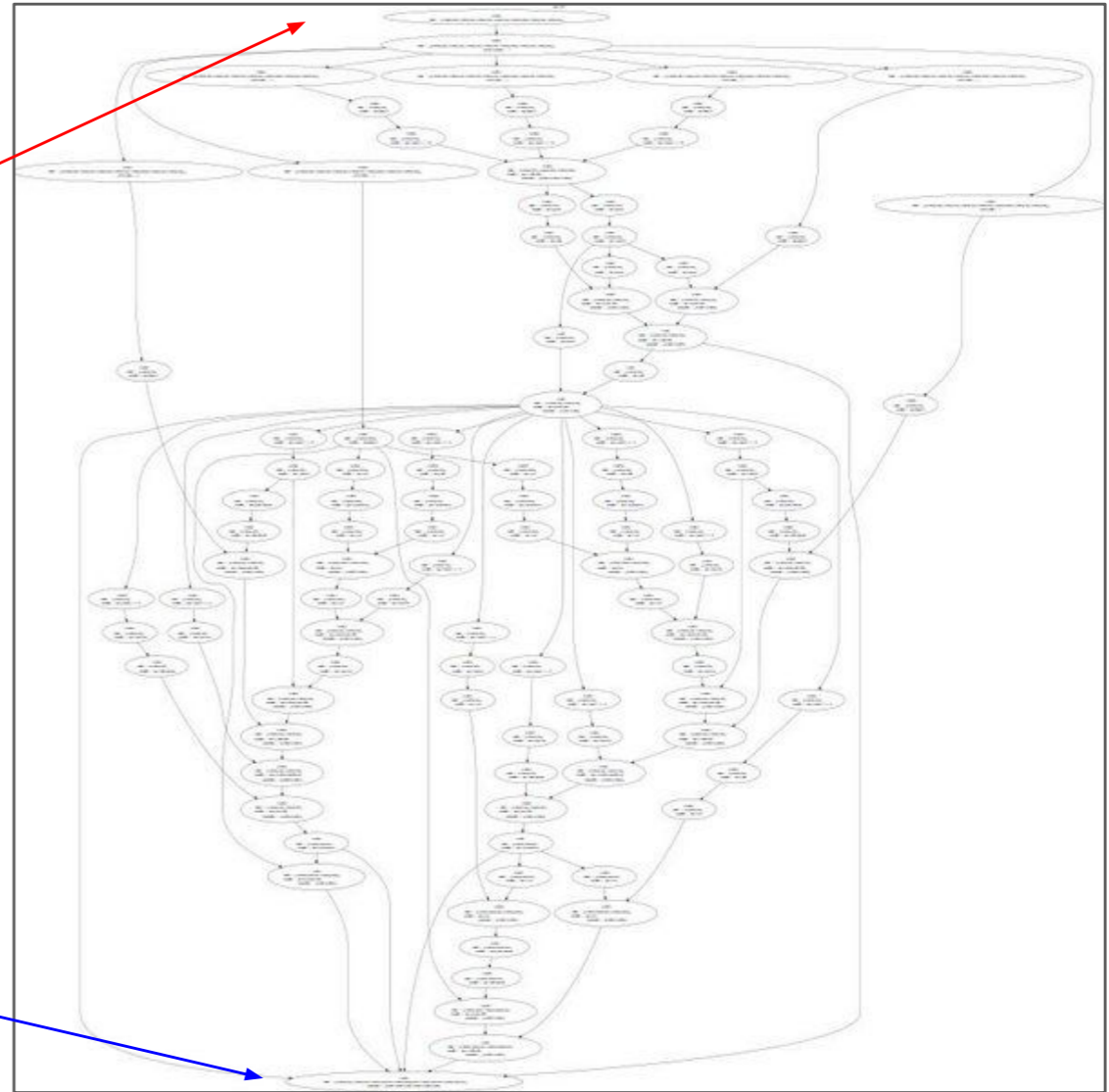


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

Neural Turing Machine

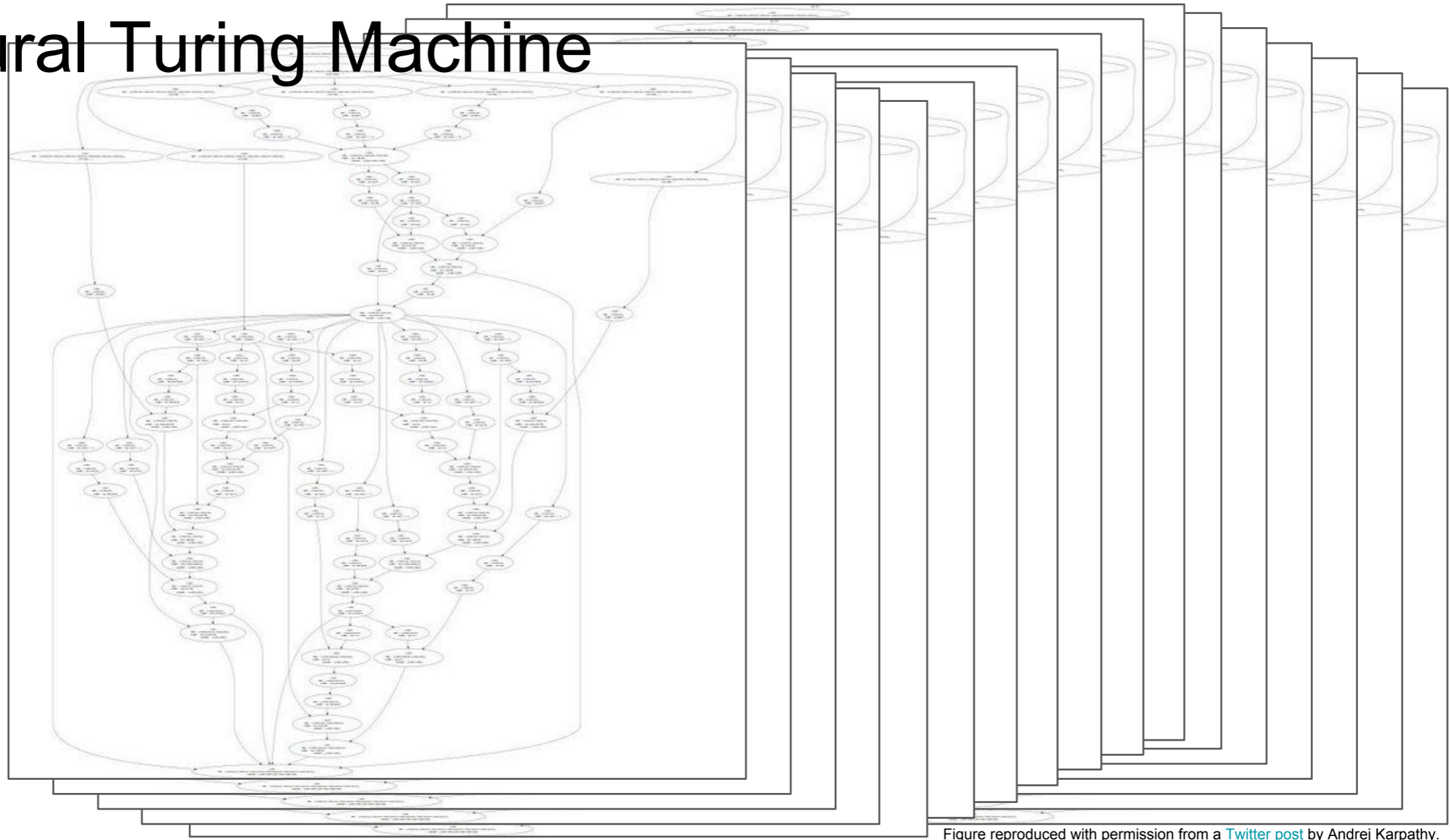


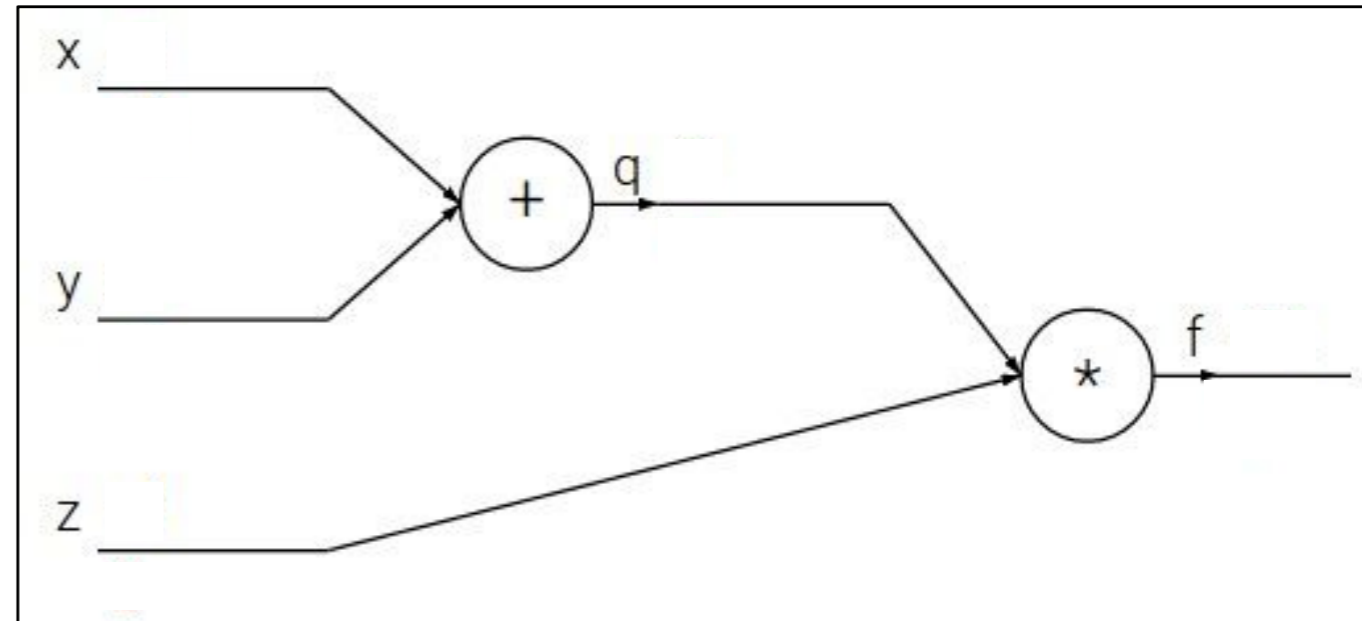
Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

Backpropagation: a simple example

$$f(x, y, z) = (x + y)z$$

Backpropagation: a simple example

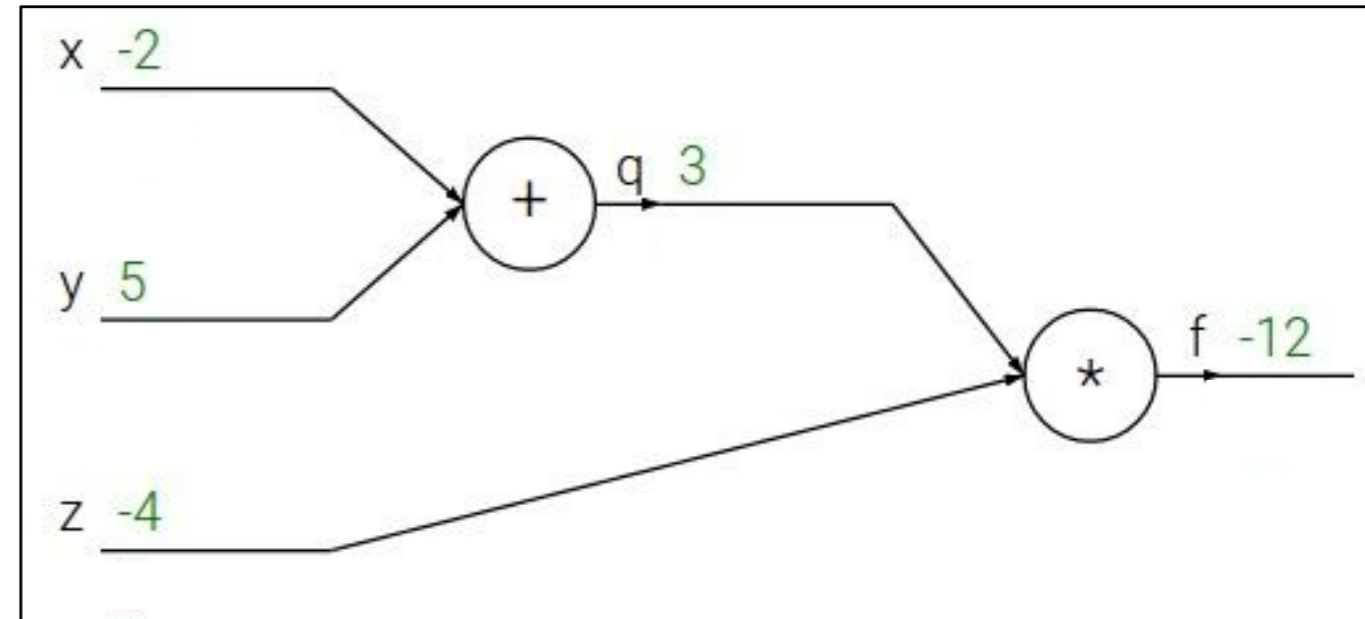
$$f(x, y, z) = (x + y)z$$



Backpropagation: a simple example

$$f(x, y, z) = (x + y)z$$

e.g. $x = -2$, $y = 5$, $z = -4$



Backpropagation: a simple example

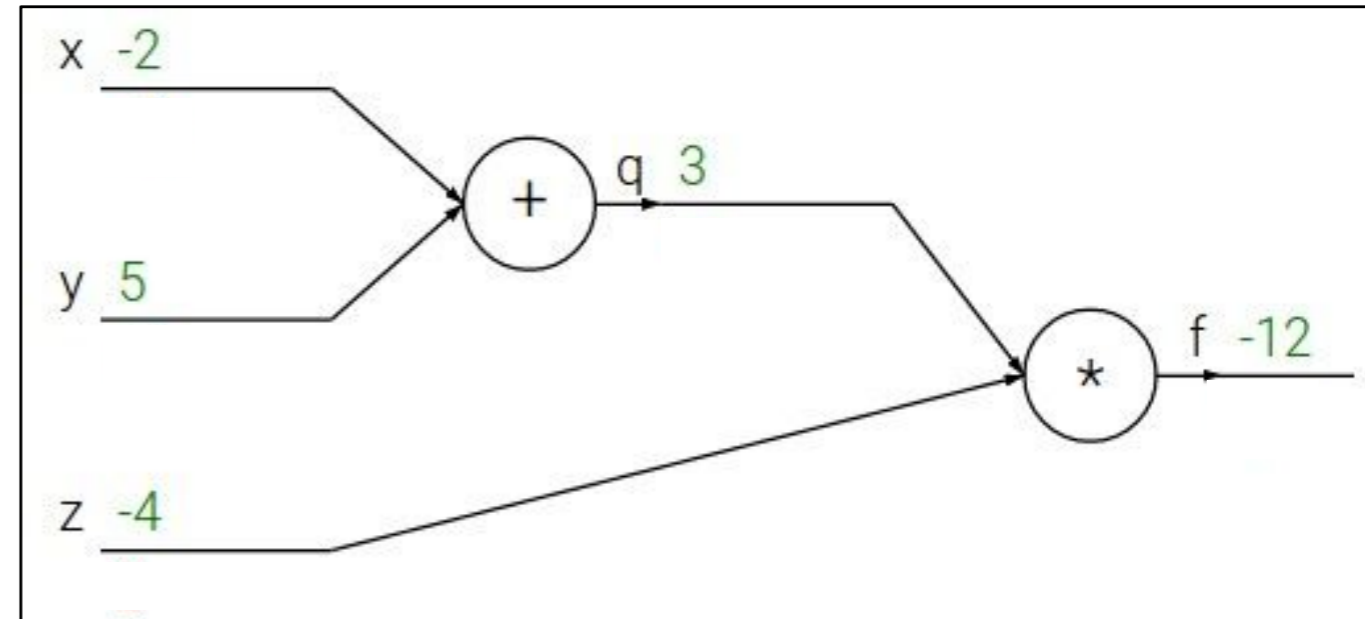
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Backpropagation: a simple example

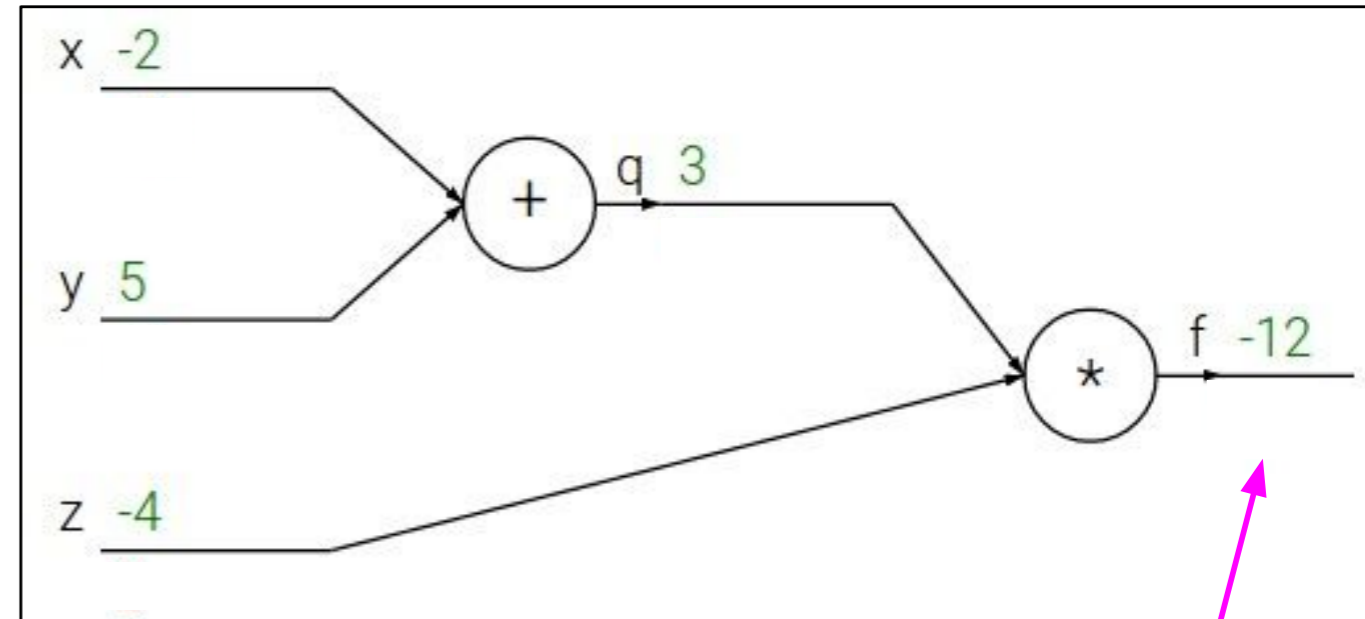
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Backpropagation: a simple example

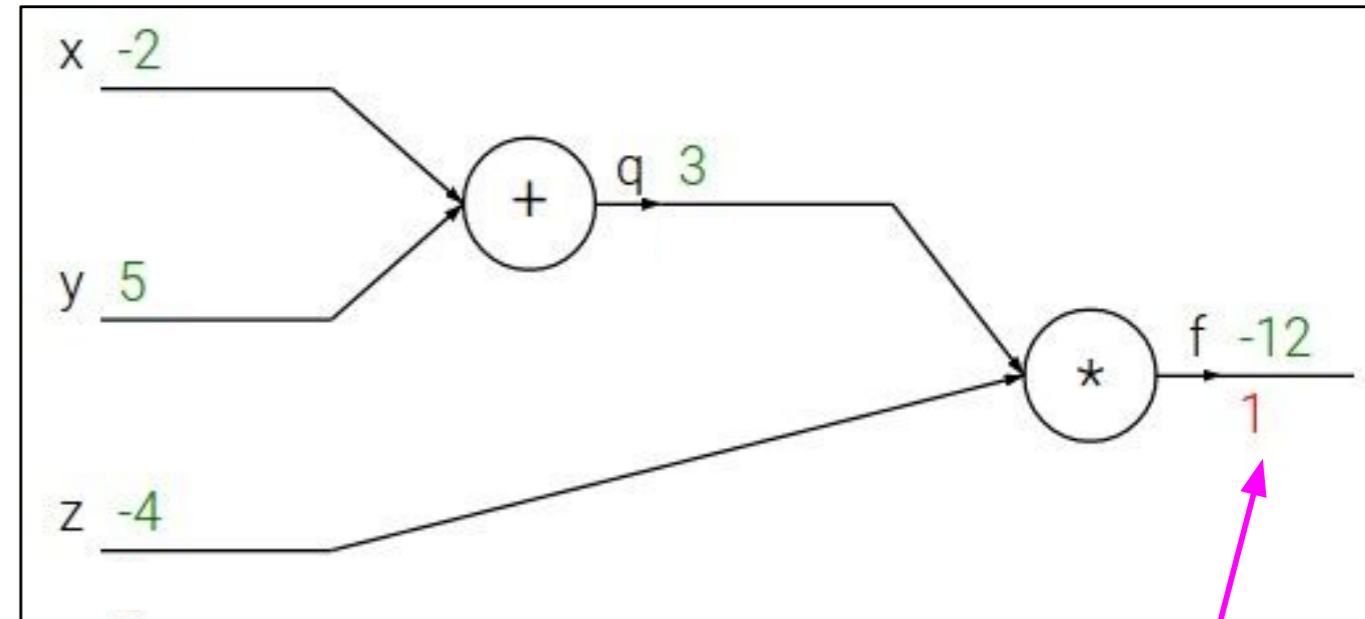
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Backpropagation: a simple example

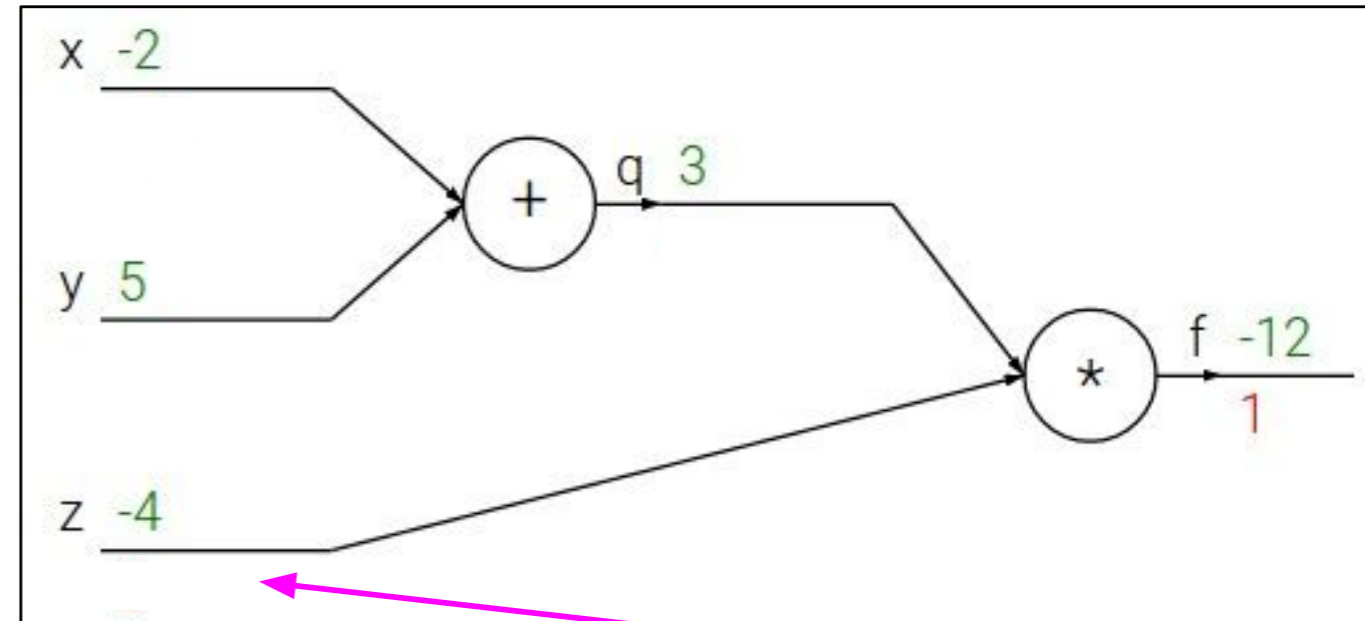
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial z}$$

Backpropagation: a simple example

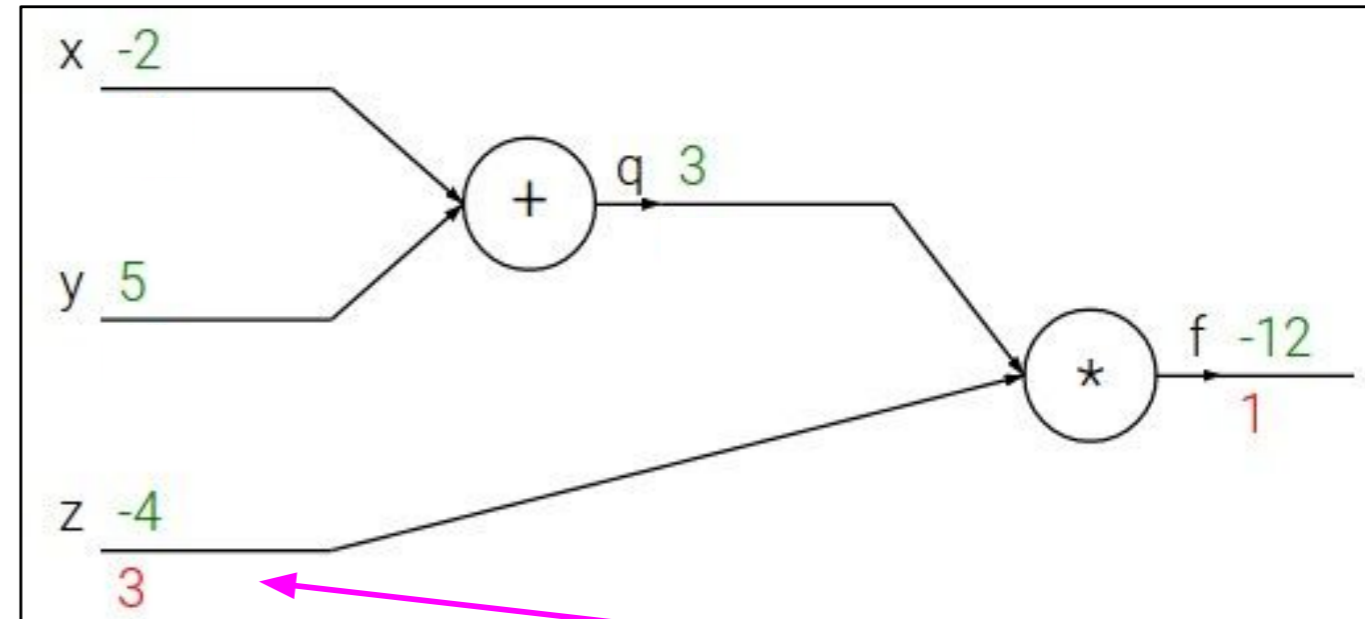
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial z}$$

Backpropagation: a simple example

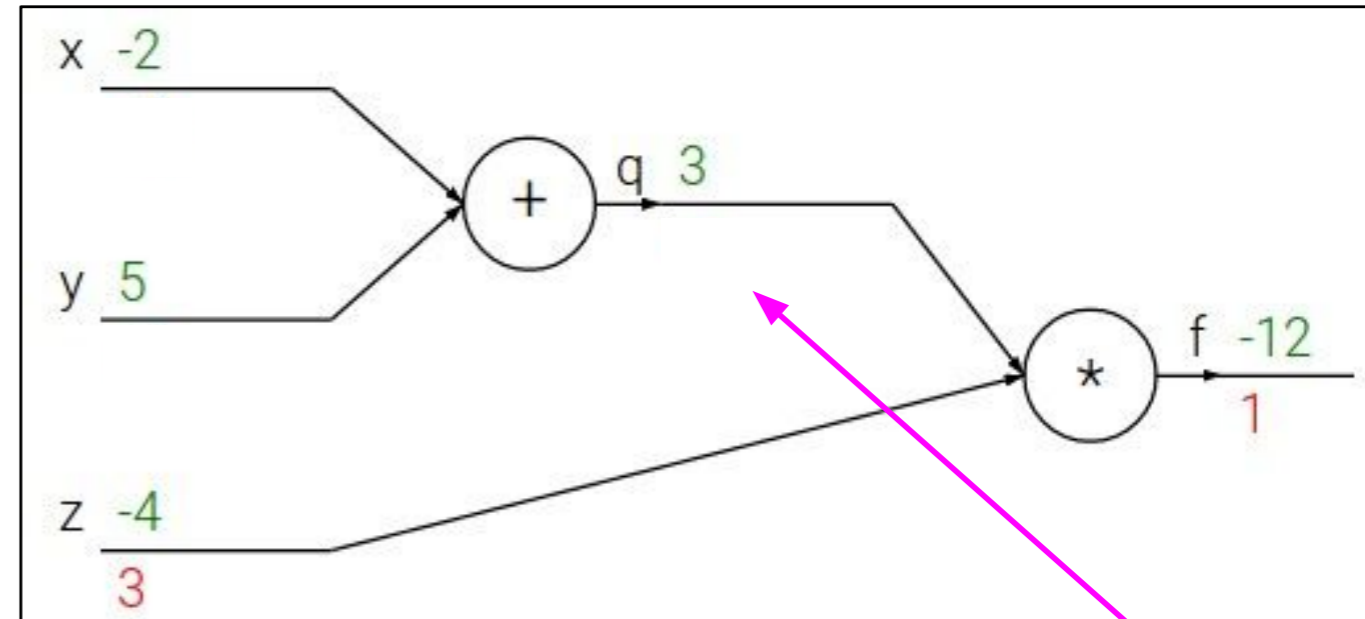
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Backpropagation: a simple example

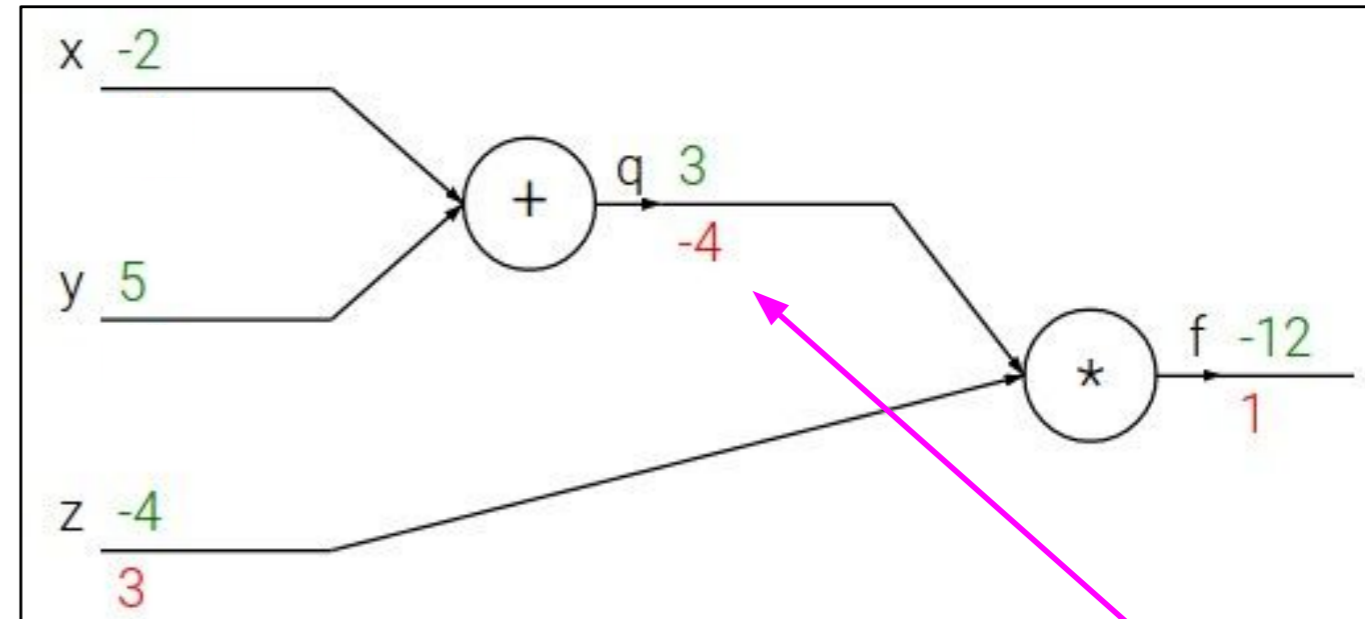
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Backpropagation: a simple example

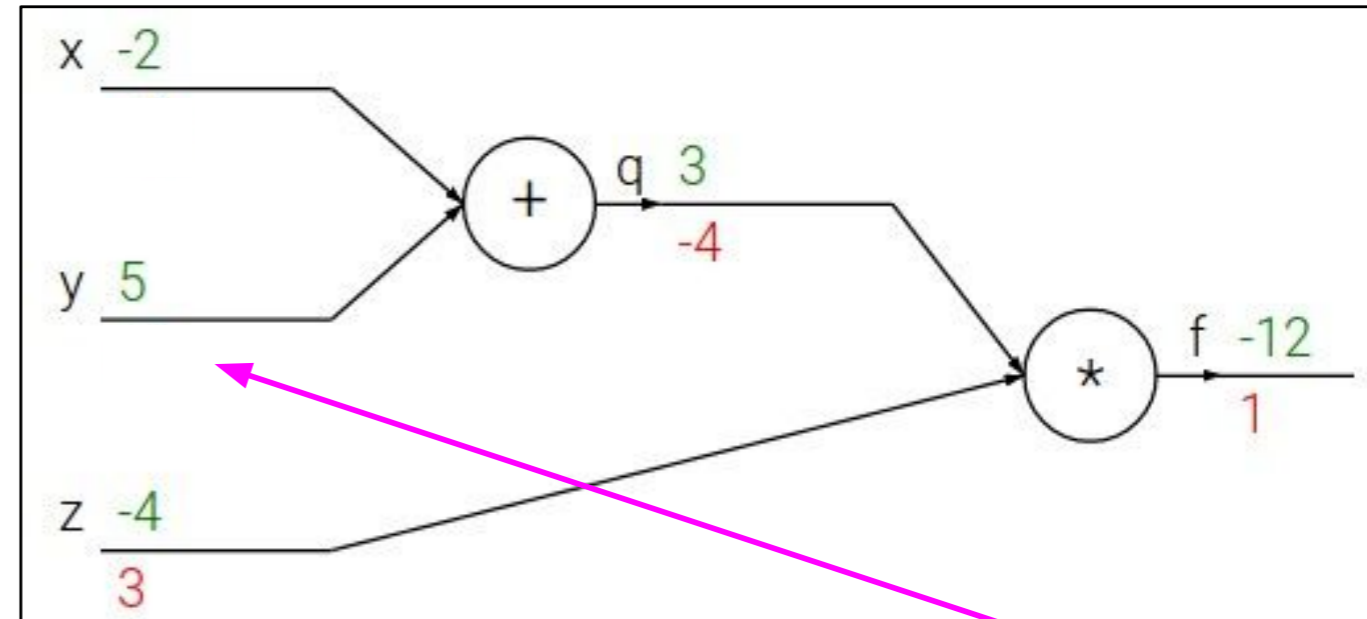
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial y}$$

Chain rule:

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

Upstream
gradient

Local
gradient

Backpropagation: a simple example

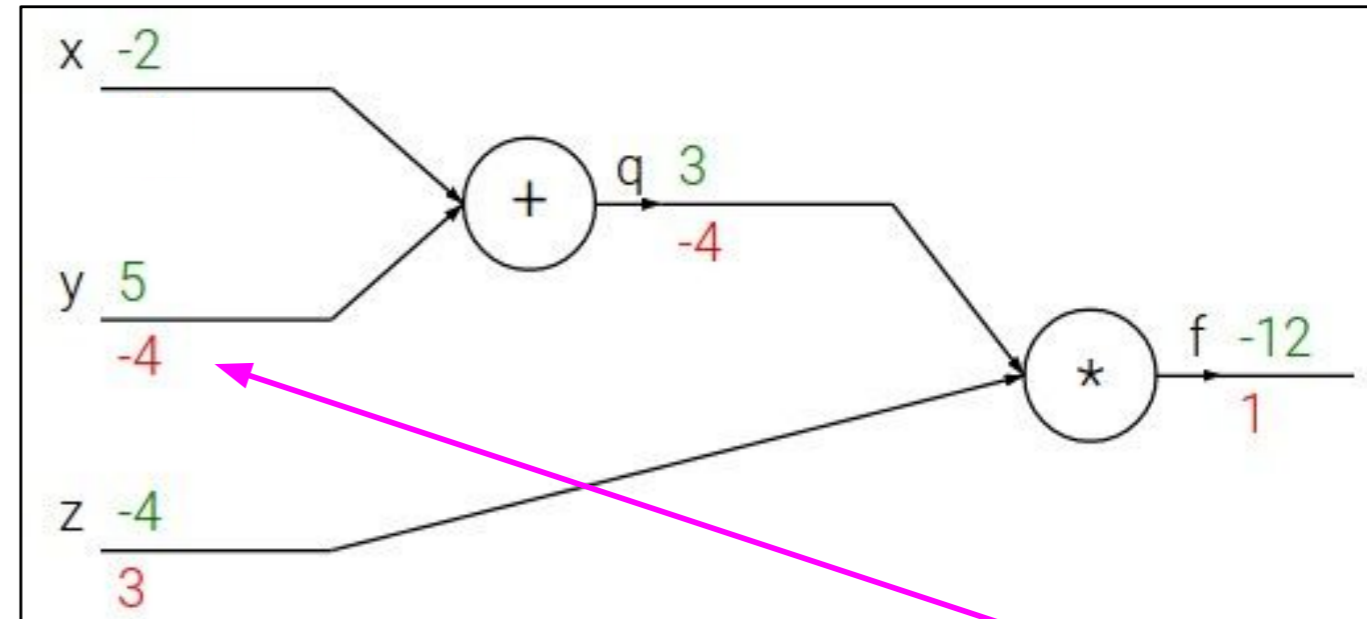
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial f}{\partial y}$$

Chain rule:

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

Upstream
gradient

Local
gradient

Backpropagation: a simple example

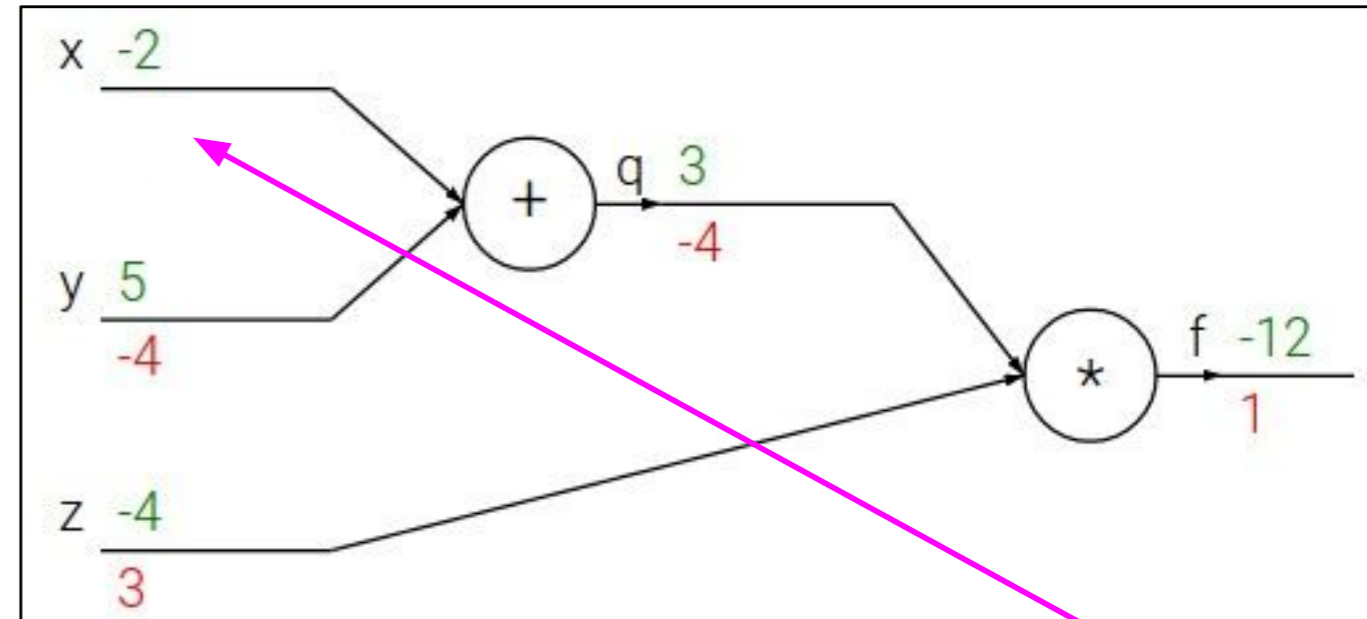
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Chain rule:

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

Upstream
gradient

Local
gradient

Backpropagation: a simple example

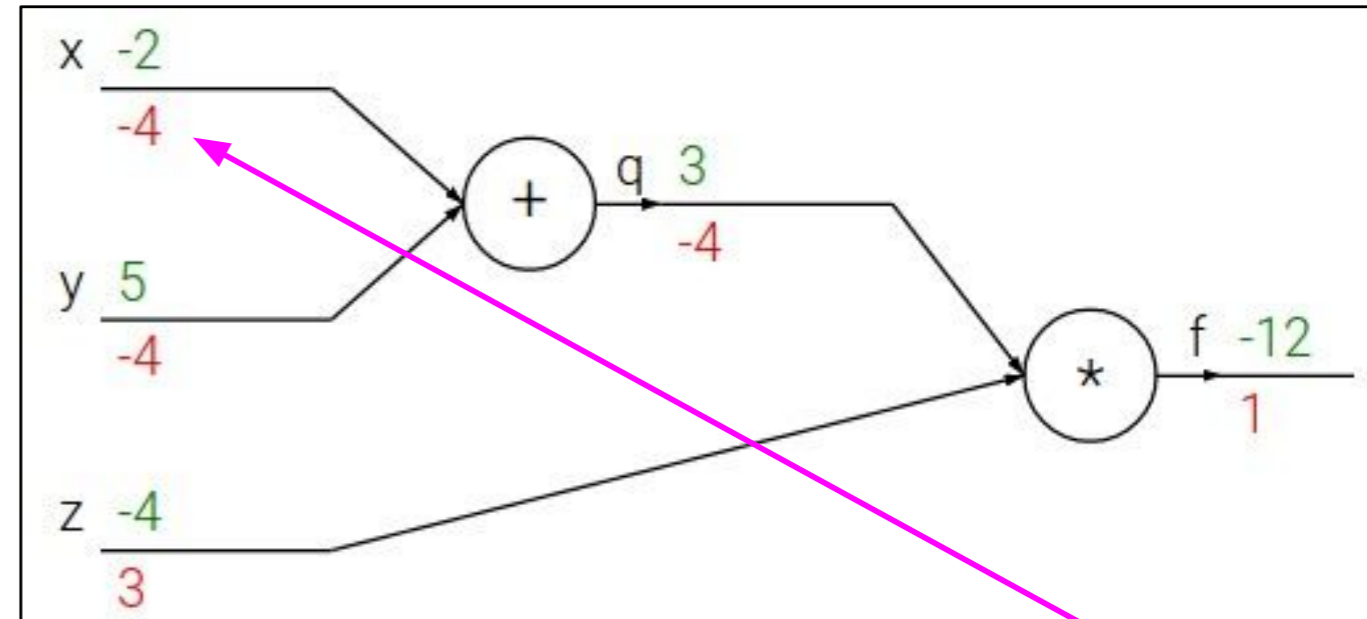
$$f(x, y, z) = (x + y)z$$

e.g. $x = -2, y = 5, z = -4$

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

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

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



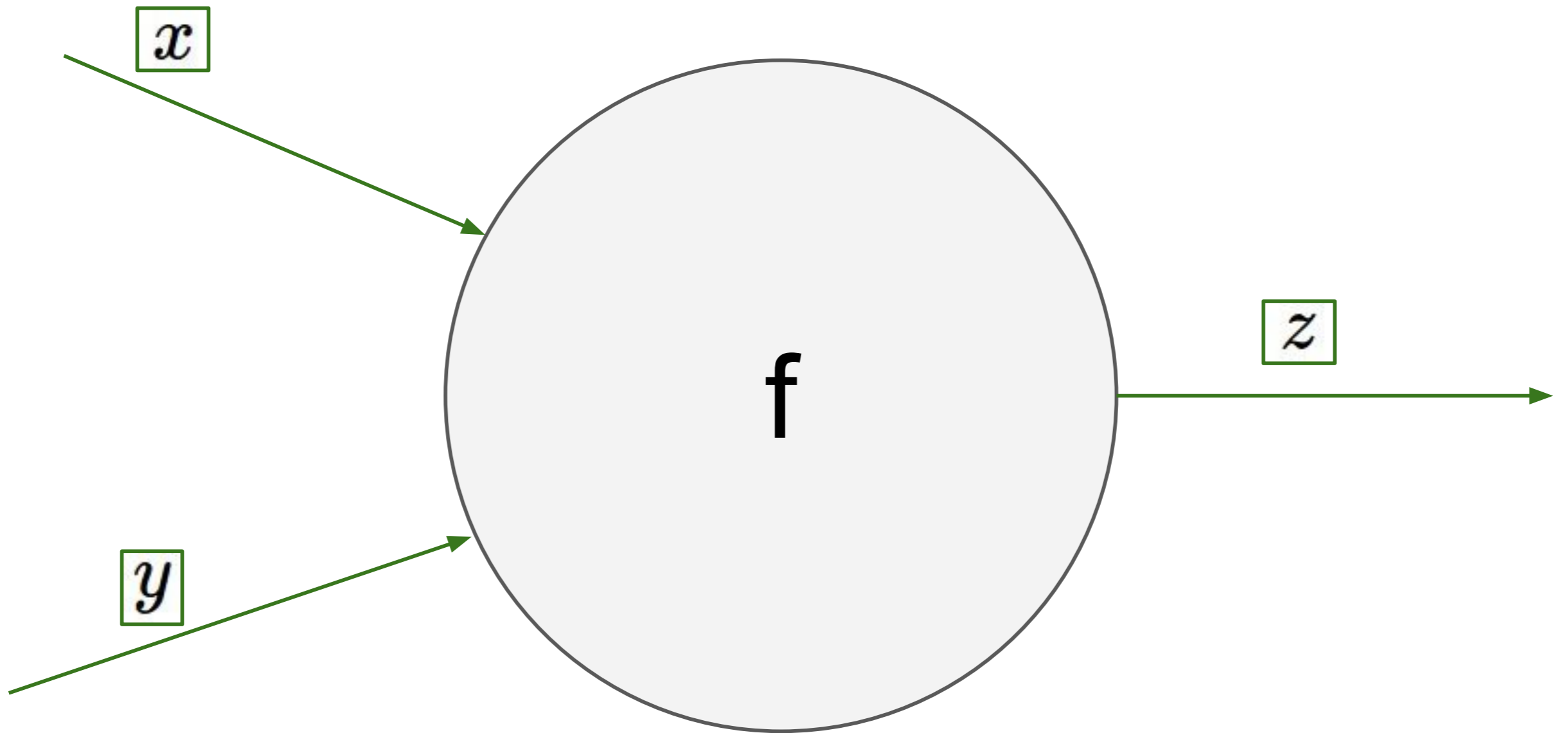
$$\frac{\partial f}{\partial x}$$

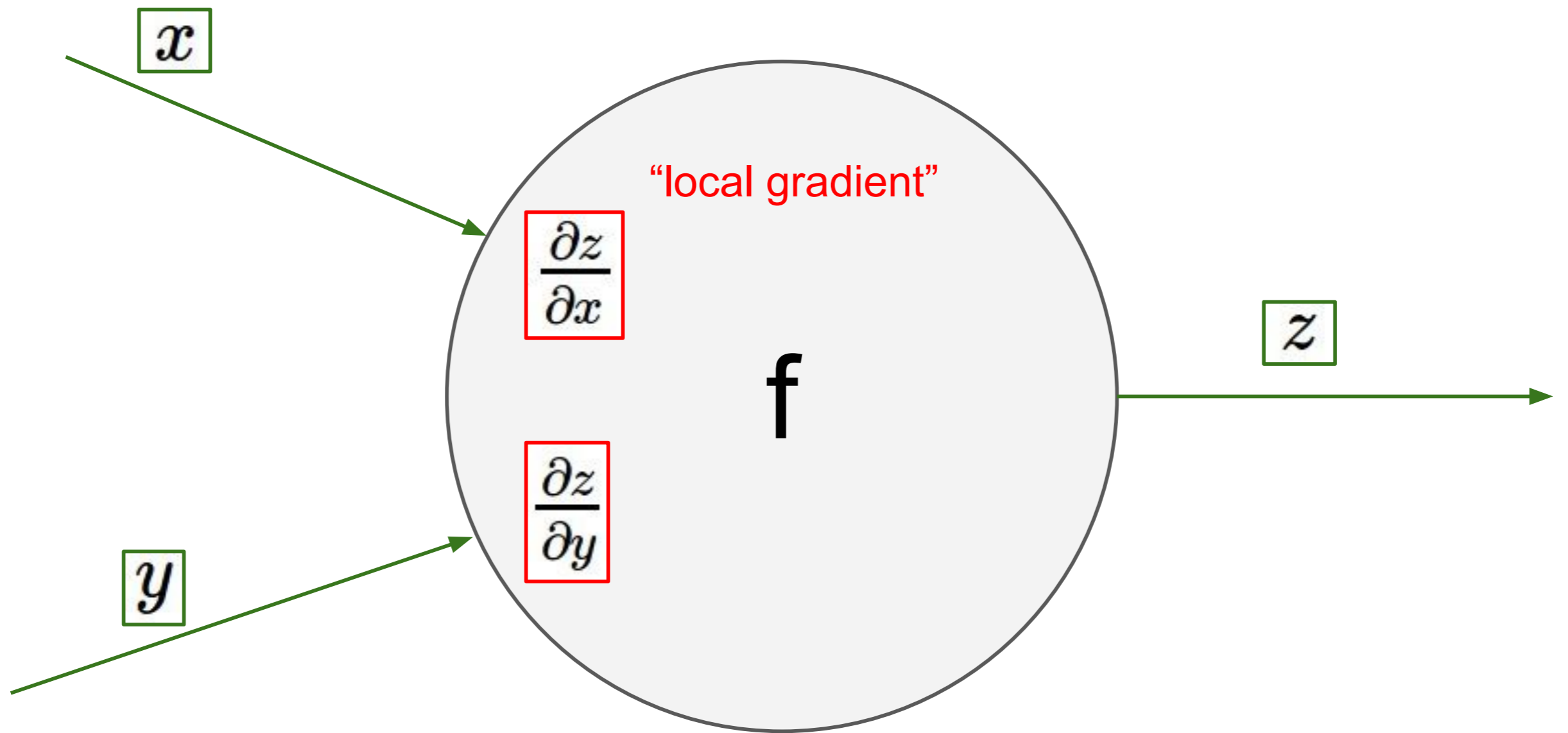
Chain rule:

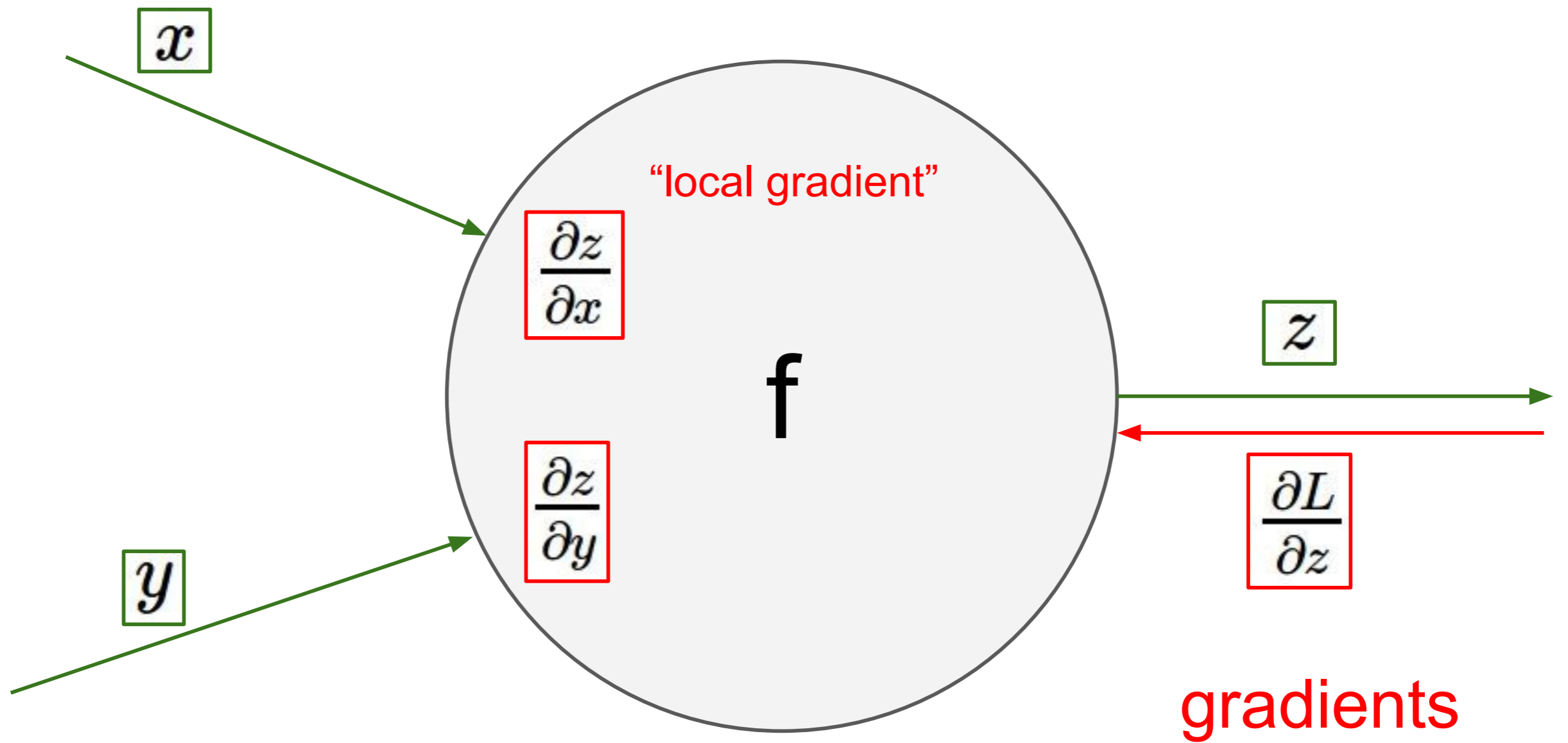
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

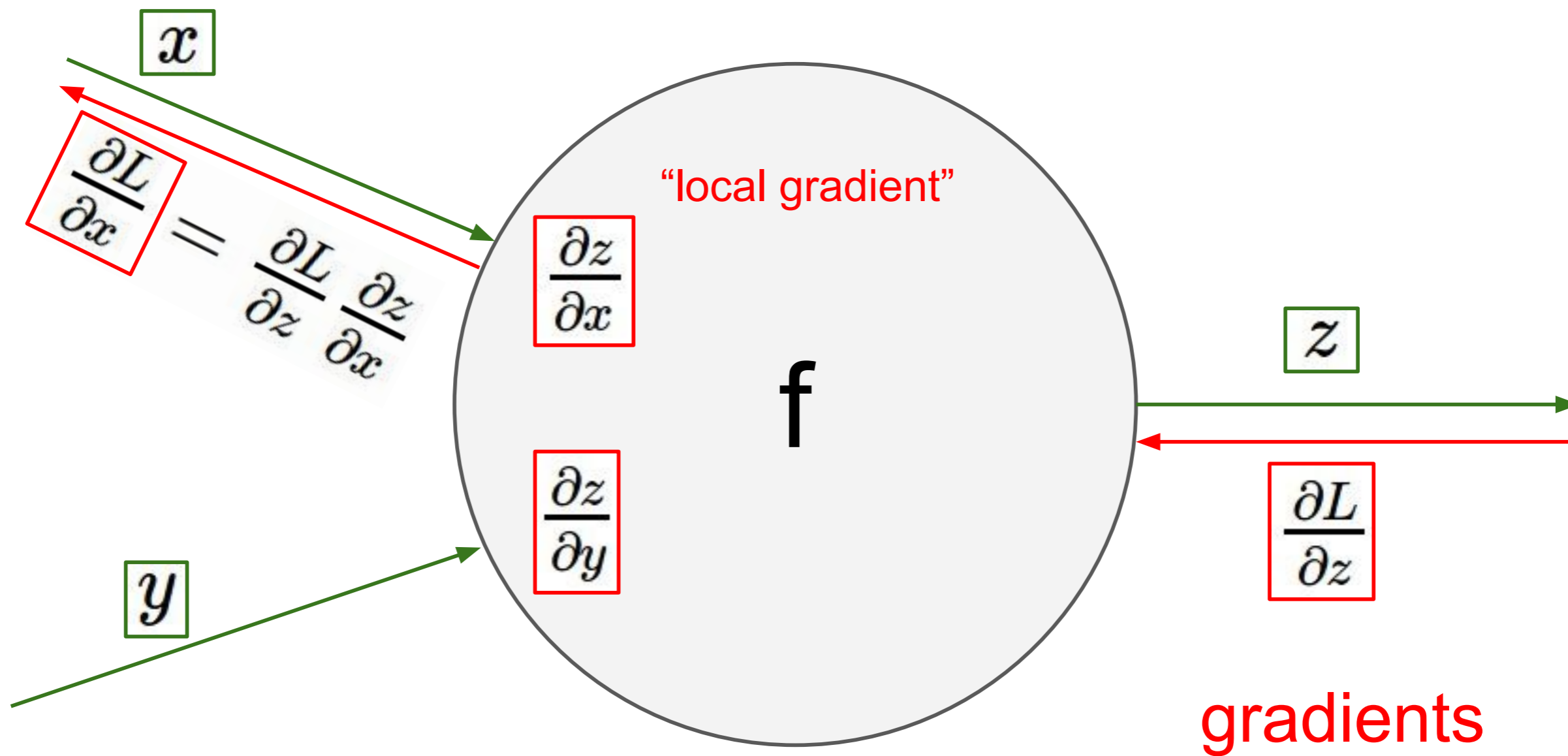
Upstream
gradient

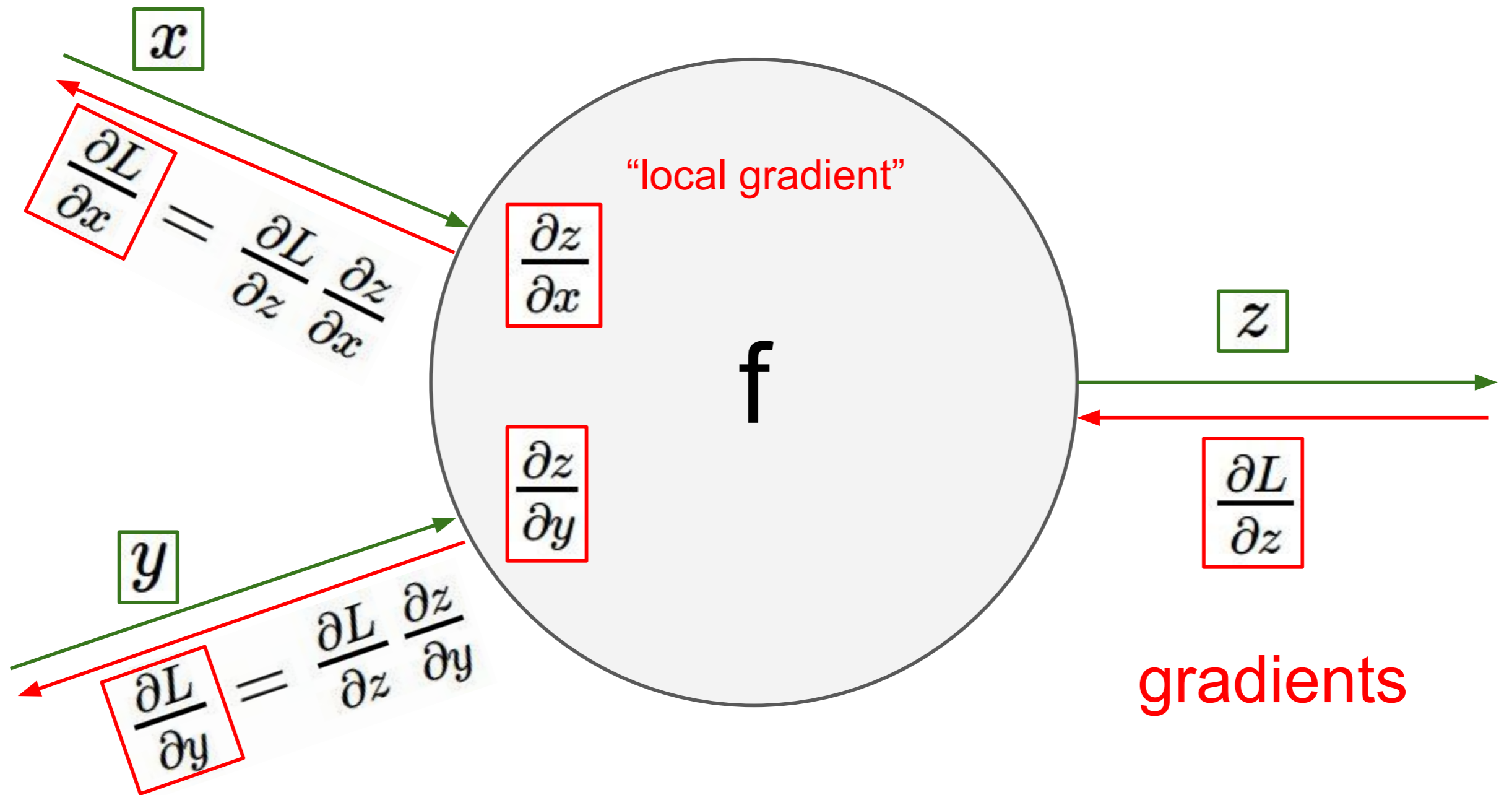
Local
gradient

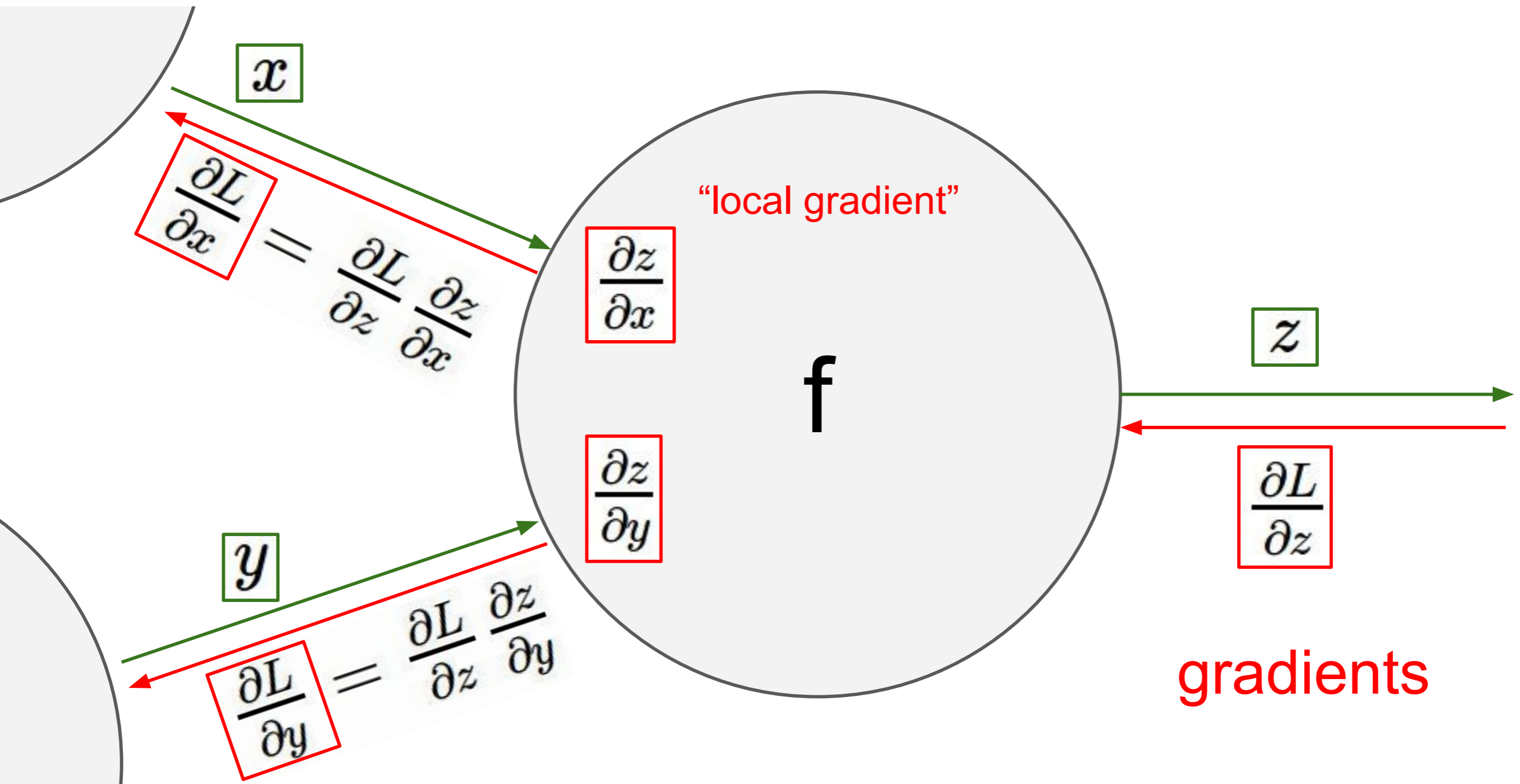






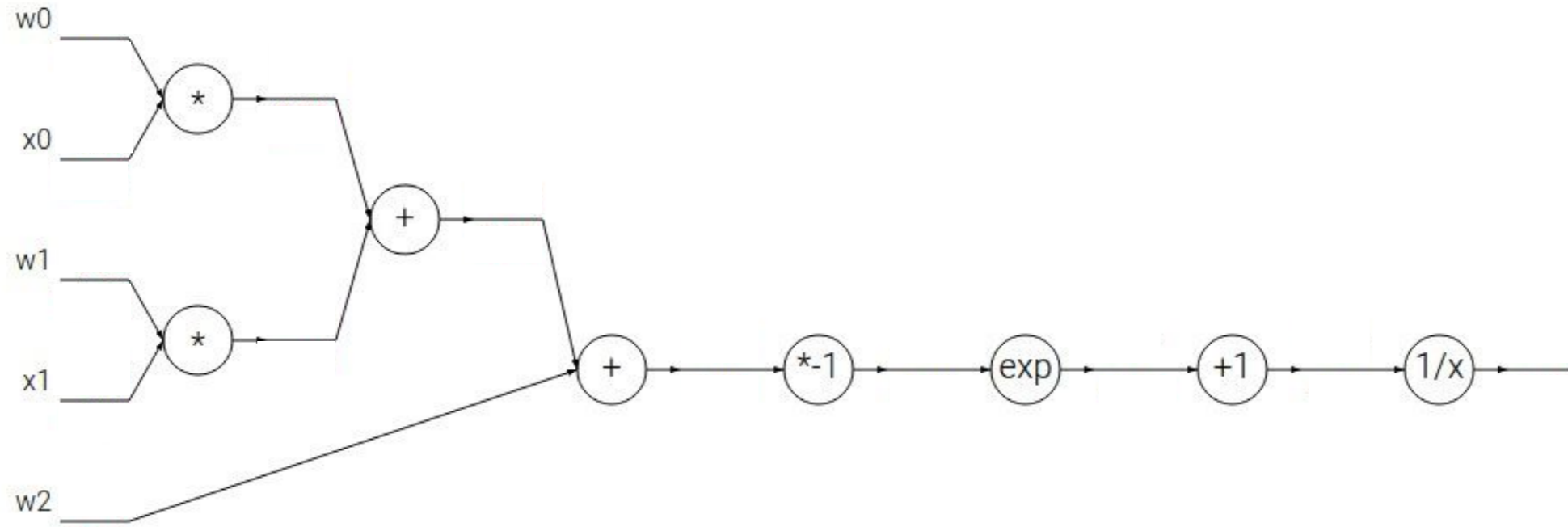






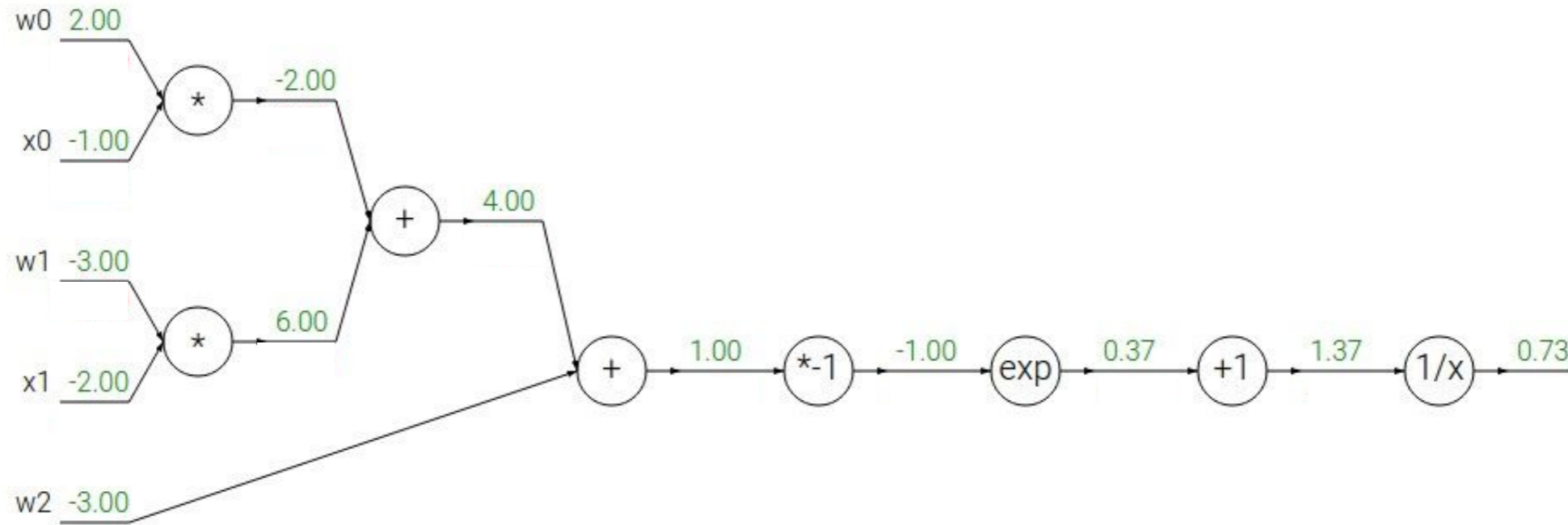
Another example:

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



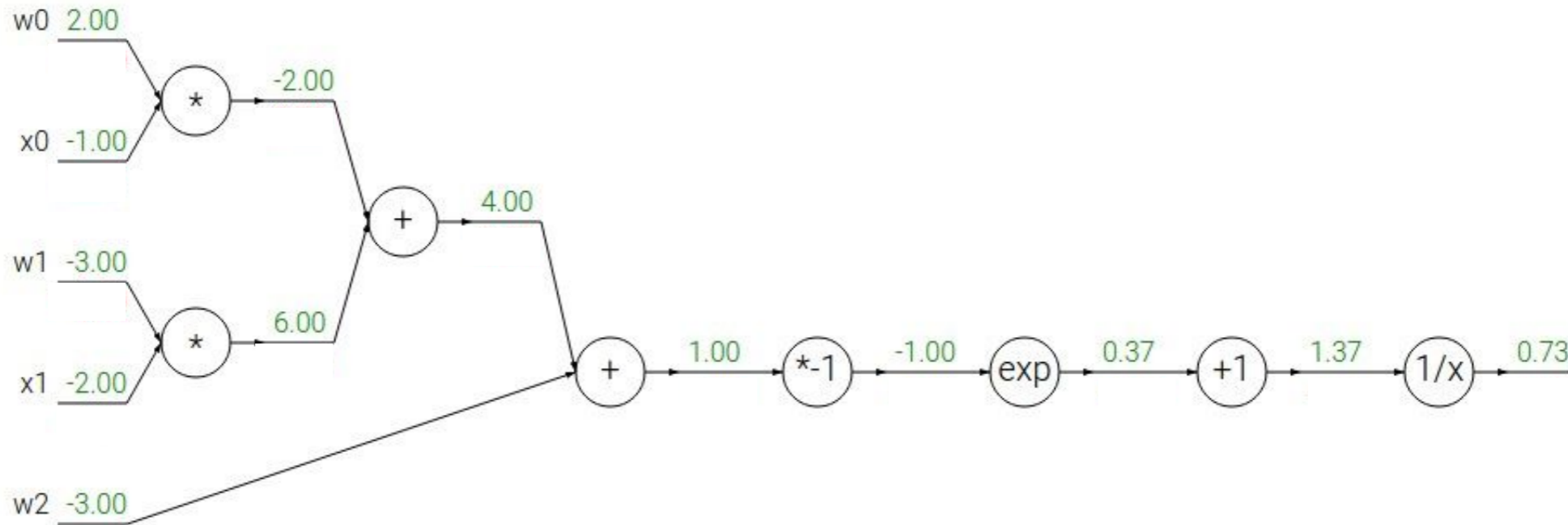
Another example:

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



Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

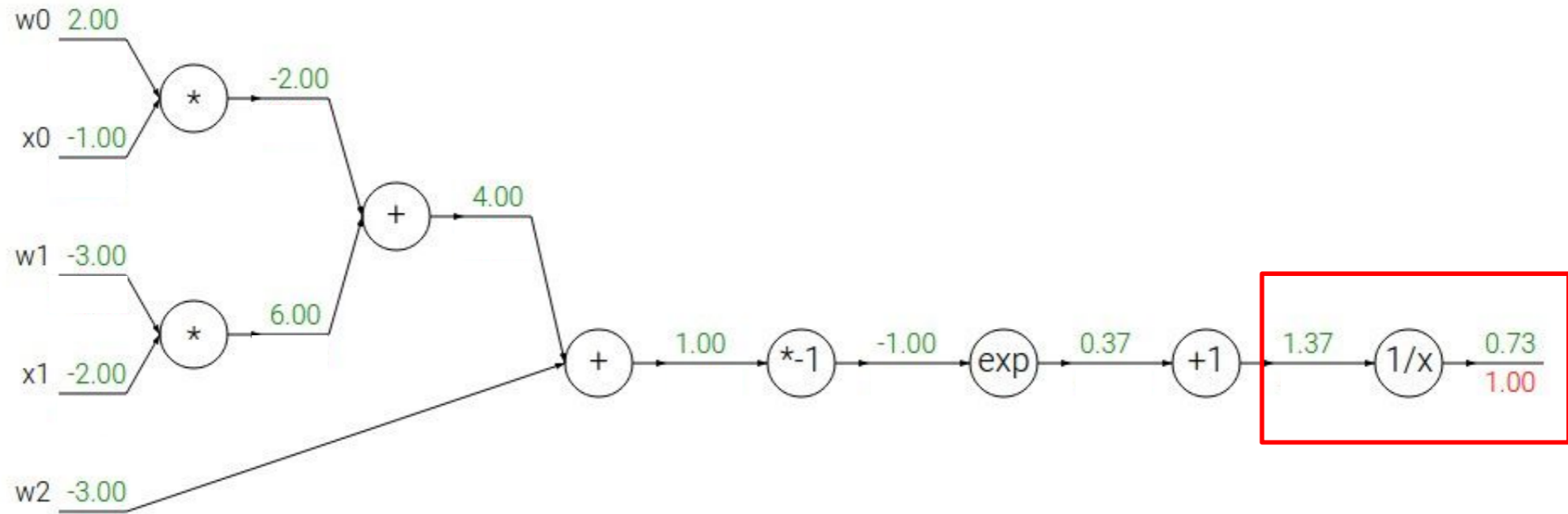
$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

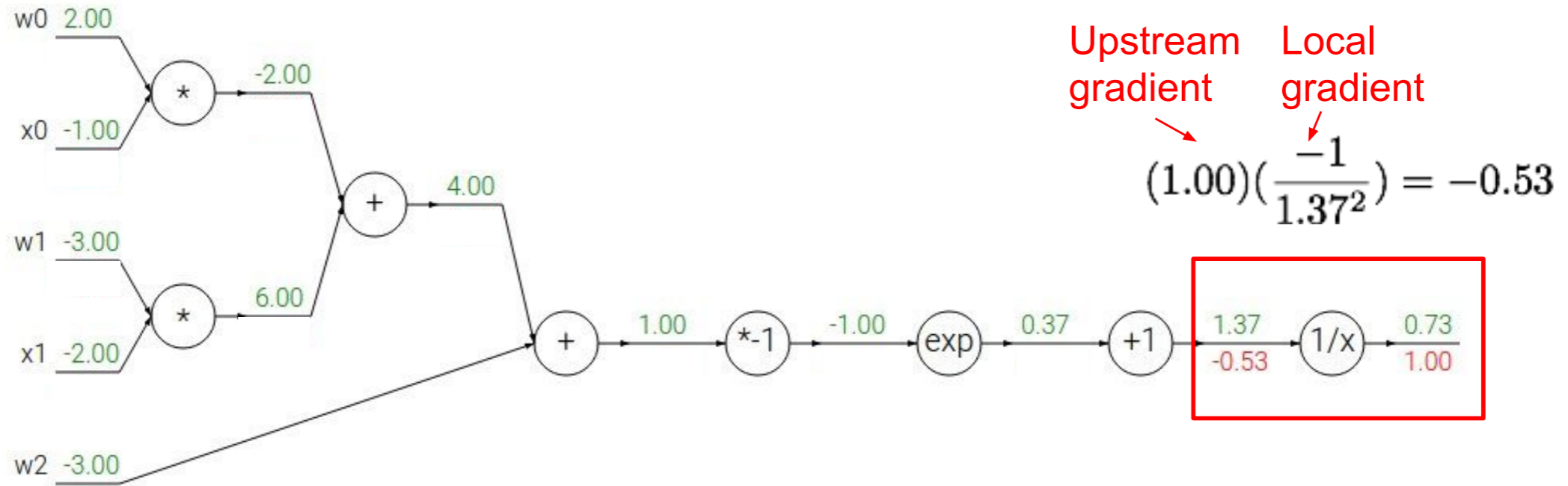
$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x$$

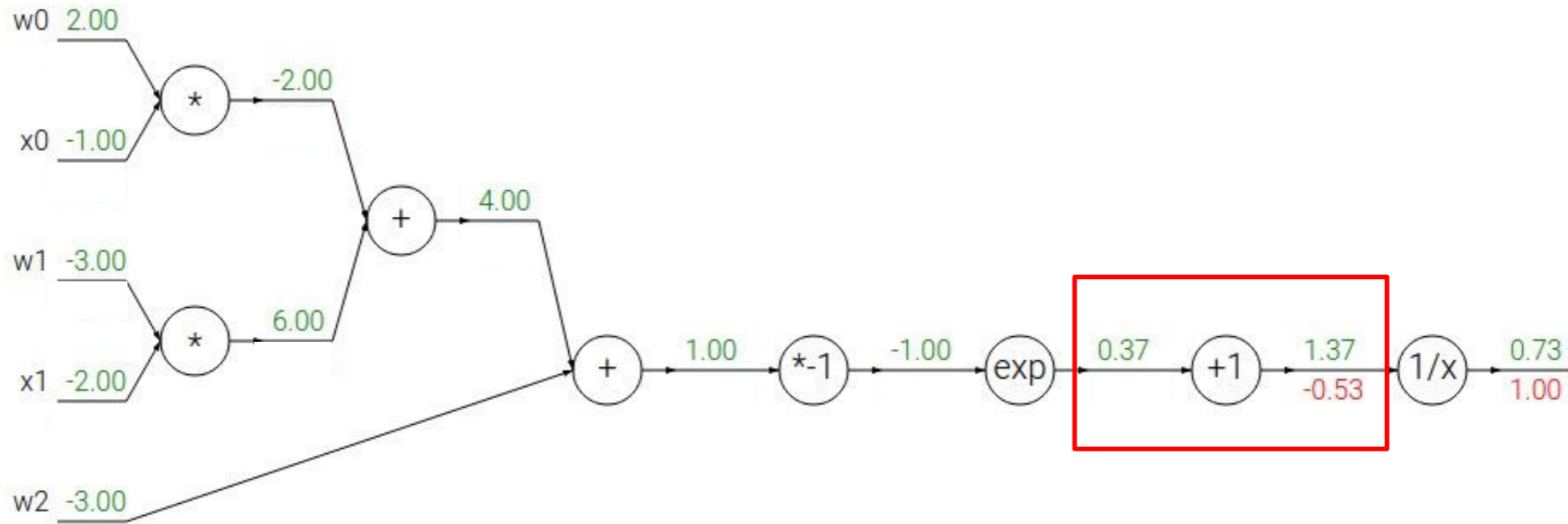
Upstream gradient

→

$$\frac{df}{dx} = 1$$

Another example:

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



$$f(x) = e^x$$

\rightarrow

$$\frac{df}{dx} = e^x$$

$$f(x) = \frac{1}{x}$$

\rightarrow

$$\frac{df}{dx} = -1/x^2$$

$$f_a(x) = ax$$

\rightarrow

$$\frac{df}{dx} = a$$

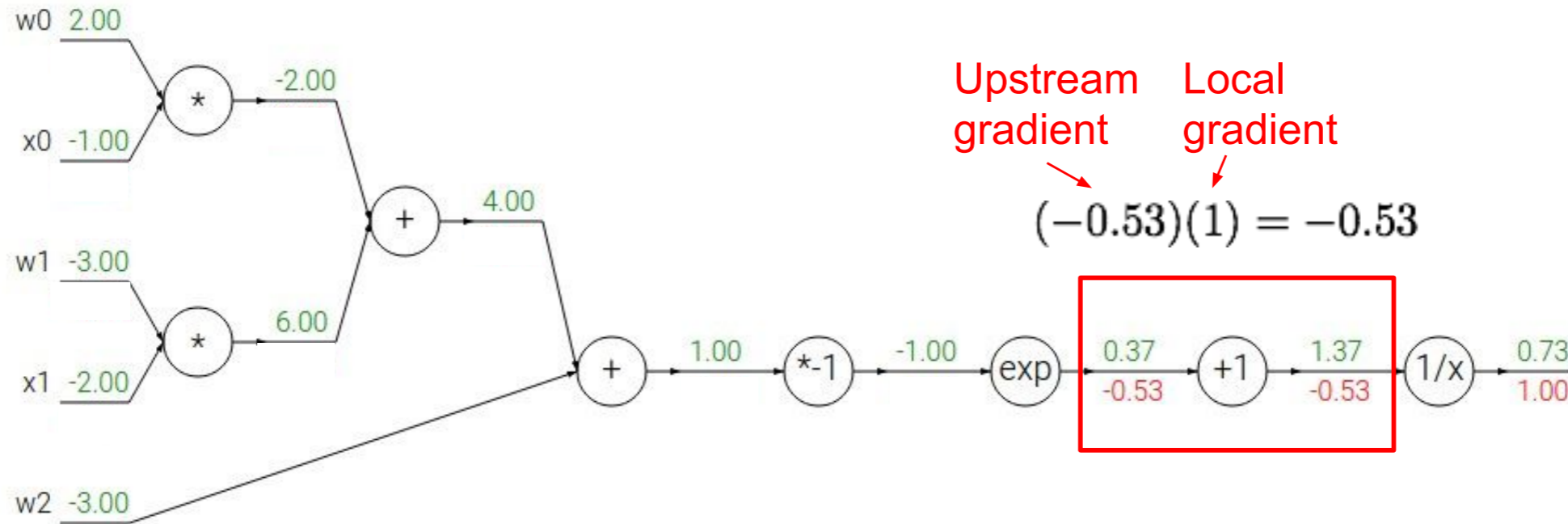
$$f_c(x) = c + x$$

\rightarrow

$$\frac{df}{dx} = 1$$

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

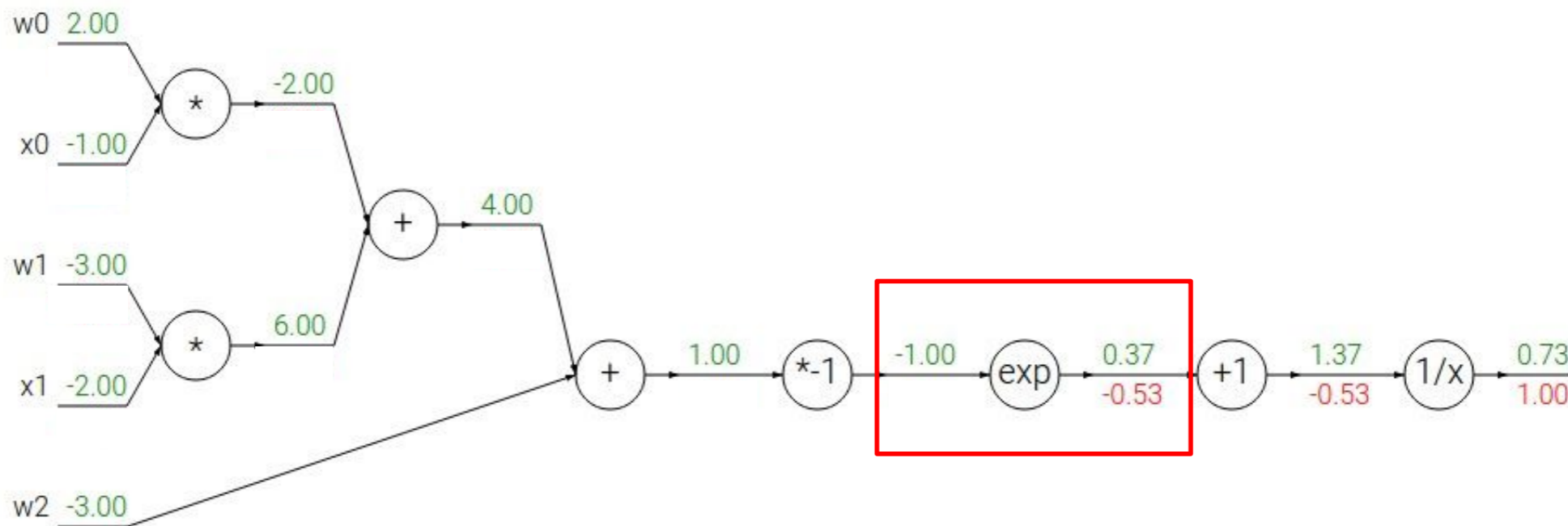
$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

Another example:

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



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

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

$$f(x) = \frac{1}{x}$$

$$f_c(x) = c + x$$

→

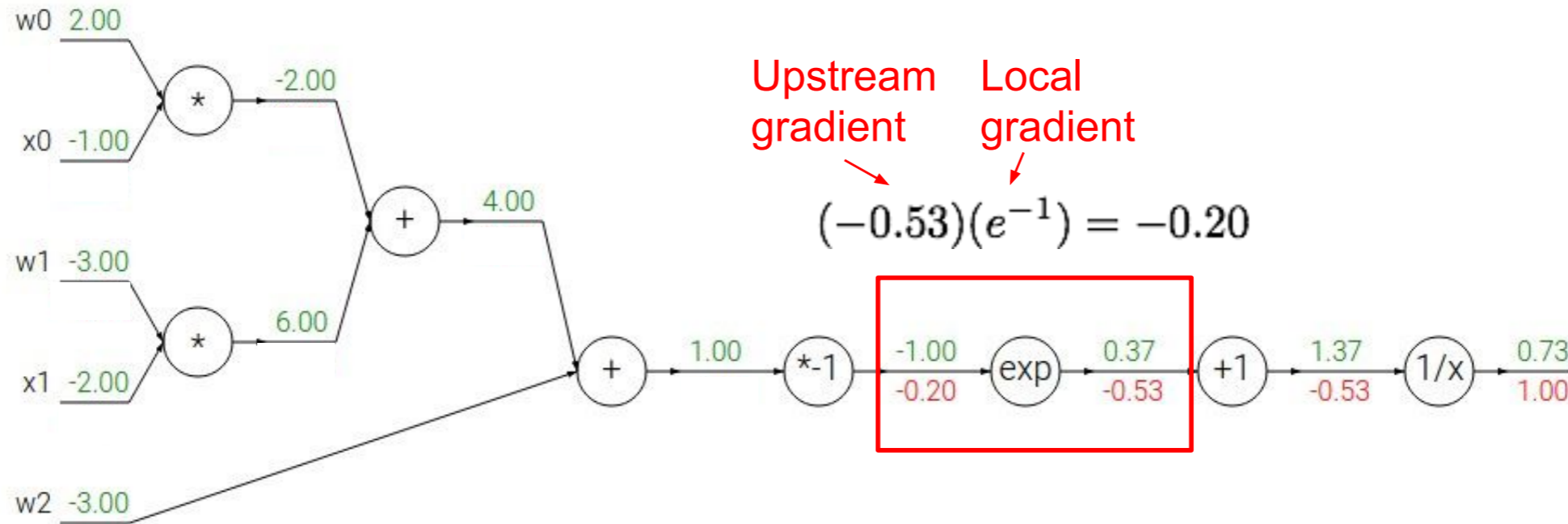
→

$$\frac{df}{dx} = -1/x^2$$

$$\frac{df}{dx} = 1$$

Another example:

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



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

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

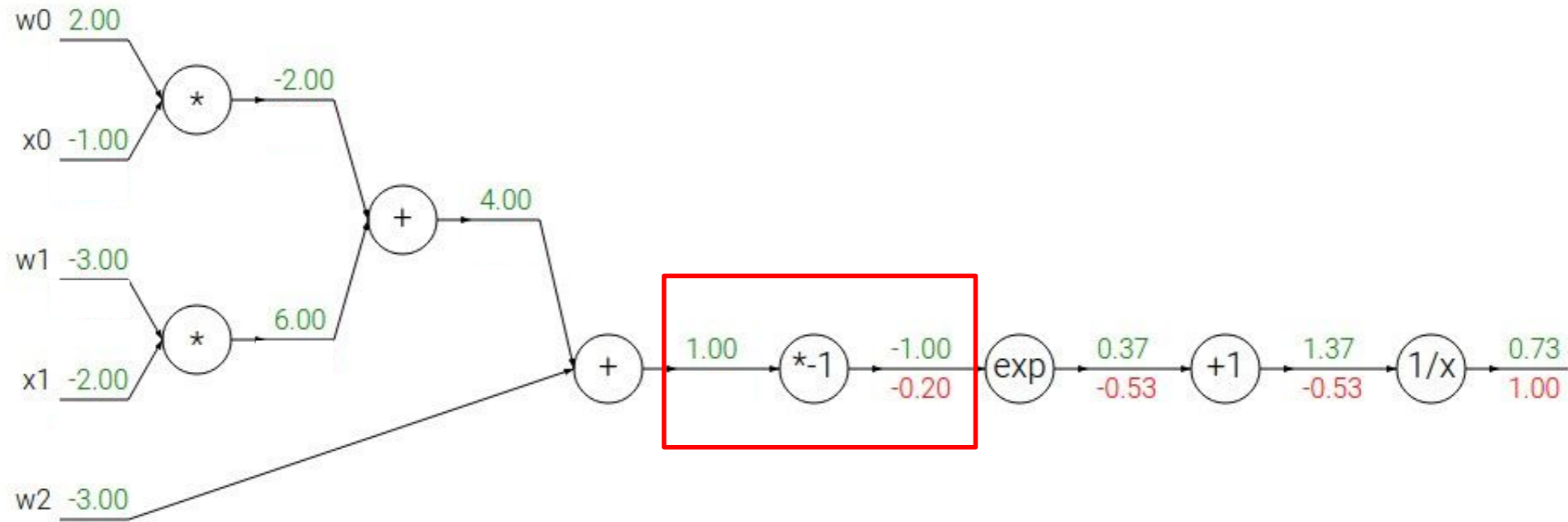
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

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

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

Another example:

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



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

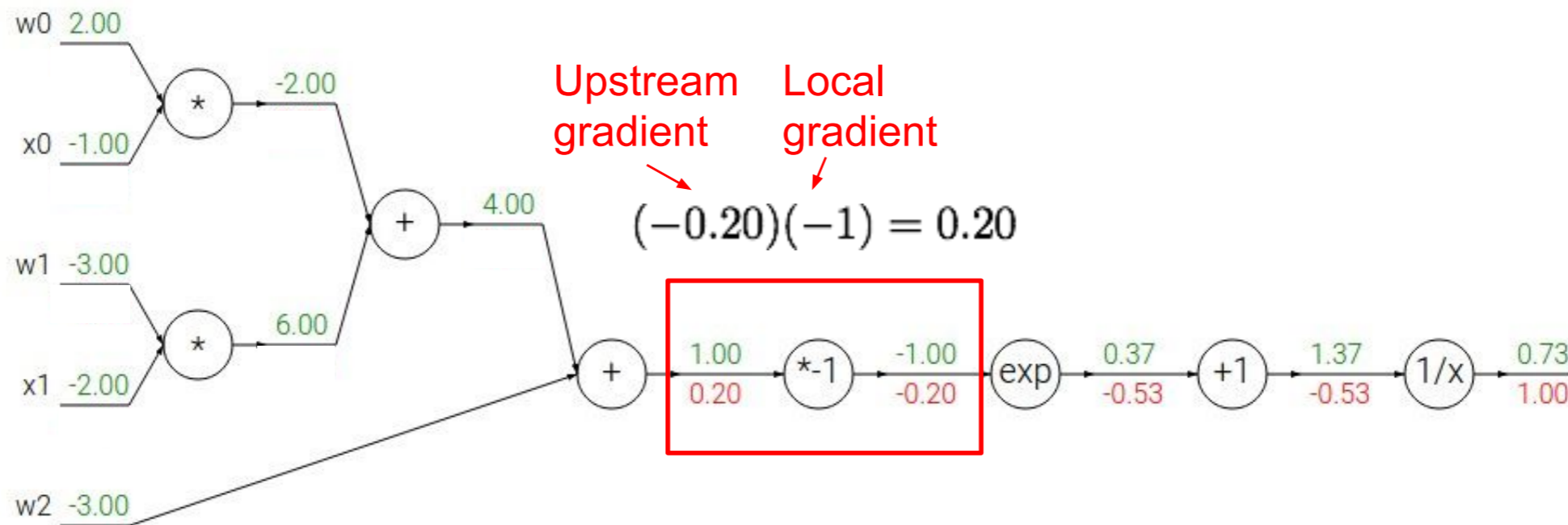
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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

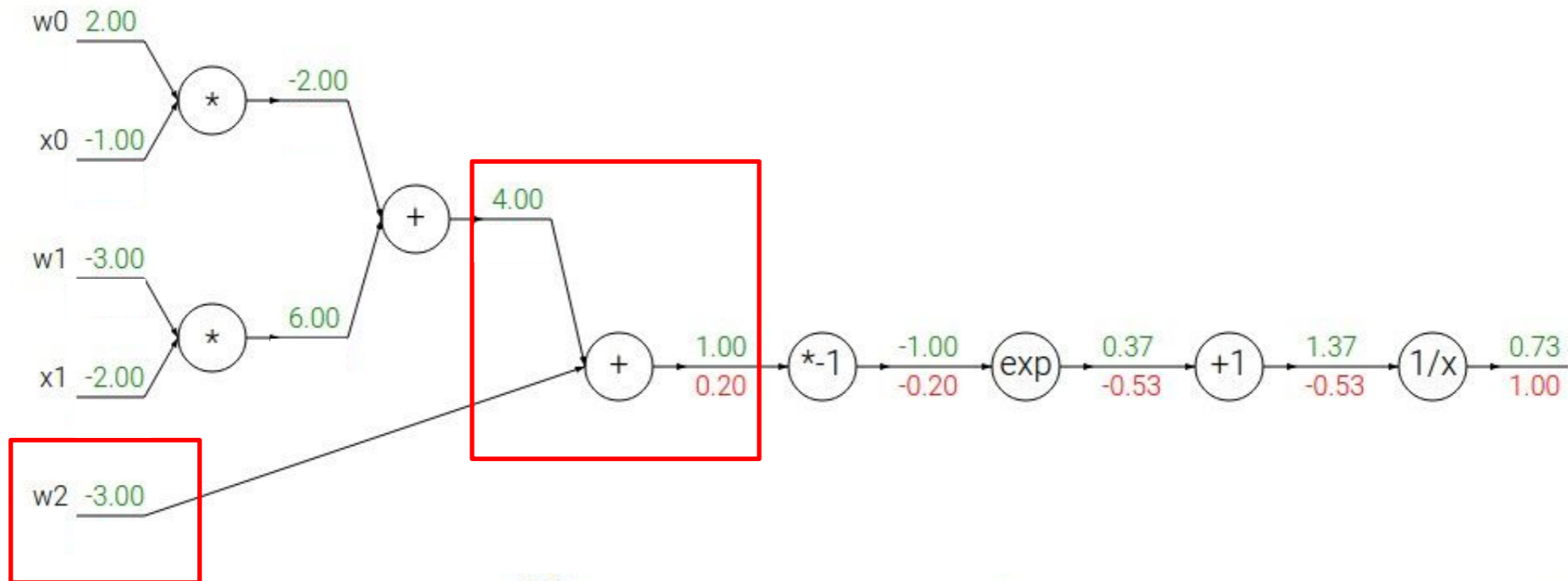


$f(x) = e^x$	\rightarrow	$\frac{df}{dx} = e^x$
$f_a(x) = ax$	\rightarrow	$\frac{df}{dx} = a$

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

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

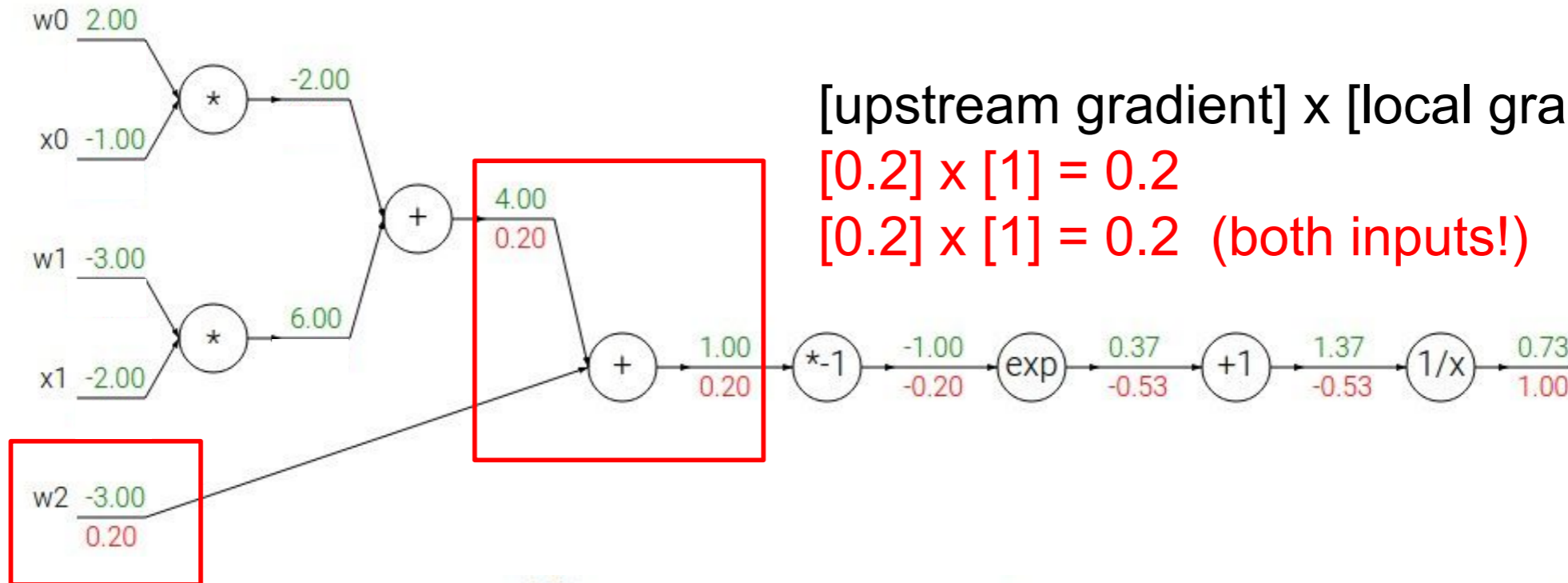
$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

Another example:

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



[upstream gradient] x [local gradient]
 [0.2] x [1] = 0.2
 [0.2] x [1] = 0.2 (both inputs!)

$$f(x) = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = e^x$$

$$\frac{df}{dx} = a$$



$$f(x) = \frac{1}{x}$$

$$f_c(x) = c + x$$

→

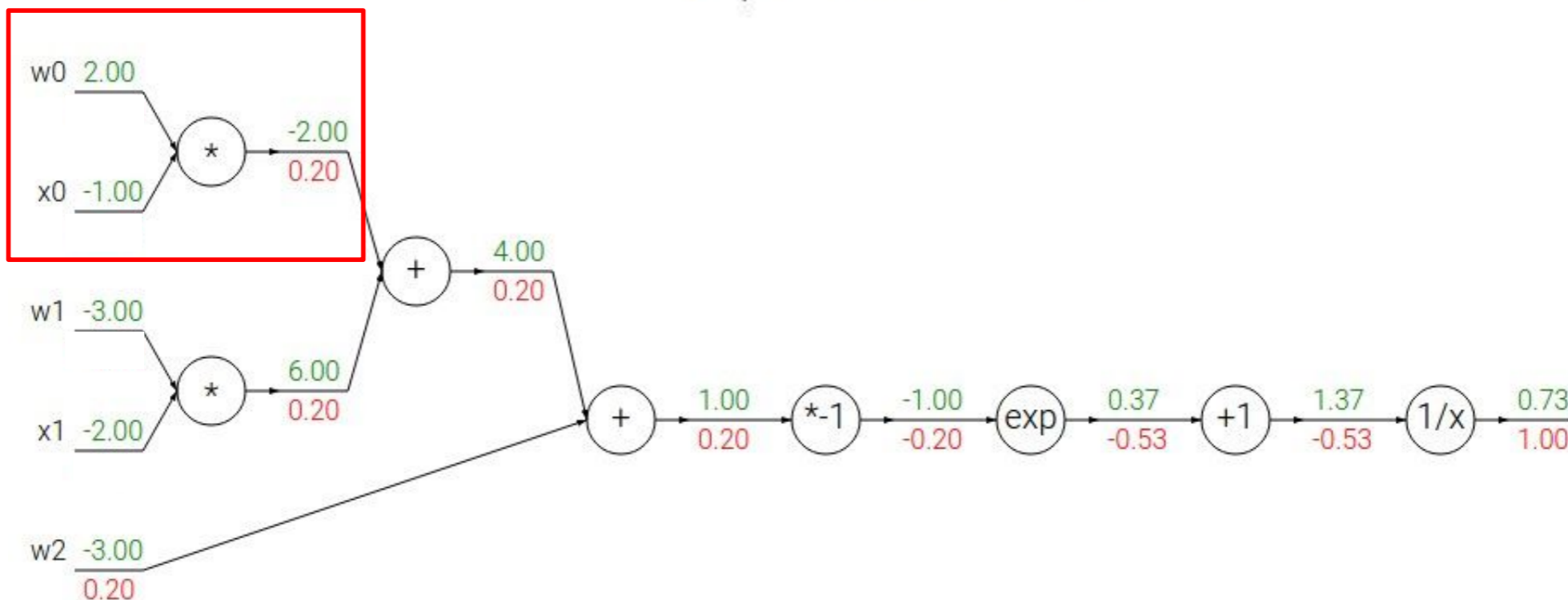
→

$$\frac{df}{dx} = -1/x^2$$

$$\frac{df}{dx} = 1$$

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

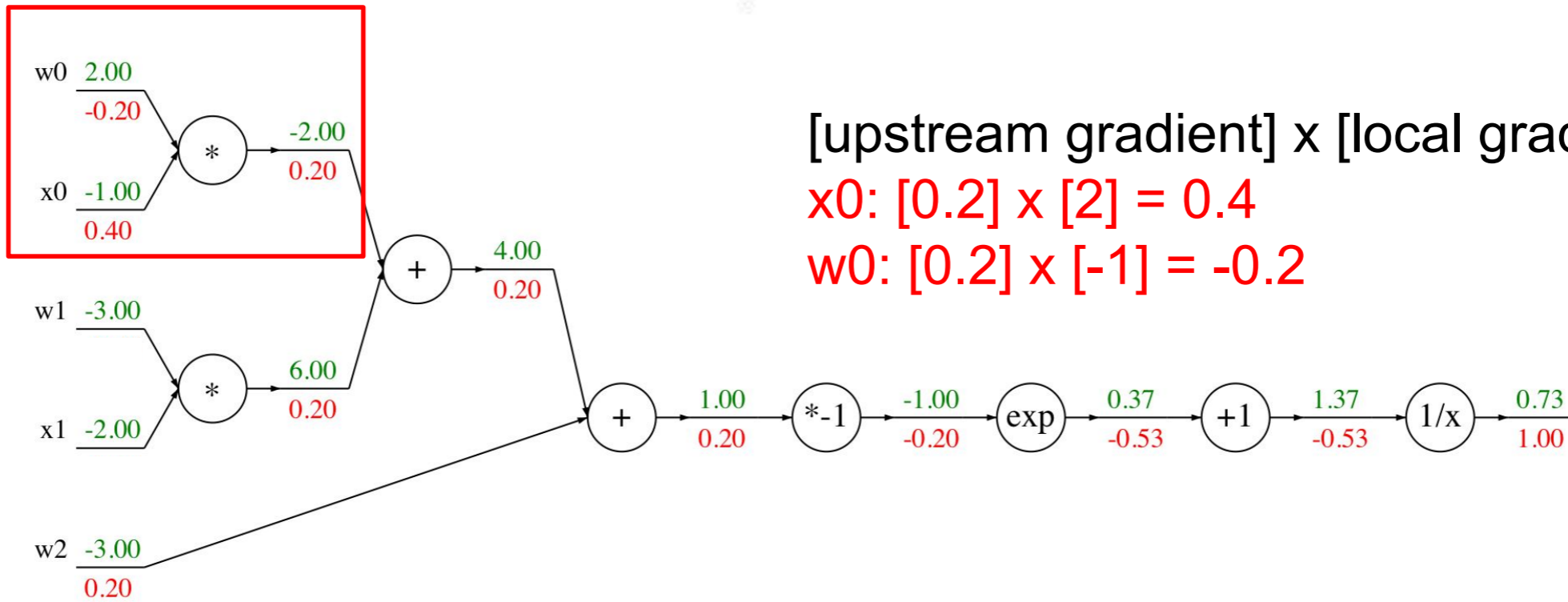
$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

Another example:

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



[upstream gradient] x [local gradient]

x_0 : $[0.2] \times [2] = 0.4$

w_0 : $[0.2] \times [-1] = -0.2$

$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

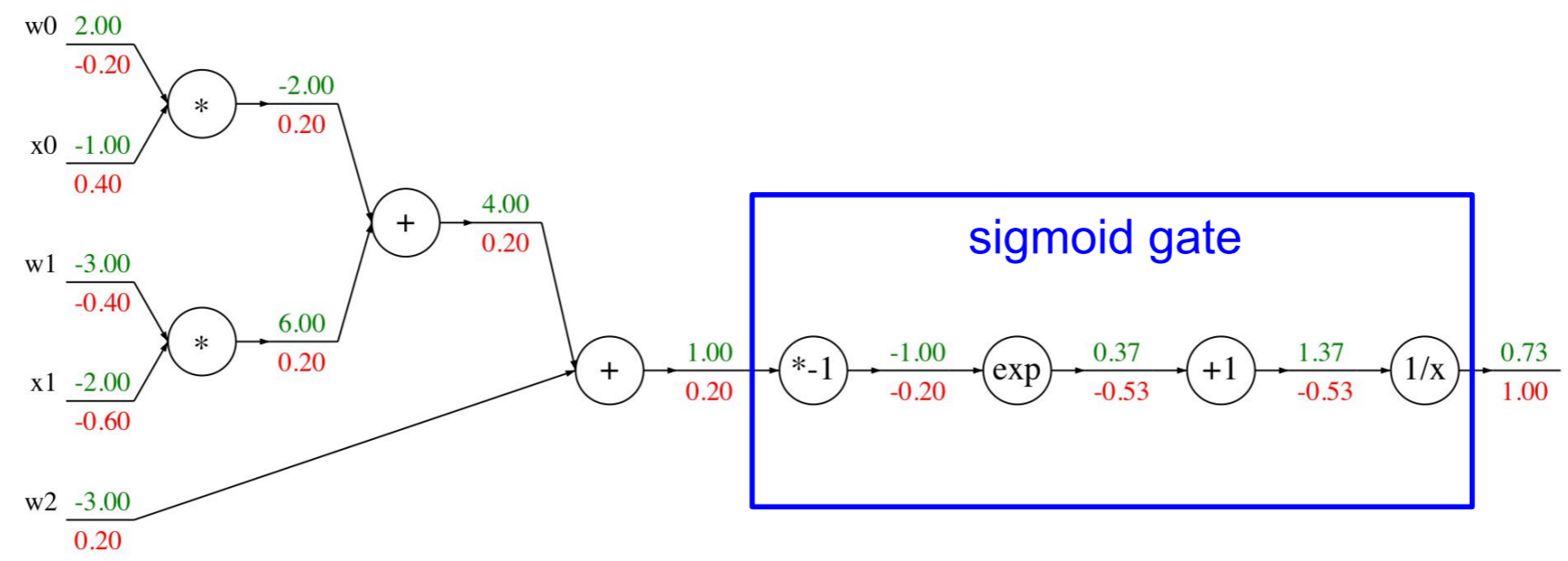
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$

Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

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

sigmoid function

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



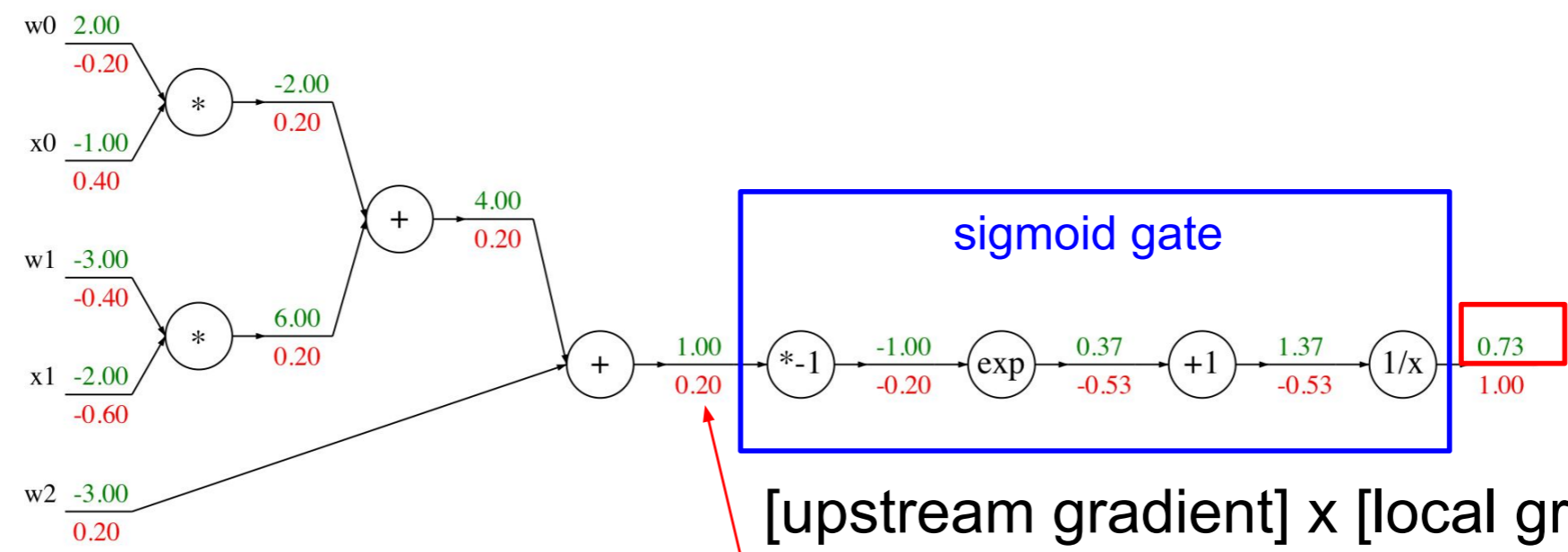
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$

Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

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

sigmoid function

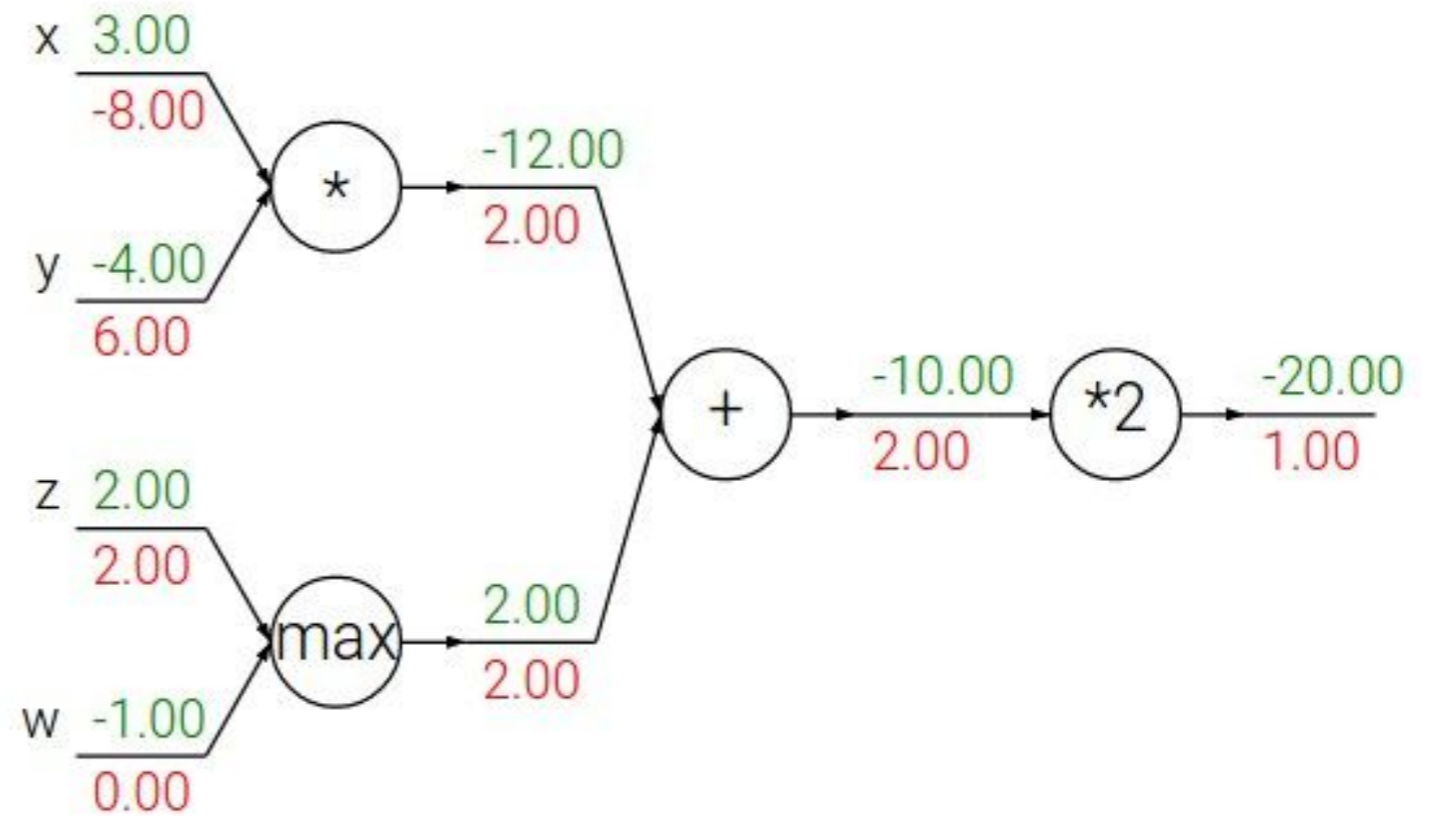
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1 + e^{-x})^2} = \left(\frac{1 + e^{-x} - 1}{1 + e^{-x}} \right) \left(\frac{1}{1 + e^{-x}} \right) = (1 - \sigma(x)) \sigma(x)$$



[upstream gradient] x [local gradient]
 $[1.00] \times [(1 - 0.73) (0.73)] = 0.2$

Patterns in backward flow

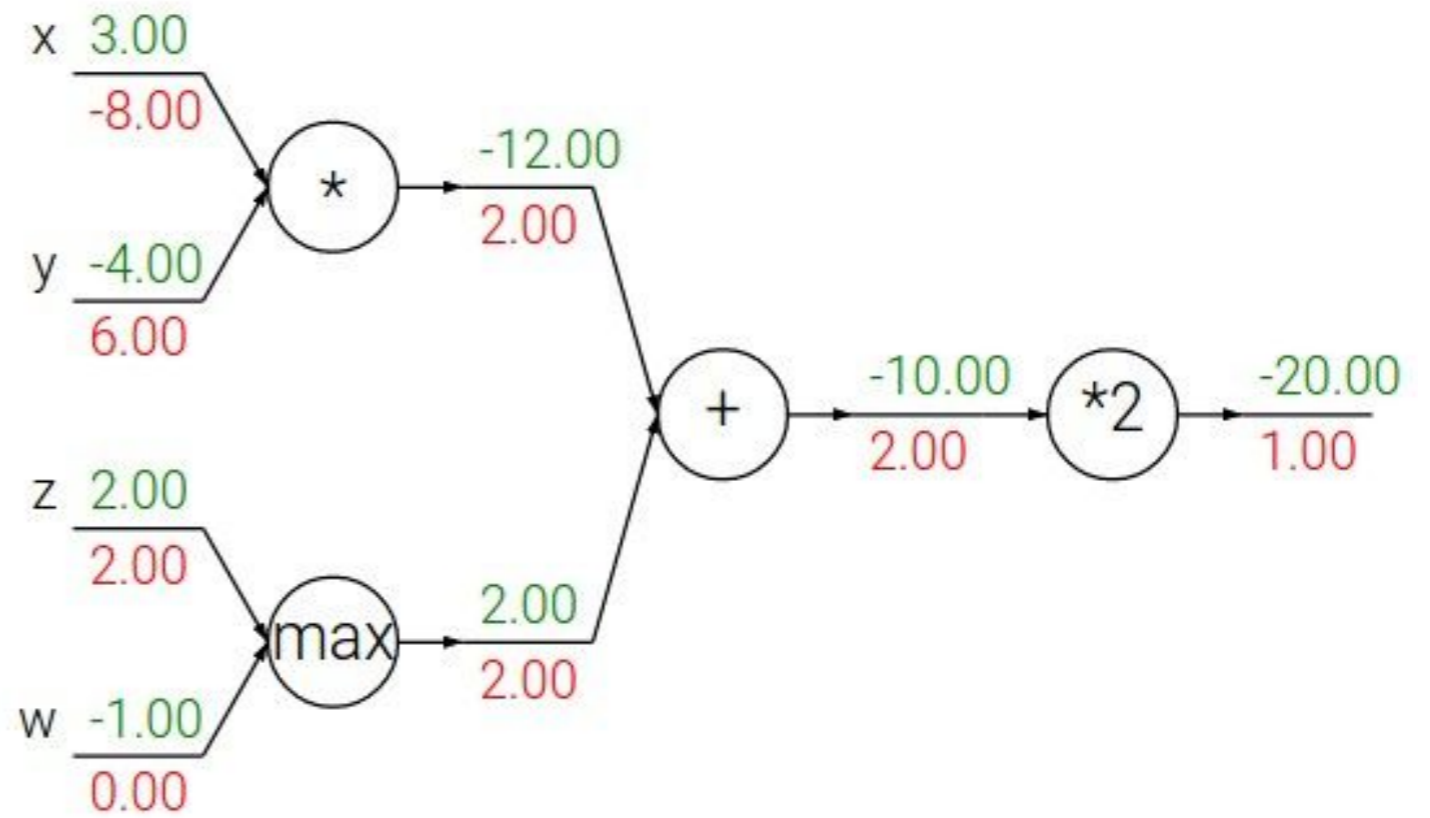
add gate: gradient distributor



Patterns in backward flow

add gate: gradient distributor

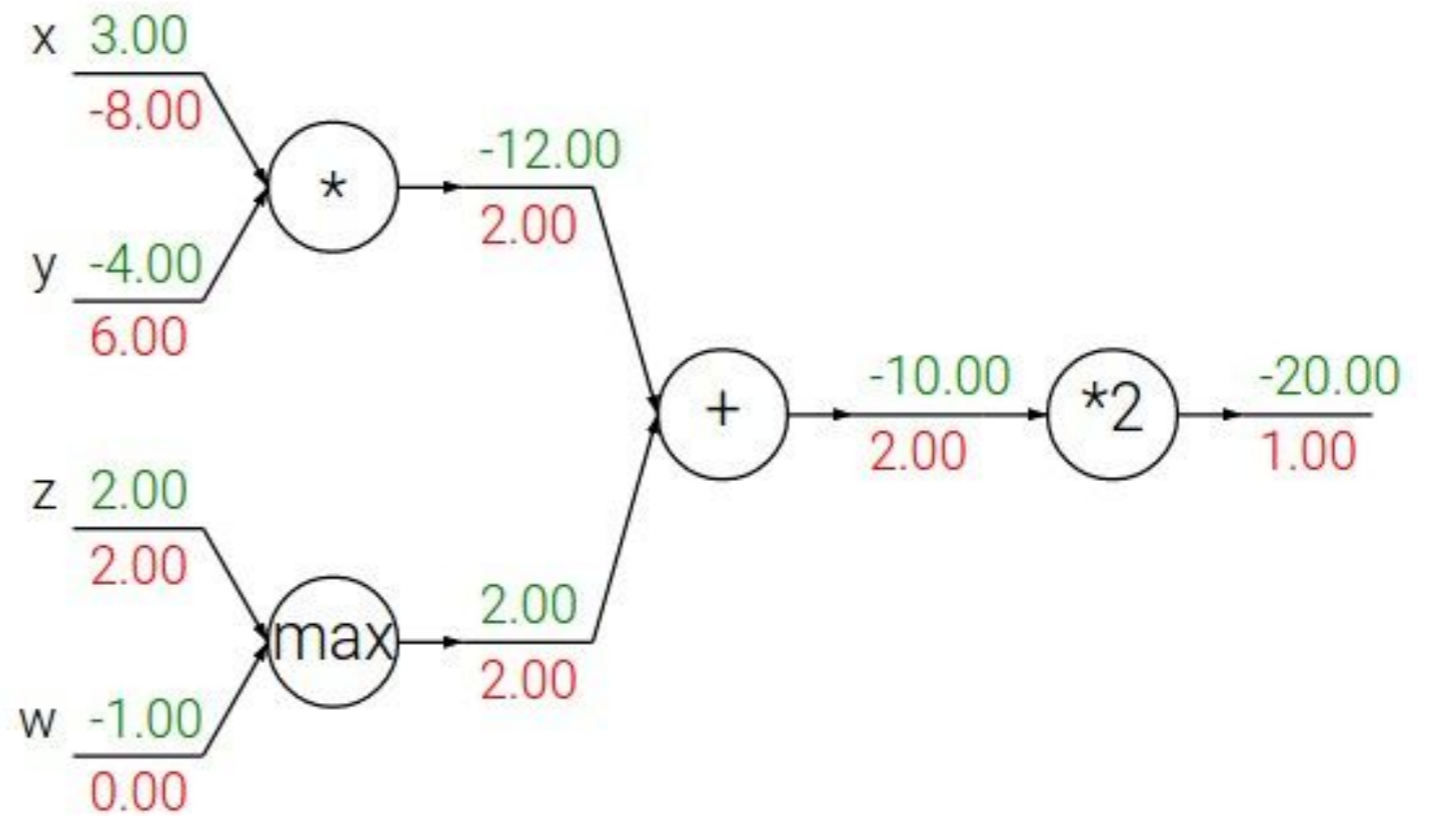
Q: What is a **max** gate?



Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

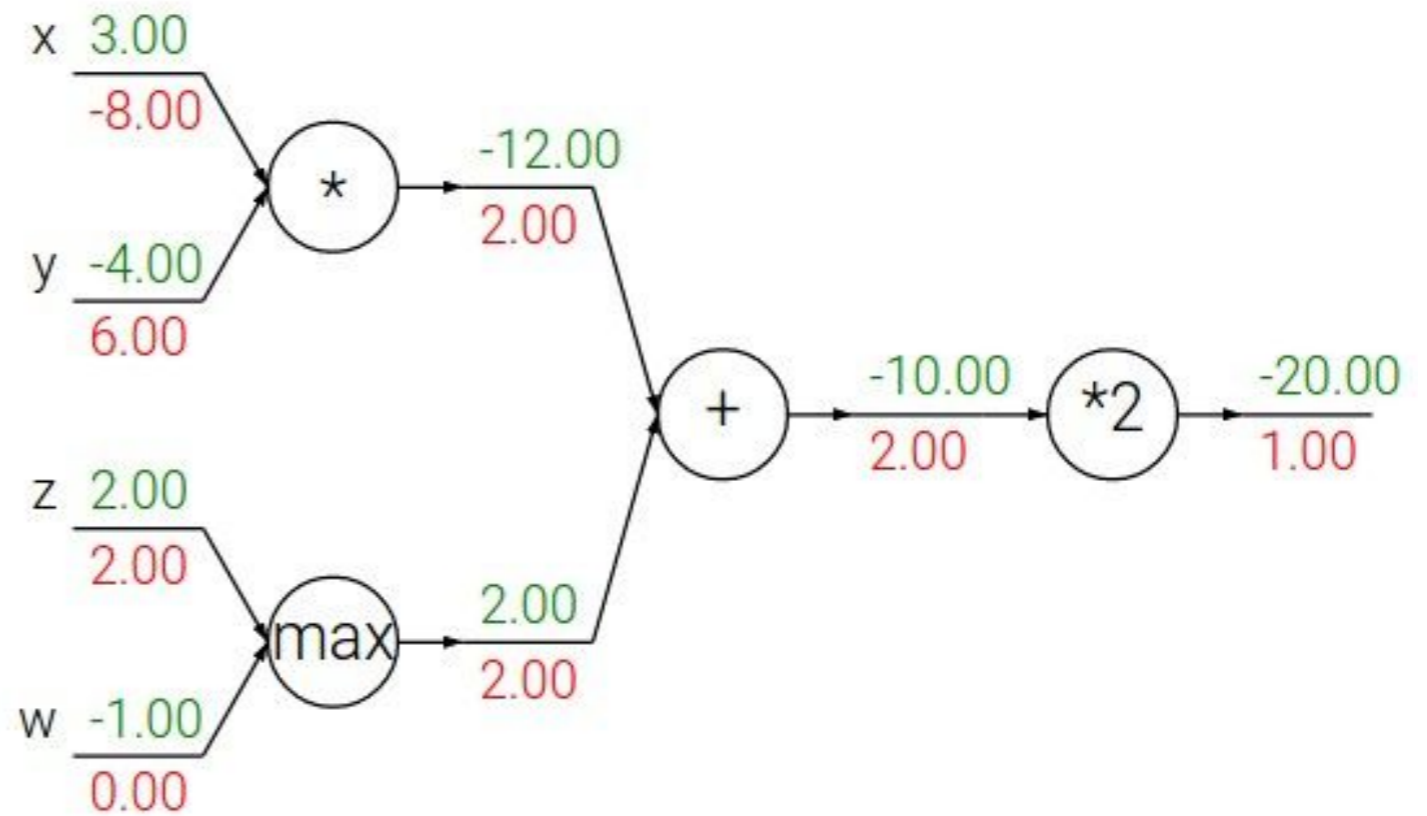


Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

Q: What is a **mul** gate?

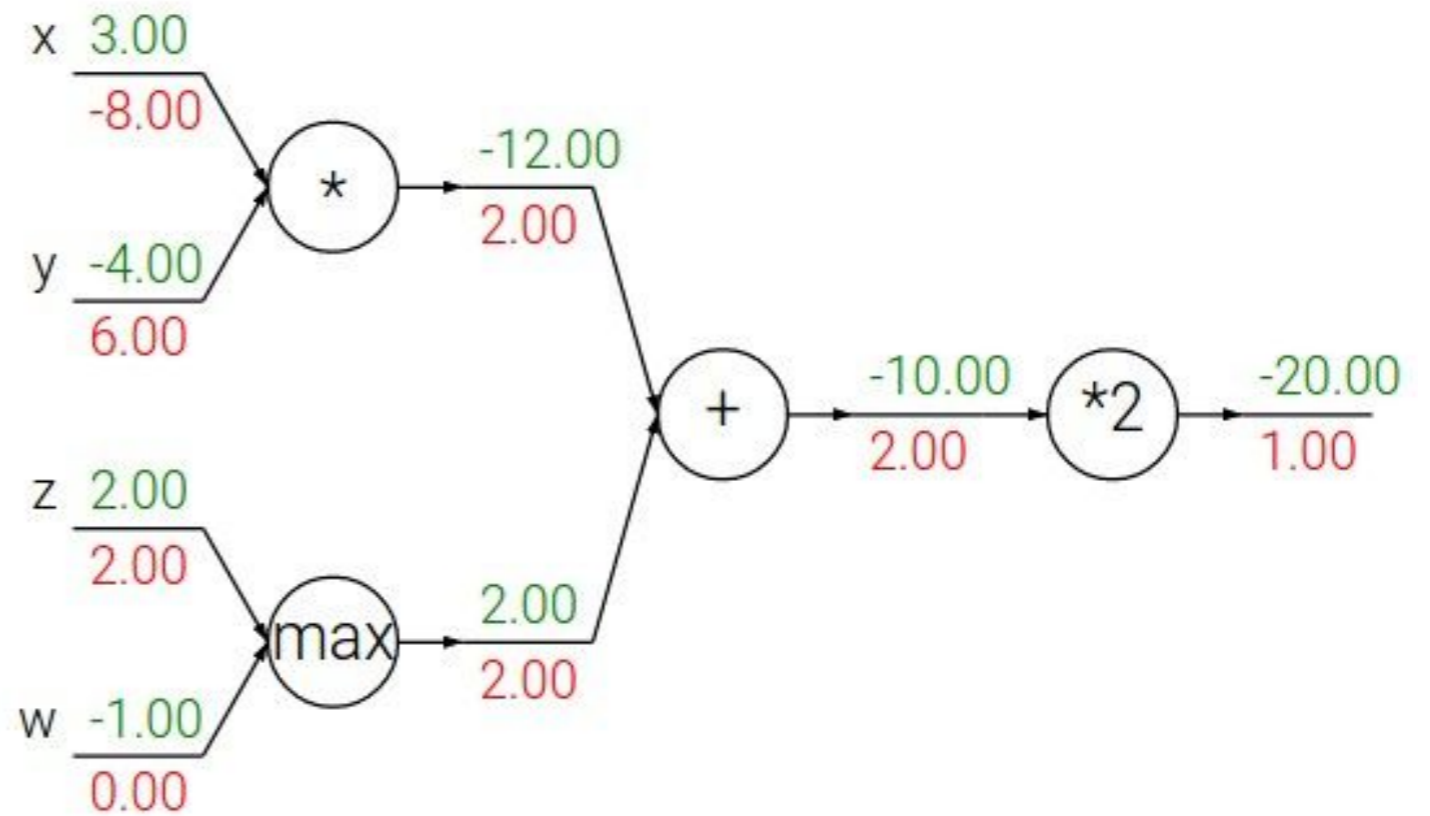


Patterns in backward flow

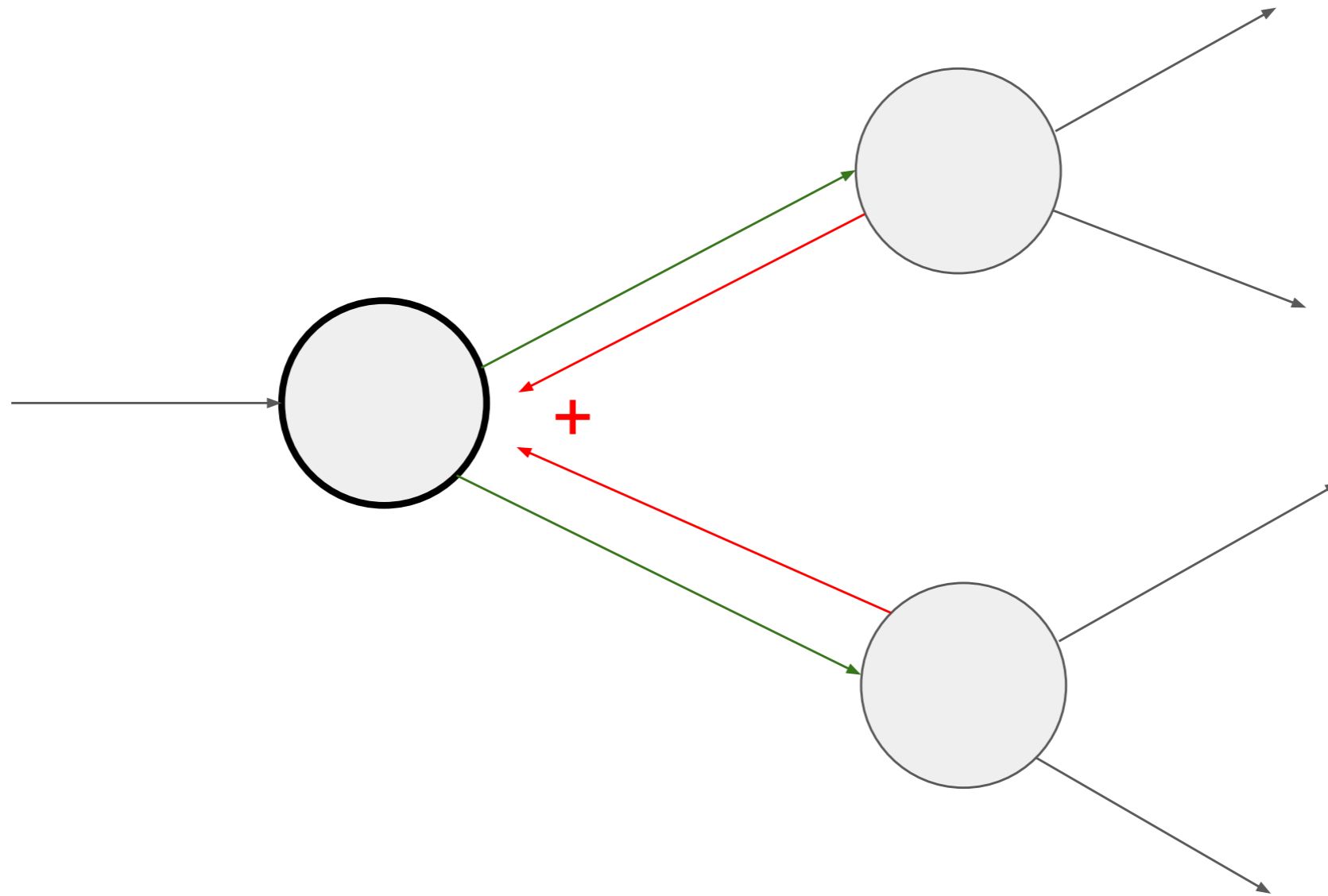
add gate: gradient distributor

max gate: gradient router

mul gate: gradient switcher



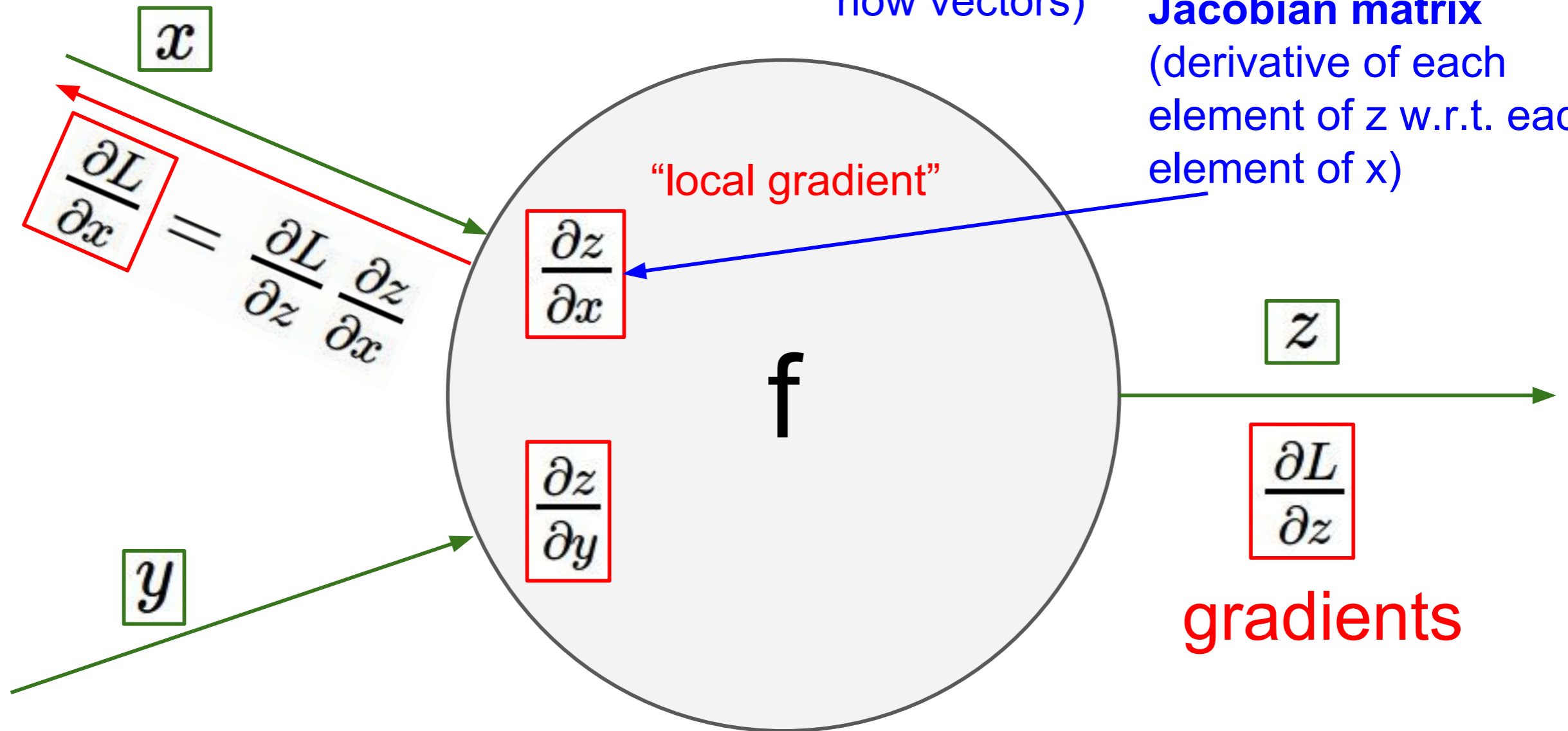
Gradients add at branches



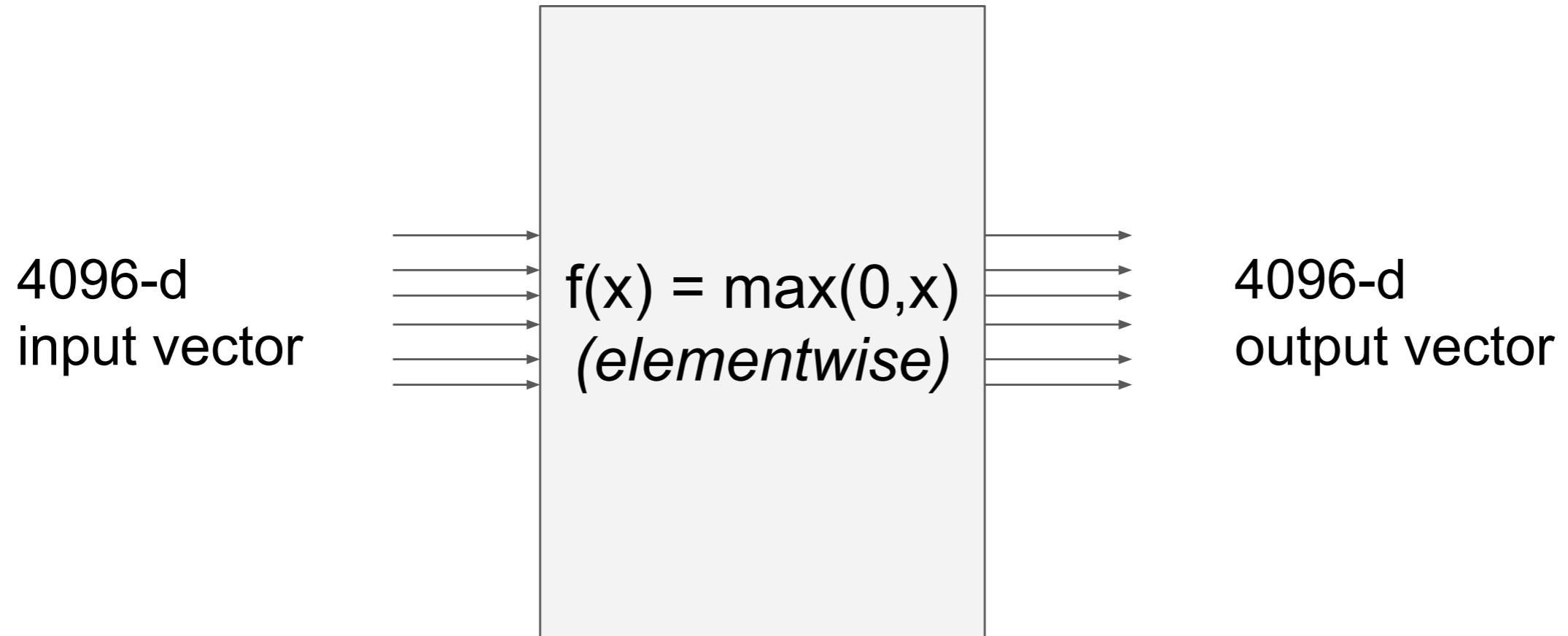
Gradients for vectorized code

(x,y,z are now vectors)

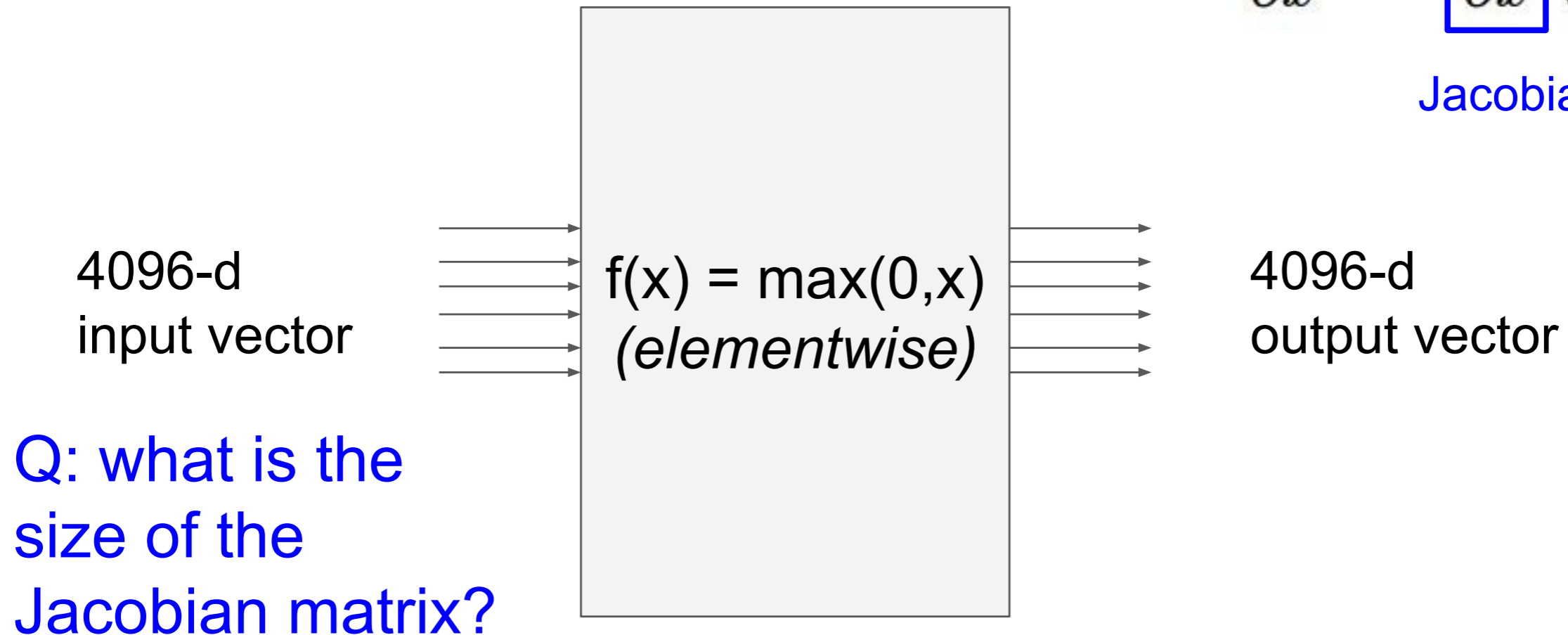
This is now the **Jacobian matrix** (derivative of each element of z w.r.t. each element of x)



Vectorized operations



Vectorized operations



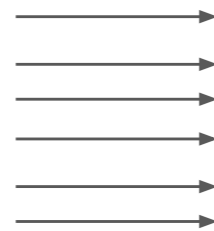
Q: what is the
size of the
Jacobian matrix?

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

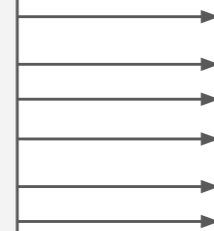
Jacobian matrix

Vectorized operations

4096-d
input vector



$f(x) = \max(0, x)$
(*elementwise*)



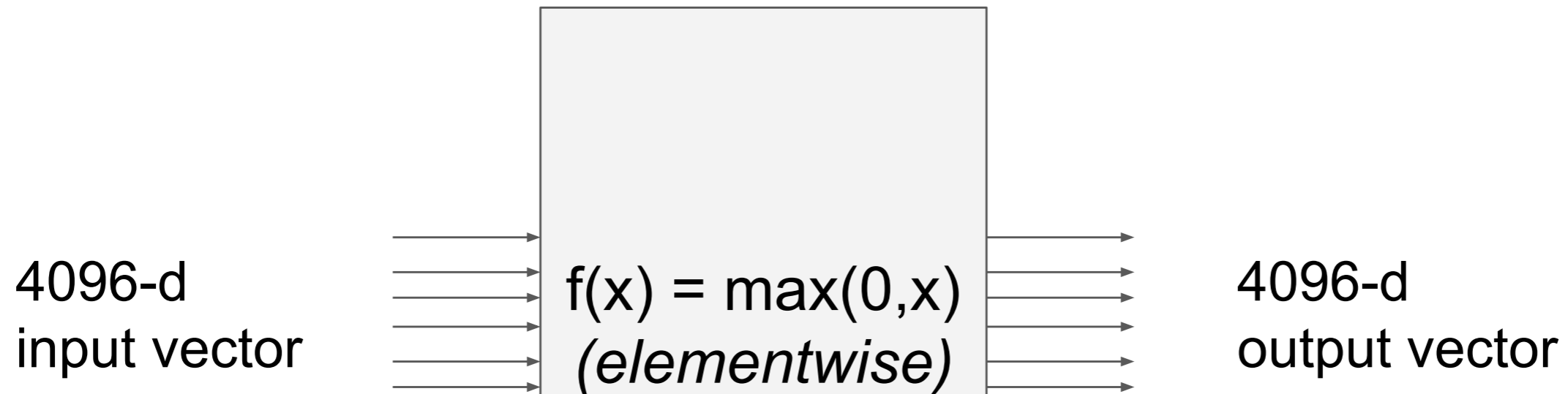
4096-d
output vector

Q: what is the
size of the
Jacobian matrix?
[4096 x 4096!]

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

Jacobian matrix

Vectorized operations



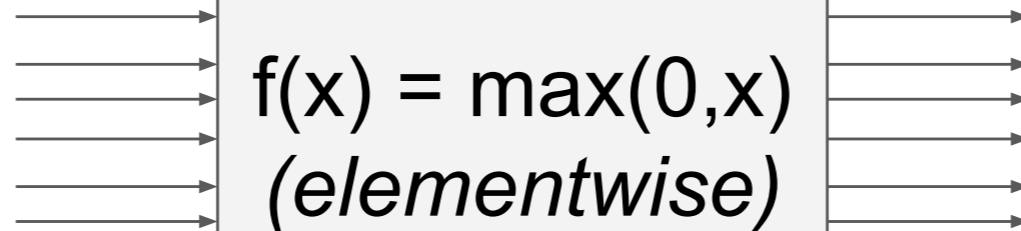
Q: what is the size of the Jacobian matrix?
[4096 x 4096!]

in practice we process an entire minibatch (e.g. 100) of examples at one time:

i.e. Jacobian would technically be a [409,600 x 409,600] matrix :\
\\

Vectorized operations

4096-d
input vector



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

Jacobian matrix

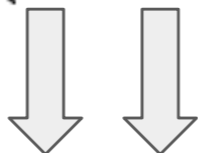
4096-d
output vector

Q: what is the
size of the
Jacobian matrix?
[4096 x 4096!]

Q2: what does it
look like?

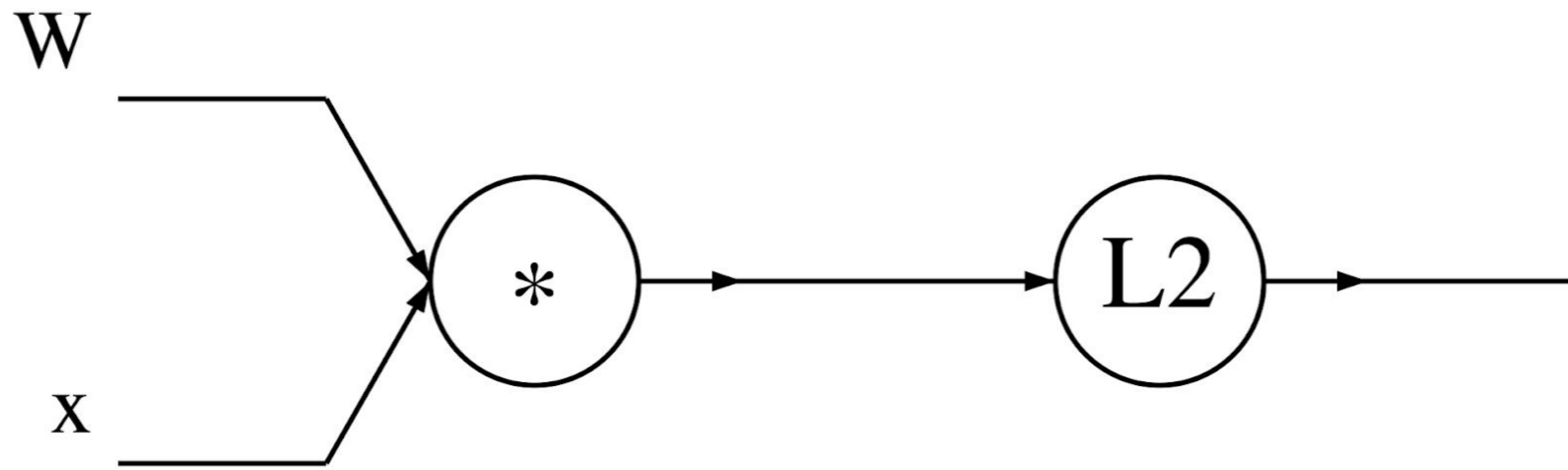
A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$



$\in \mathbb{R}^n \quad \in \mathbb{R}^{n \times n}$

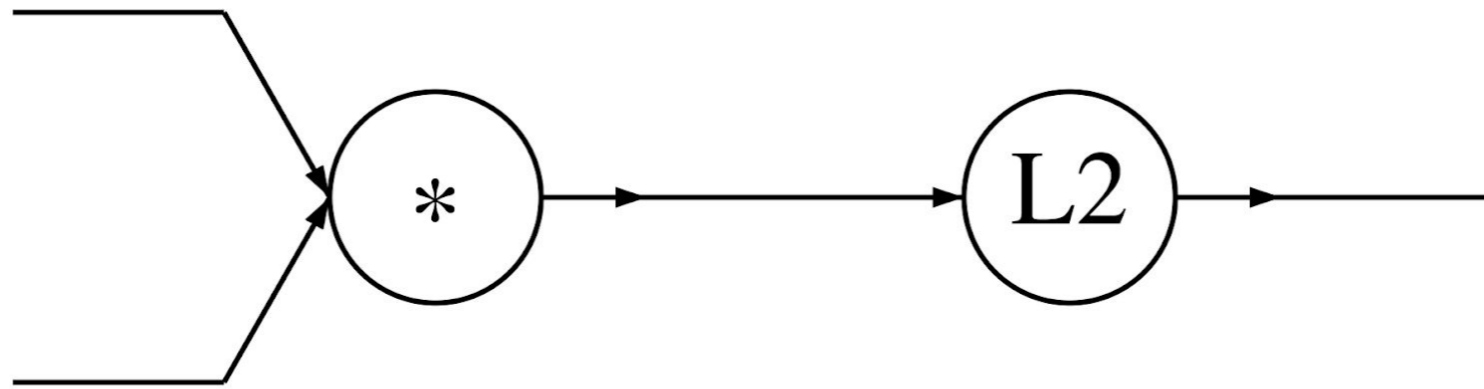
A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$



A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} W$$

$$\begin{bmatrix} 0.2 \\ 0.4 \end{bmatrix} x$$

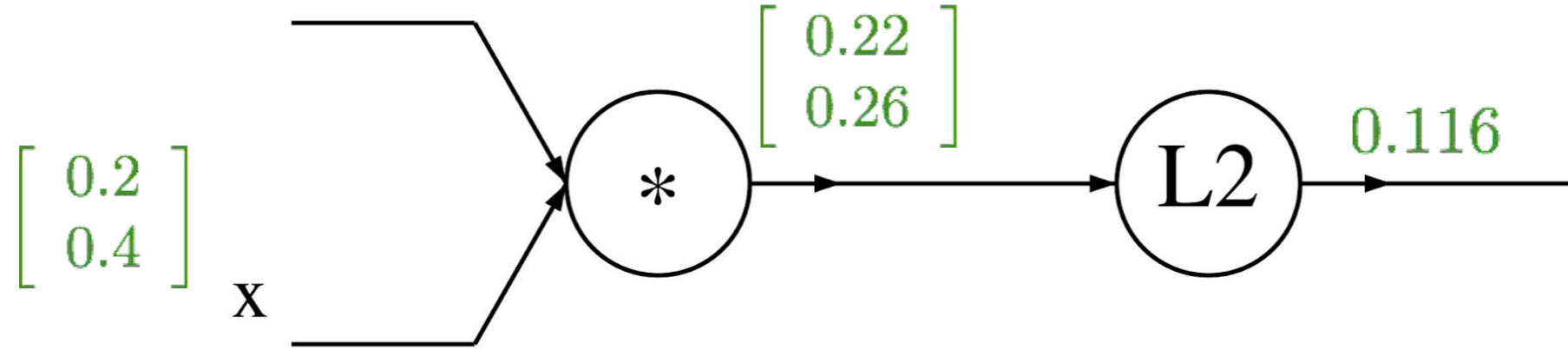


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \cdots + q_n^2$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} W$$

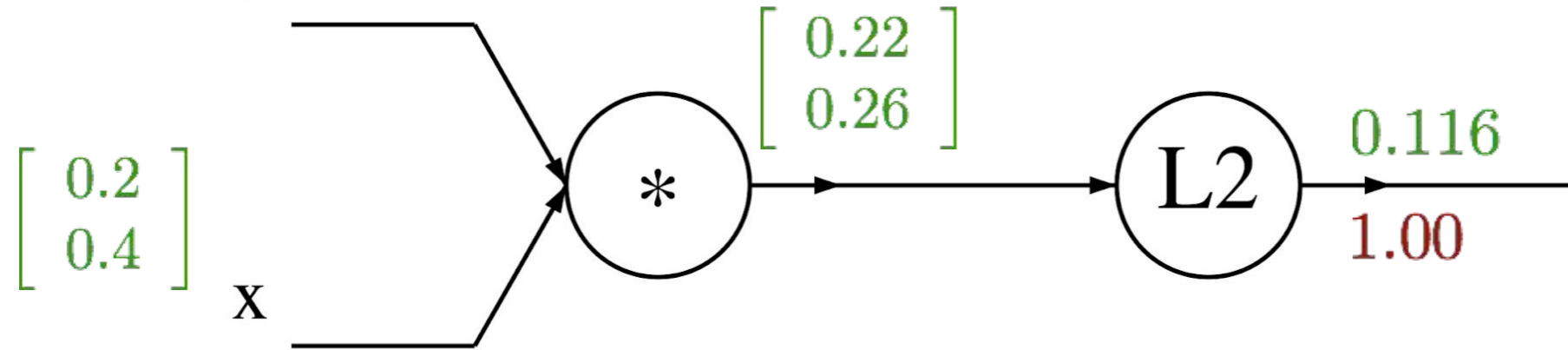


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} W$$

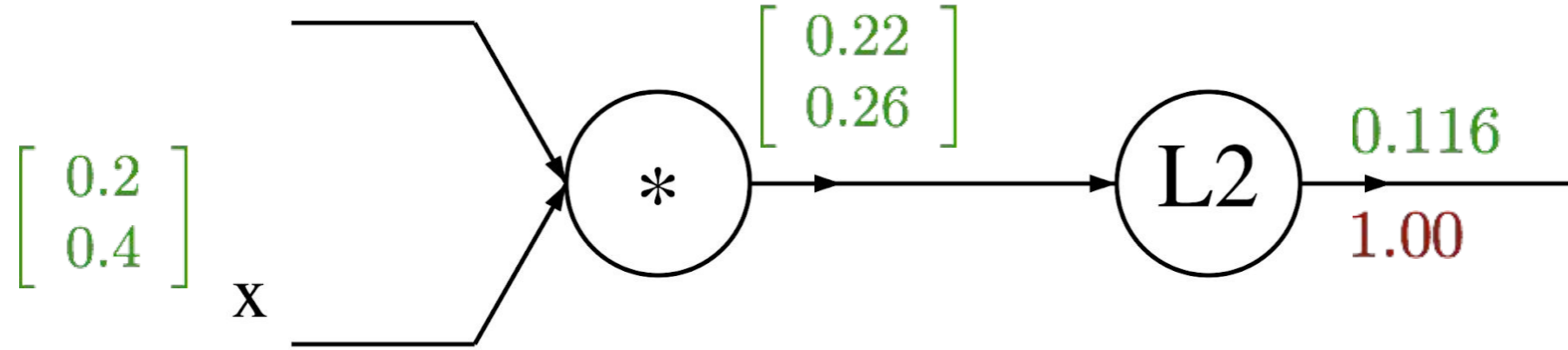


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} W$$



$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

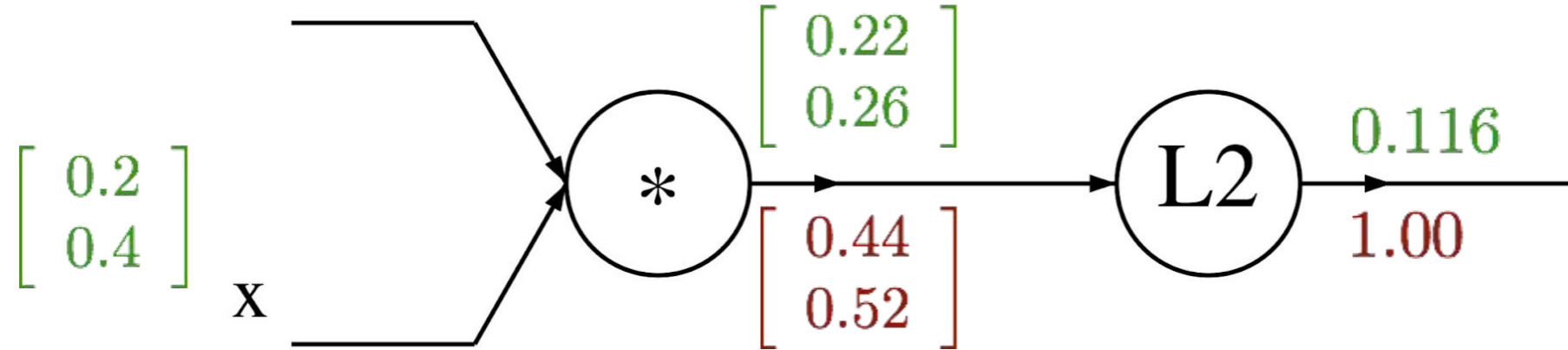
$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

$$\frac{\partial f}{\partial q_i} = 2q_i$$

$$\nabla_q f = 2q$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} W$$



$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

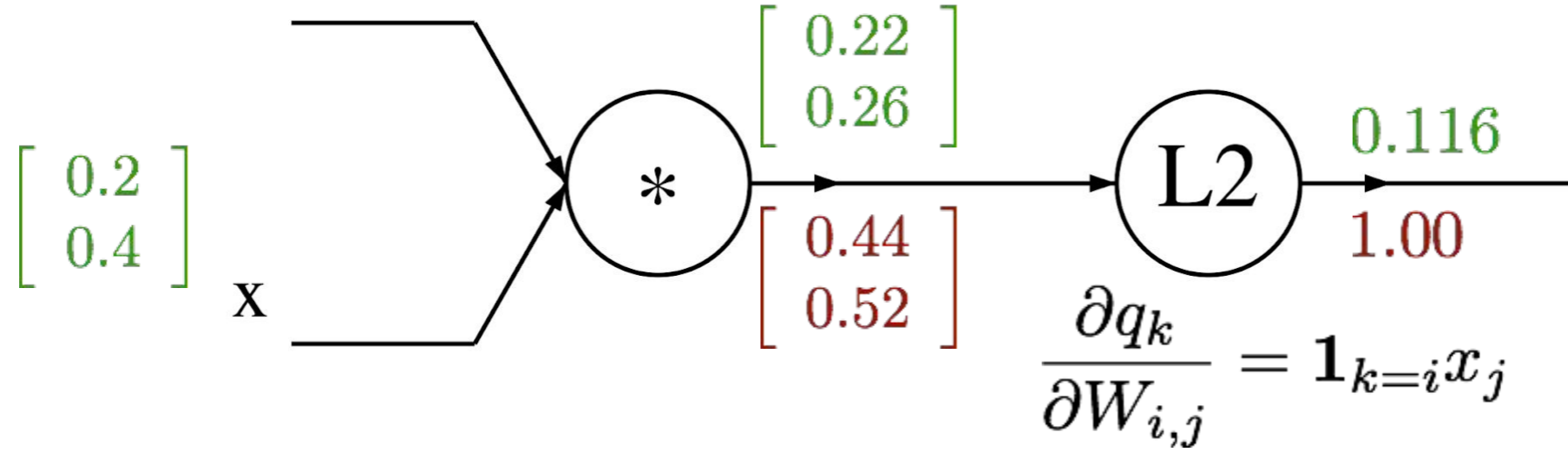
$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

$$\frac{\partial f}{\partial q_i} = 2q_i$$

$$\nabla_q f = 2q$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} W$$

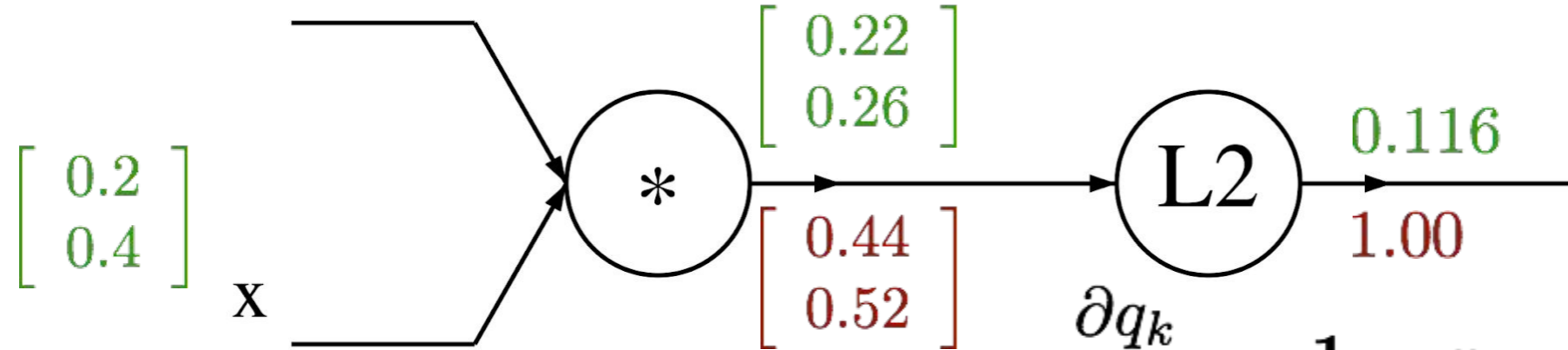


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \cdots + q_n^2$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} W$$



$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

$$\frac{\partial f}{\partial W_{i,j}} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}}$$

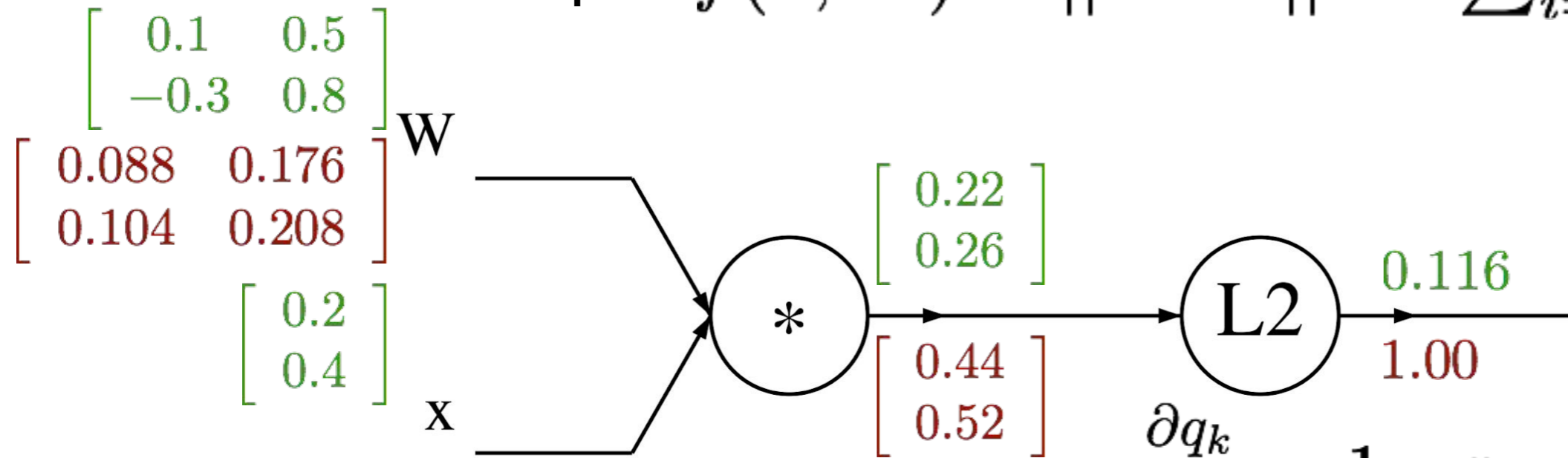
$$= \sum_k (2q_k) (\mathbf{1}_{k=i} x_j)$$

$$= 2q_i x_j$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \cdots + q_n^2$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

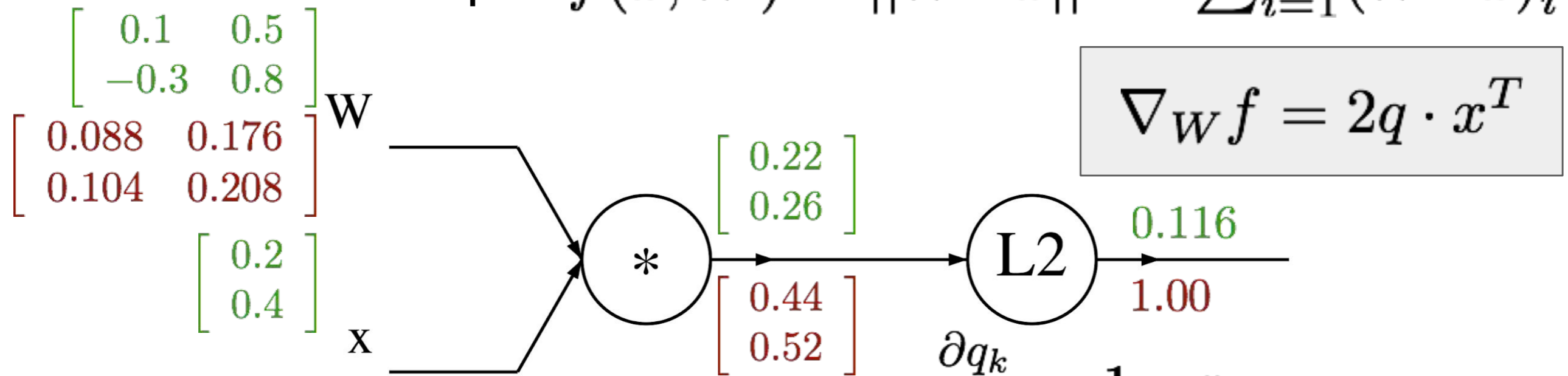


$$\begin{aligned} \frac{\partial q_k}{\partial W_{i,j}} &= \mathbf{1}_{k=i} x_j \\ \frac{\partial f}{\partial W_{i,j}} &= \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}} \\ &= \sum_k (2q_k) (\mathbf{1}_{k=i} x_j) \\ &= 2q_i x_j \end{aligned}$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$



$$\nabla_W f = 2q \cdot x^T$$

$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

$$\frac{\partial f}{\partial W_{i,j}} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}}$$

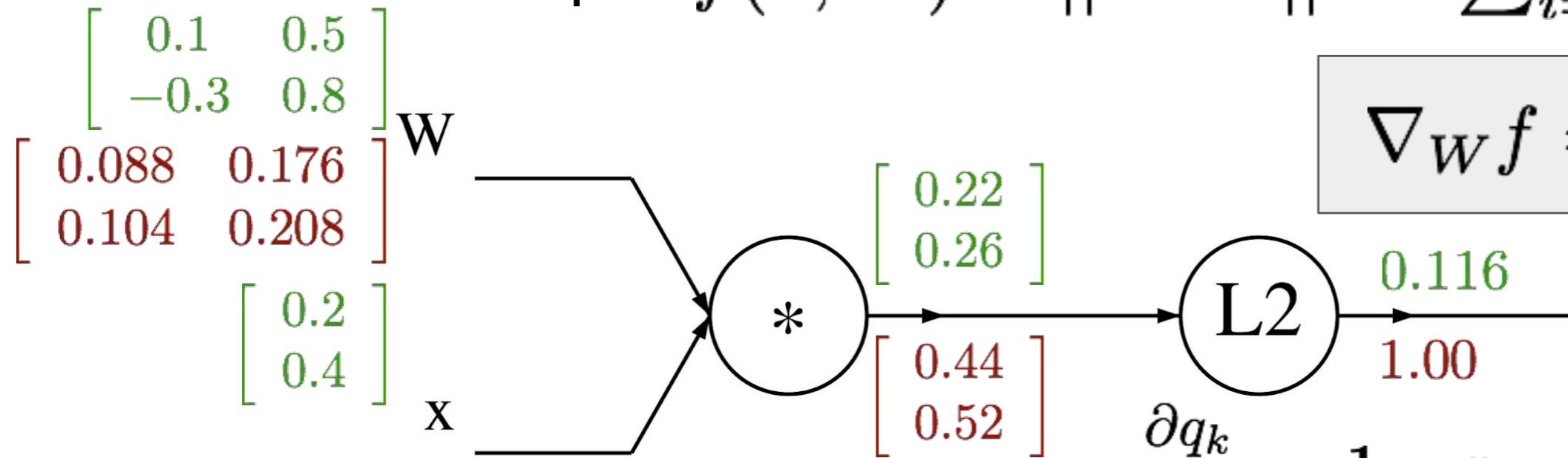
$$= \sum_k (2q_k) (\mathbf{1}_{k=i} x_j)$$

$$= 2q_i x_j$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$



$$\nabla_W f = 2q \cdot x^T$$

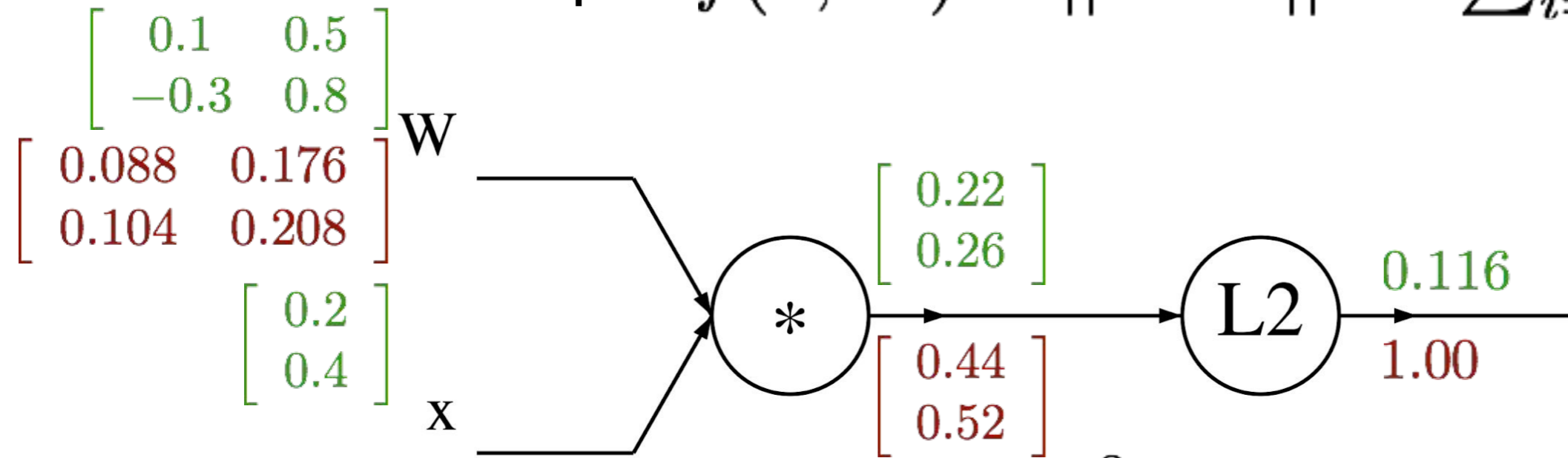
Always check: The gradient with respect to a variable should have the same shape as the variable

$$\begin{aligned} \frac{\partial q_k}{\partial W_{i,j}} &= \mathbf{1}_{k=i} x_j \\ \frac{\partial f}{\partial W_{i,j}} &= \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}} \\ &= \sum_k (2q_k) (\mathbf{1}_{k=i} x_j) \\ &= 2q_i x_j \end{aligned}$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

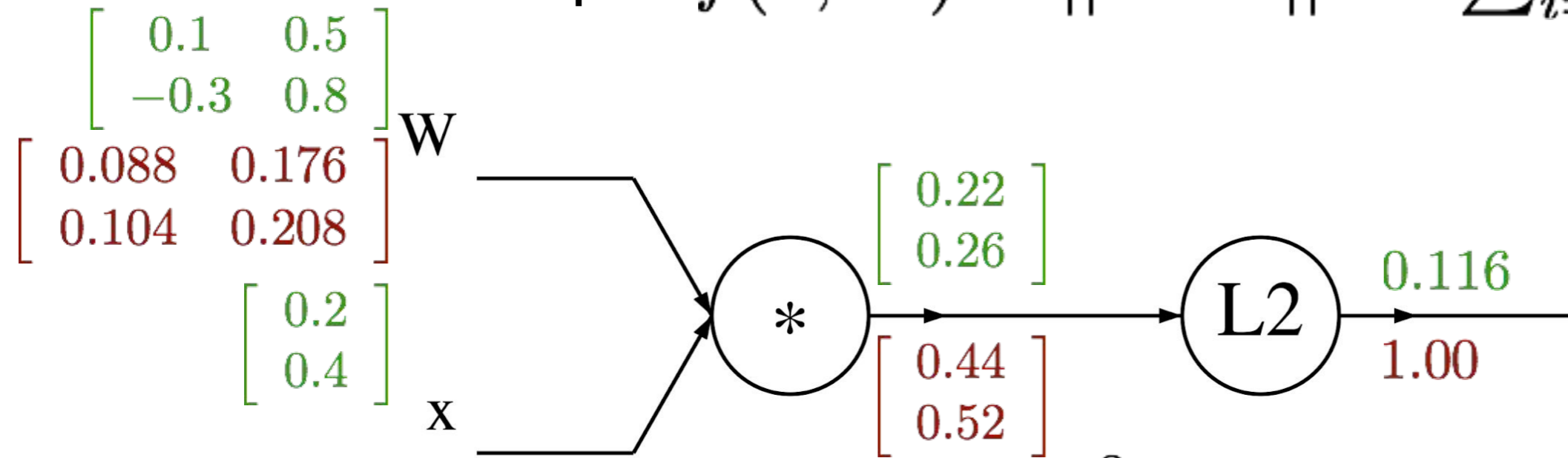


$$\frac{\partial q_k}{\partial x_i} = W_{k,i}$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

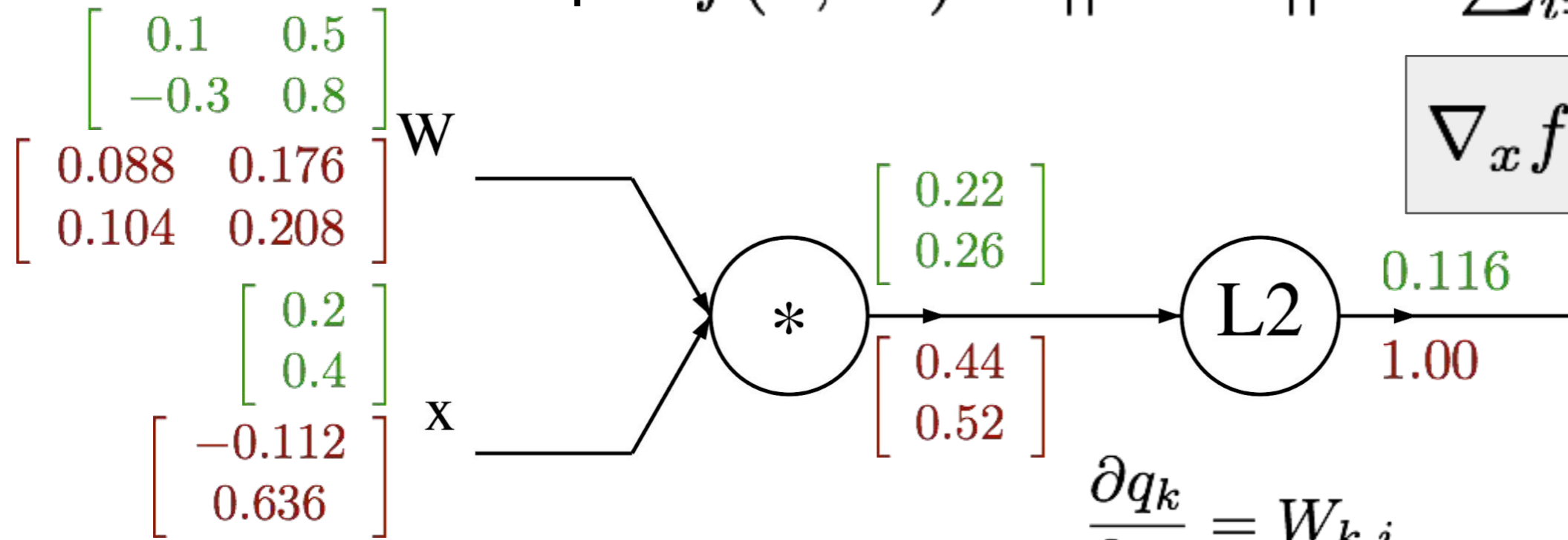


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

$$\begin{aligned} \frac{\partial q_k}{\partial x_i} &= W_{k,i} \\ \frac{\partial f}{\partial x_i} &= \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i} \\ &= \sum_k 2q_k W_{k,i} \end{aligned}$$

A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$



$$\nabla_x f = 2W^T \cdot q$$

$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \dots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \dots + W_{n,n}x_n \end{pmatrix}$$

$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

$$\begin{aligned} \frac{\partial q_k}{\partial x_i} &= W_{k,i} \\ \frac{\partial f}{\partial x_i} &= \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i} \\ &= \sum_k 2q_k W_{k,i} \end{aligned}$$

In discussion section: A matrix example...

$$z_1 = XW_1$$

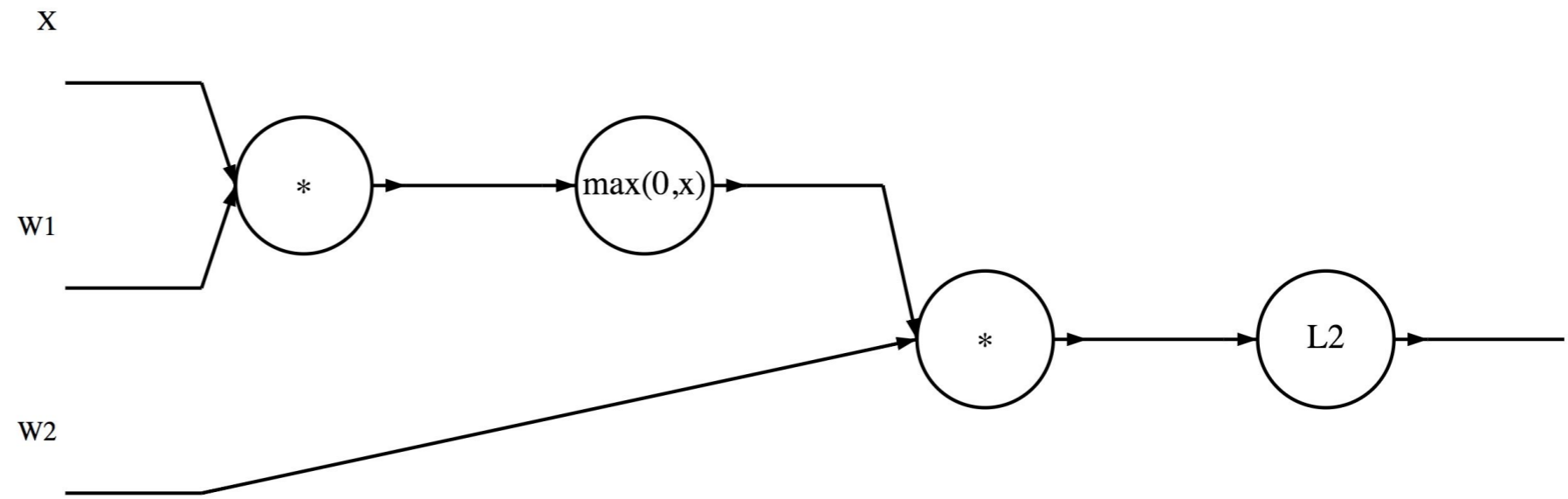
$$h_1 = \text{ReLU}(z_1)$$

$$\hat{y} = h_1 W_2$$

$$L = \|\hat{y}\|_2^2$$

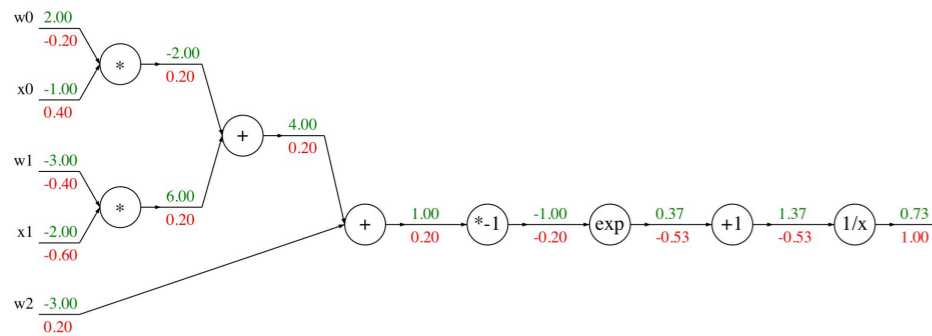
$$\frac{\partial L}{\partial W_2} = ?$$

$$\frac{\partial L}{\partial W_1} = ?$$



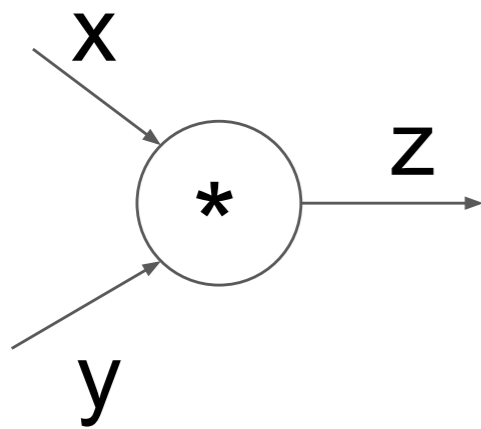
Modularized implementation: forward / backward API

Graph (or Net) object (*rough pseudo code*)



```
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
```

Modularized implementation: forward / backward API



(x,y,z are scalars)

```
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]  
        return [dx, dy]
```

Local gradient

Upstream gradient variable

Example: Caffe layers

Branch: master | [caffe / src / caffe / layers /](#) | [Create new file](#) | [Upload files](#) | [Find file](#) | [History](#)

shelhamer committed on GitHub Merge pull request #4630 from BiGene/load_hdf5_fix Latest commit e687a71 21 days ago

..		
absval_layer.cpp	dismantle layer headers	a year ago
absval_layer.cu	dismantle layer headers	a year ago
accuracy_layer.cpp	dismantle layer headers	a year ago
argmax_layer.cpp	dismantle layer headers	a year ago
base_conv_layer.cpp	enable dilated deconvolution	a year ago
base_data_layer.cpp	Using default from proto for prefetch	3 months ago
base_data_layer.cu	Switched multi-GPU to NCCL	3 months ago
batch_norm_layer.cpp	Add missing spaces besides equal signs in batch_norm_layer.cpp	4 months ago
batch_norm_layer.cu	dismantle layer headers	a year ago
batch_reindex_layer.cpp	dismantle layer headers	a year ago
batch_reindex_layer.cu	dismantle layer headers	a year ago
bias_layer.cpp	Remove incorrect cast of gemm int arg to Dtype in BiasLayer	a year ago
bias_layer.cu	Separation and generalization of ChannelwiseAffineLayer into BiasLayer	a year ago
bnll_layer.cpp	dismantle layer headers	a year ago
bnll_layer.cu	dismantle layer headers	a year ago
concat_layer.cpp	dismantle layer headers	a year ago
concat_layer.cu	dismantle layer headers	a year ago
contrastive_loss_layer.cpp	dismantle layer headers	a year ago
contrastive_loss_layer.cu	dismantle layer headers	a year ago
conv_layer.cpp	add support for 2D dilated convolution	a year ago
conv_layer.cu	dismantle layer headers	a year ago
crop_layer.cpp	remove redundant operations in Crop layer (#5138)	2 months ago
crop_layer.cu	remove redundant operations in Crop layer (#5138)	2 months ago
cudnn_conv_layer.cpp	dismantle layer headers	a year ago
cudnn_conv_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago

cudnn_lcn_layer.cpp	dismantle layer headers	a year ago
cudnn_lcn_layer.cu	dismantle layer headers	a year ago
cudnn_lrn_layer.cpp	dismantle layer headers	a year ago
cudnn_lrn_layer.cu	dismantle layer headers	a year ago
cudnn_pooling_layer.cpp	dismantle layer headers	a year ago
cudnn_pooling_layer.cu	dismantle layer headers	a year ago
cudnn_relu_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_relu_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_softmax_layer.cpp	dismantle layer headers	a year ago
cudnn_softmax_layer.cu	dismantle layer headers	a year ago
cudnn_tanh_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_tanh_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
data_layer.cpp	Switched multi-GPU to NCCL	3 months ago
deconv_layer.cpp	enable dilated deconvolution	a year ago
deconv_layer.cu	dismantle layer headers	a year ago
dropout_layer.cpp	supporting N-D Blobs in Dropout layer Reshape	a year ago
dropout_layer.cu	dismantle layer headers	a year ago
dummy_data_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cu	dismantle layer headers	a year ago
elu_layer.cpp	ELU layer with basic tests	a year ago
elu_layer.cu	ELU layer with basic tests	a year ago
embed_layer.cpp	dismantle layer headers	a year ago
embed_layer.cu	dismantle layer headers	a year ago
euclidean_loss_layer.cpp	dismantle layer headers	a year ago
euclidean_loss_layer.cu	dismantle layer headers	a year ago
exp_layer.cpp	Solving issue with exp layer with base e	a year ago
exp_layer.cu	dismantle layer headers	a year ago

Caffe is licensed under [BSD 2-Clause](#)

Caffe Sigmoid Layer

```
1 #include <cmath>
2 #include <vector>
3
4 #include "caffe/layers/sigmoid_layer.hpp"
5
6 namespace caffe {
7
8 template <typename Dtype>
9 inline Dtype sigmoid(Dtype x) {
10     return 1. / (1. + exp(-x));
11 }
12
13 template <typename Dtype>
14 void SigmoidLayer<Dtype>::Forward_cpu(const vector<Blob<Dtype>*>& bottom,
15     const vector<Blob<Dtype>*>& top) {
16     const Dtype* bottom_data = bottom[0]->cpu_data();
17     Dtype* top_data = top[0]->mutable_cpu_data();
18     const int count = bottom[0]->count();
19     for (int i = 0; i < count; ++i) {
20         top_data[i] = sigmoid(bottom_data[i]);
21     }
22 }
23
24 template <typename Dtype>
25 void SigmoidLayer<Dtype>::Backward_cpu(const vector<Blob<Dtype>*>& top,
26     const vector<bool>& propagate_down,
27     const vector<Blob<Dtype>*>& bottom) {
28     if (propagate_down[0]) {
29         const Dtype* top_data = top[0]->cpu_data();
30         const Dtype* top_diff = top[0]->cpu_diff();
31         Dtype* bottom_diff = bottom[0]->mutable_cpu_diff();
32         const int count = bottom[0]->count();
33         for (int i = 0; i < count; ++i) {
34             const Dtype sigmoid_x = top_data[i];
35             bottom_diff[i] = top_diff[i] * sigmoid_x * (1. - sigmoid_x);
36         }
37     }
38 }
39
40 #ifdef CPU_ONLY
41 STUB_GPU(SigmoidLayer);
42 #endif
43
44 INSTANTIATE_CLASS(SigmoidLayer);
45
46 } // namespace caffe
```

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

$$(1 - \sigma(x)) \sigma(x) * \text{top_diff} \text{ (chain rule)}$$

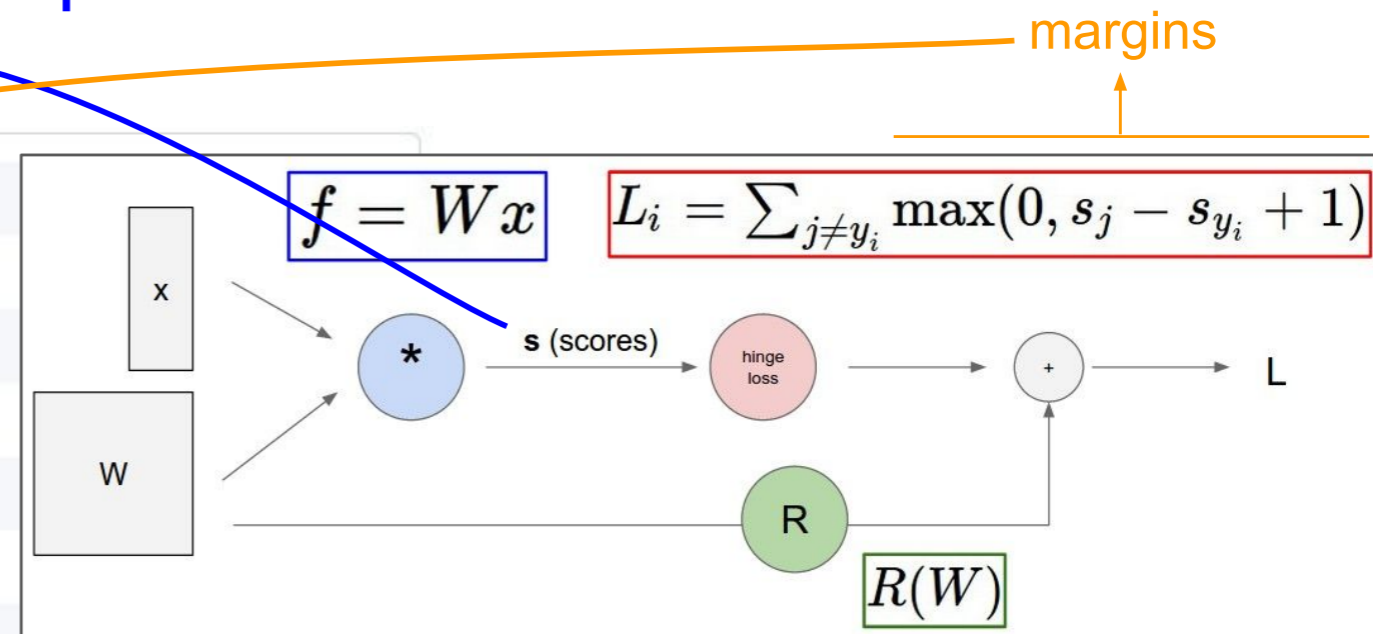
Caffe is licensed under [BSD 2-Clause](#)

In Assignment 1: Writing SVM / Softmax

Stage your forward/backward computation!

E.g. for the SVM:

```
# receive W (weights), X (data)
# forward pass (we have 8 lines)
scores = #...
margins = #...
data_loss = #...
reg_loss = #...
loss = data_loss + reg_loss
# backward pass (we have 5 lines)
dmargins = # ... (optionally, we go direct to dscores)
dscores = #...
dW = #...
```



Summary so far...

- neural nets will be very large: impractical to write down gradient formula by hand for all parameters
- **backpropagation** = recursive application of the chain rule along a computational graph to compute the gradients of all inputs/parameters/intermediates
- implementations maintain a graph structure, where the nodes implement the **forward()** / **backward()** API
- **forward**: compute result of an operation and save any intermediates needed for gradient computation in memory
- **backward**: apply the chain rule to compute the gradient of the loss function with respect to the inputs

Next: Neural Networks

Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

Neural networks: without the brain stuff

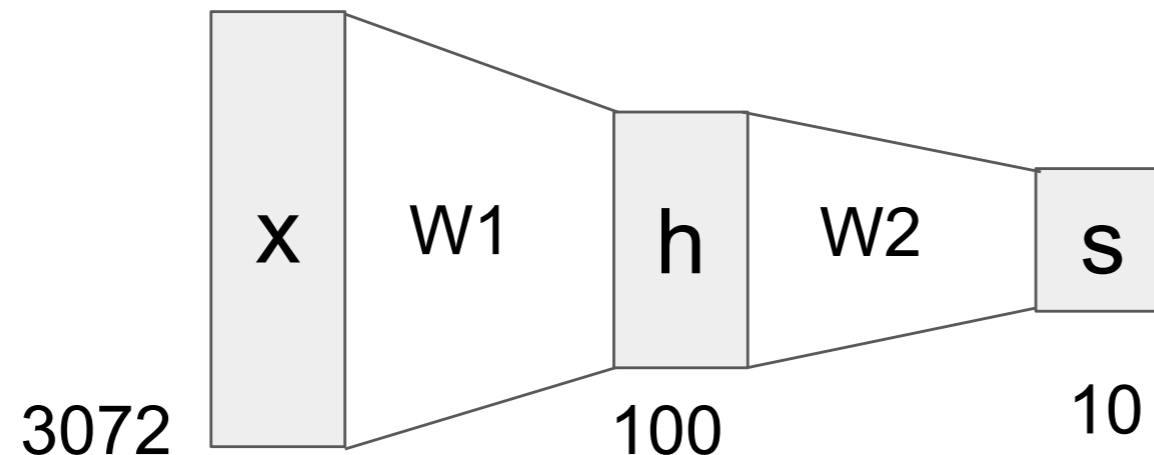
(Before) Linear score function: $f = Wx$

(Now) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

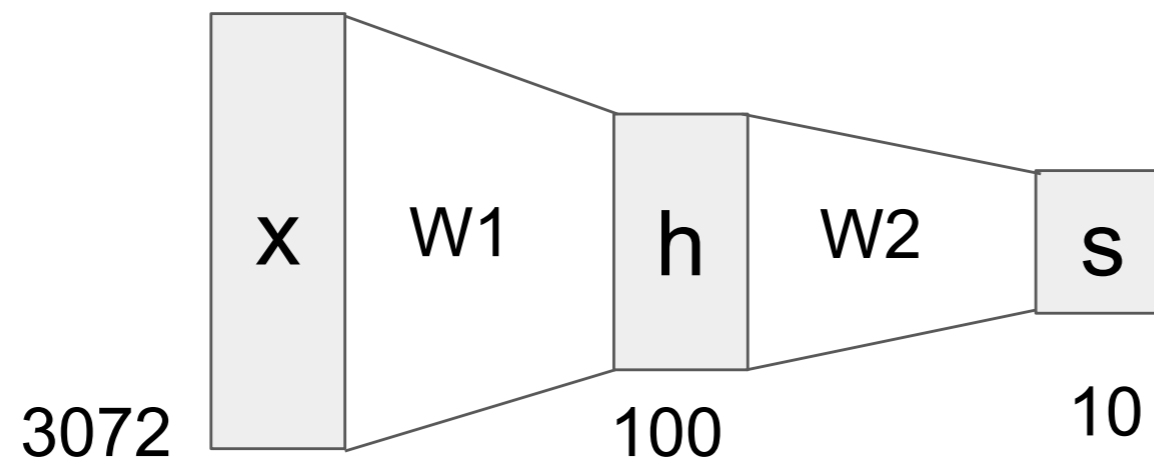
(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$



Neural networks: without the brain stuff

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$



Neural networks: without the brain stuff

(Before) Linear score function: $f = Wx$

(Now) 2-layer Neural Network
or 3-layer Neural Network $f = W_2 \max(0, W_1 x)$

$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
1 import numpy as np
2 from numpy.random import randn
3
4 N, D_in, H, D_out = 64, 1000, 100, 10
5 x, y = randn(N, D_in), randn(N, D_out)
6 w1, w2 = randn(D_in, H), randn(H, D_out)
7
8 for t in range(2000):
9     h = 1 / (1 + np.exp(-x.dot(w1)))
10    y_pred = h.dot(w2)
11    loss = np.square(y_pred - y).sum()
12    print(t, loss)
13
14    grad_y_pred = 2.0 * (y_pred - y)
15    grad_w2 = h.T.dot(grad_y_pred)
16    grad_h = grad_y_pred.dot(w2.T)
17    grad_w1 = x.T.dot(grad_h * h * (1 - h))
18
19    w1 -= 1e-4 * grad_w1
20    w2 -= 1e-4 * grad_w2
```

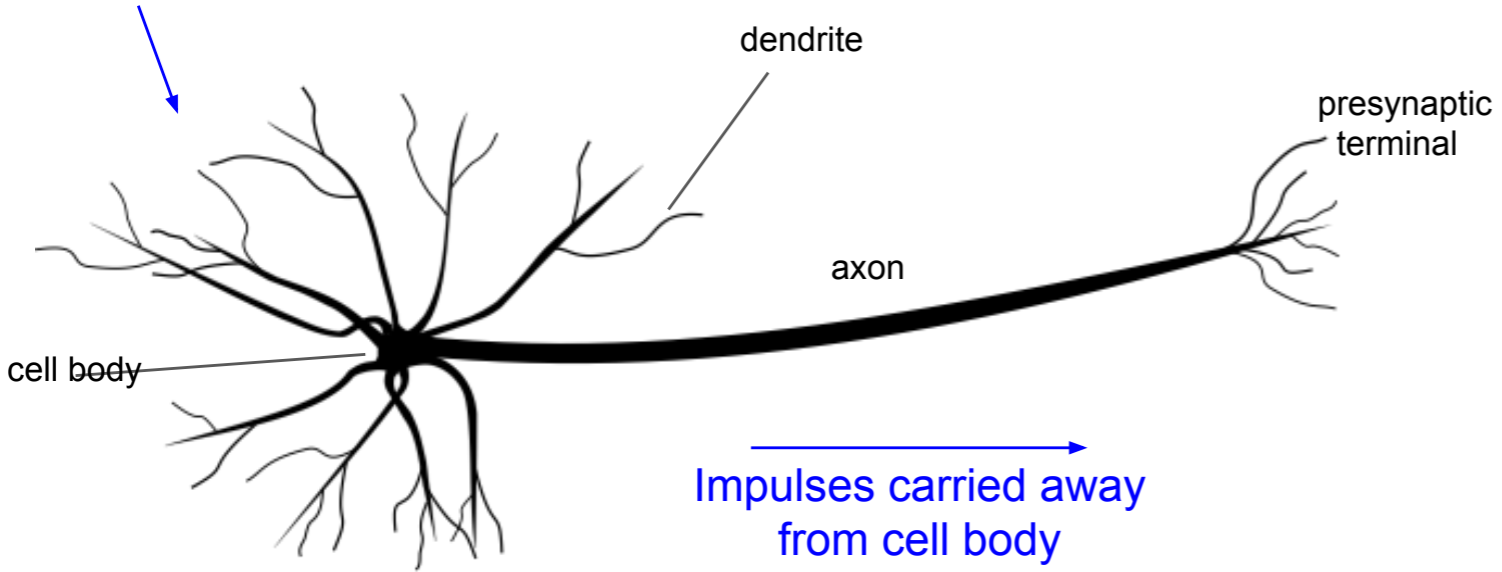
In HW: Writing a 2-layer net

```
# receive W1,W2,b1,b2 (weights/biases), X (data)
# forward pass:
h1 = #... function of X,W1,b1
scores = #... function of h1,W2,b2
loss = #... (several lines of code to evaluate Softmax loss)
# backward pass:
dscores = #...
dh1,dW2,db2 = #...
dW1,db1 = #...
```



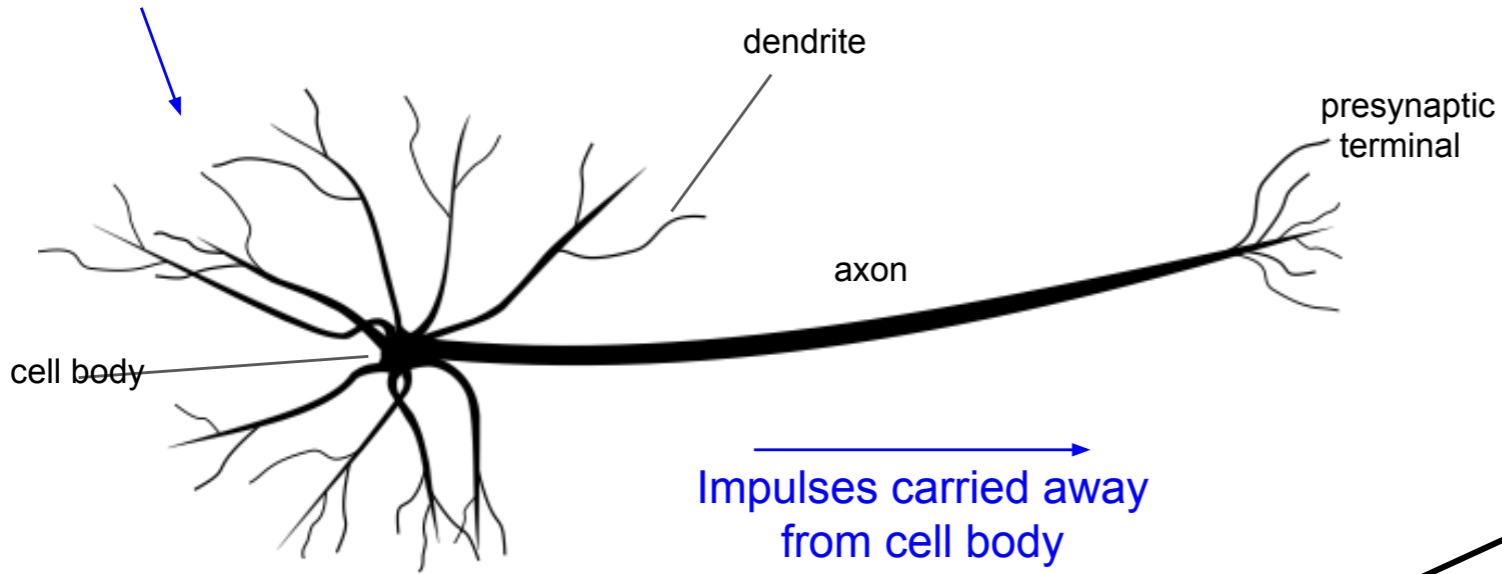

[This image](#) by [Fotis Bobolas](#) is licensed under [CC-BY 2.0](#)

Impulses carried toward cell body

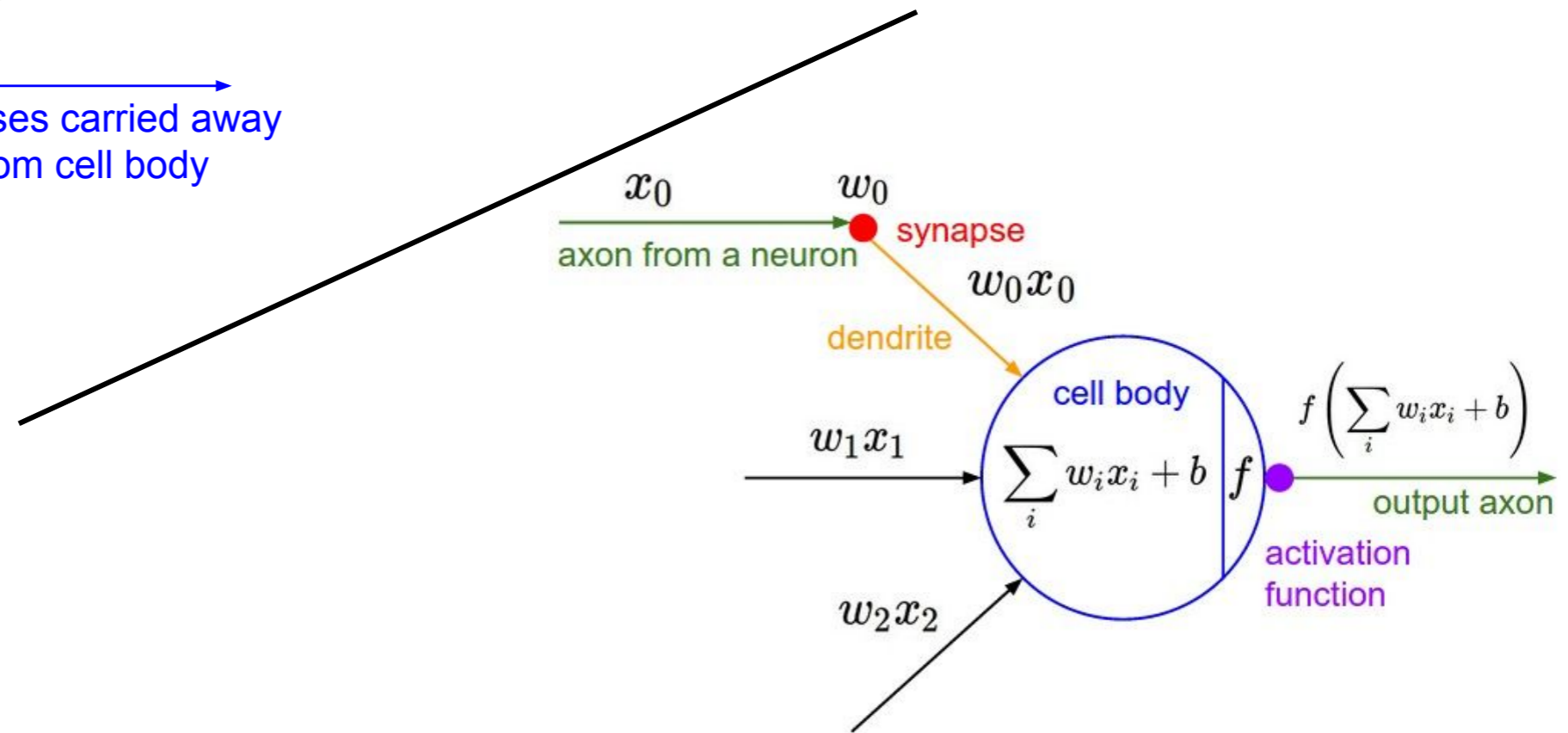


[This image](#) by Felipe Perucho is licensed under [CC-BY 3.0](#)

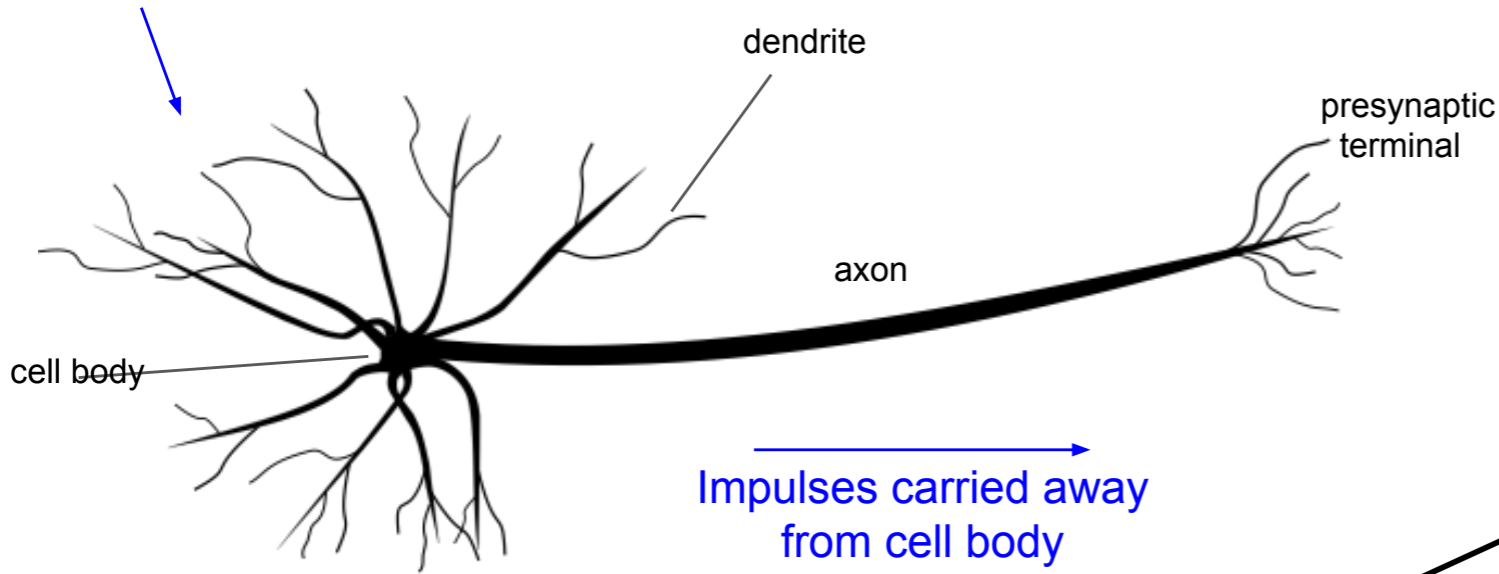
Impulses carried toward cell body



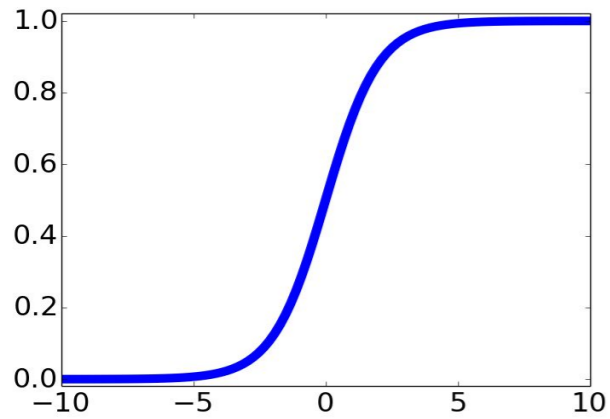
This image by Felipe Perucho is licensed under [CC-BY 3.0](https://creativecommons.org/licenses/by/3.0/)



Impulses carried toward cell body

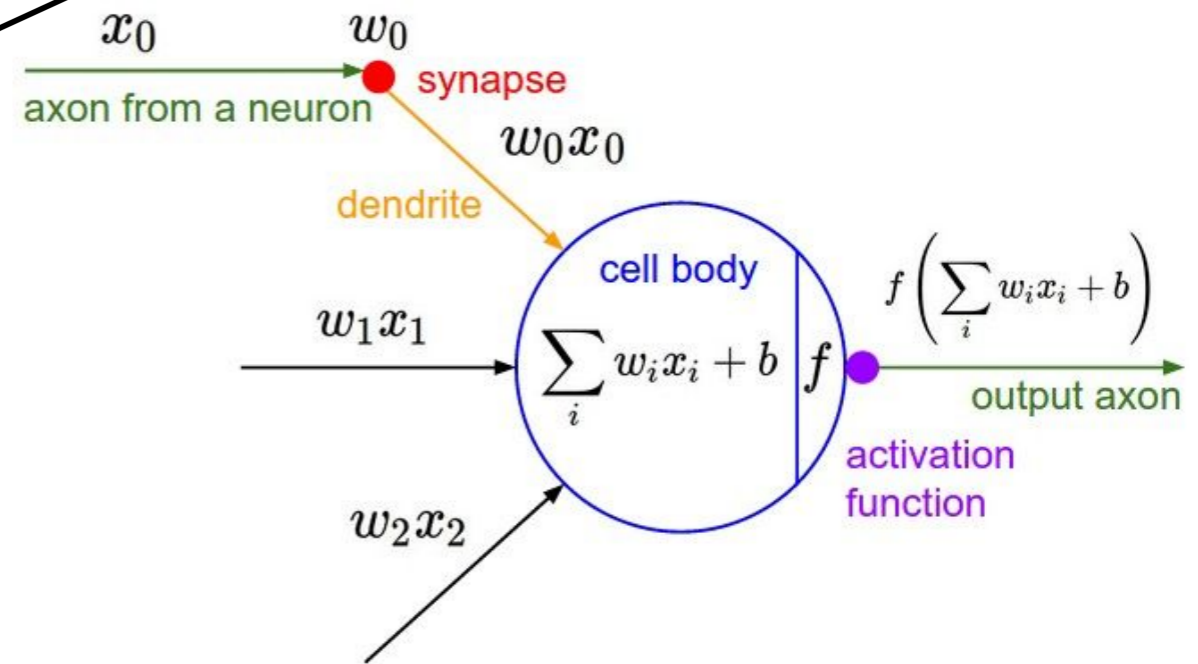


This image by Felipe Perucho is licensed under [CC-BY 3.0](https://creativecommons.org/licenses/by/3.0/)

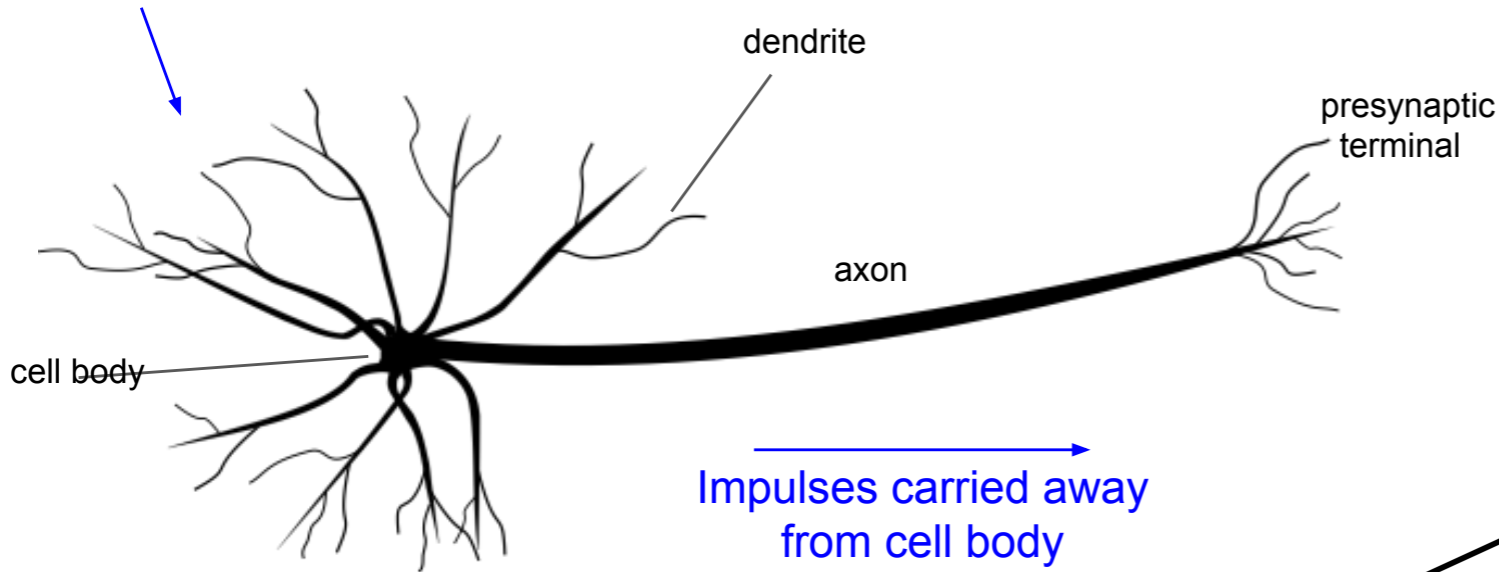


sigmoid activation function

$$\frac{1}{1 + e^{-x}}$$

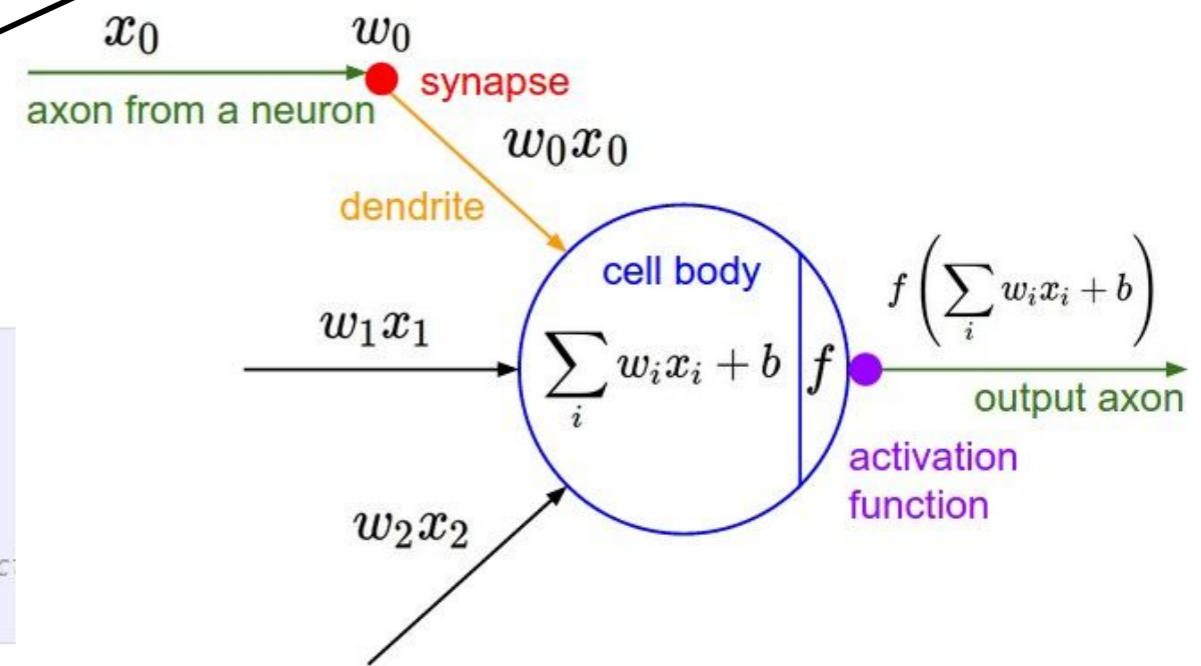


Impulses carried toward cell body



This image by Felipe Perucho is licensed under [CC-BY 3.0](https://creativecommons.org/licenses/by/3.0/)

```
class Neuron:
    # ...
    def neuron_tick(inputs):
        """ assume inputs and weights are 1-D numpy arrays and bias is a number """
        cell_body_sum = np.sum(inputs * self.weights) + self.bias
        firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation func
        return firing_rate
```



Be very careful with your brain analogies!

Biological Neurons:

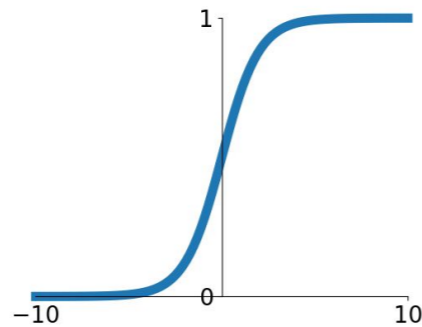
- Many different types
- Dendrites can perform complex non-linear computations
- Synapses are not a single weight but a complex non-linear dynamical system
- Rate code may not be adequate

[Dendritic Computation. London and Hausser]

Activation functions

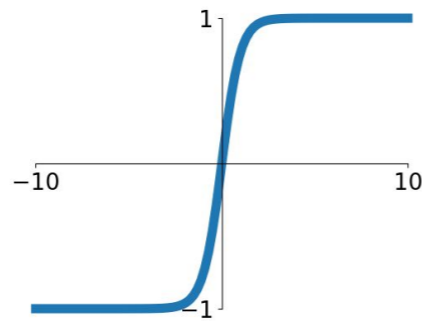
Sigmoid

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



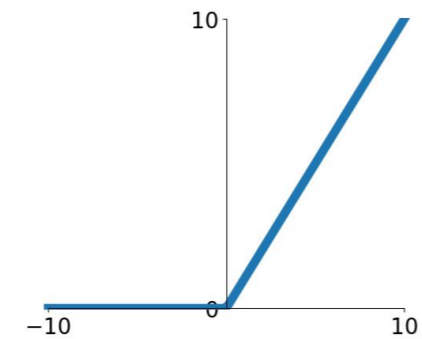
tanh

$$\tanh(x)$$



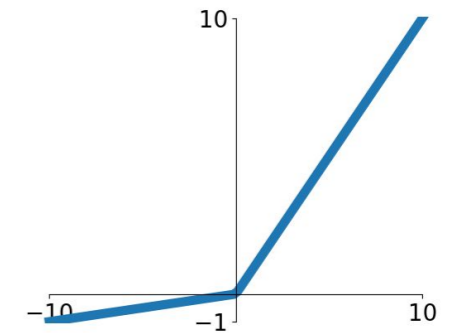
ReLU

$$\max(0, x)$$



Leaky ReLU

$$\max(0.1x, x)$$

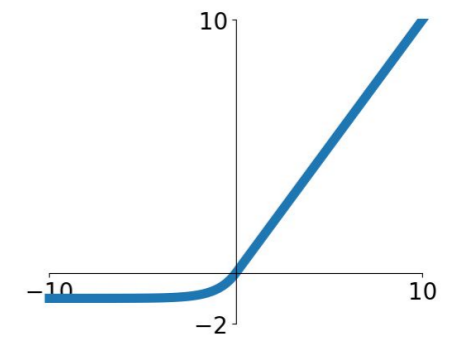


Maxout

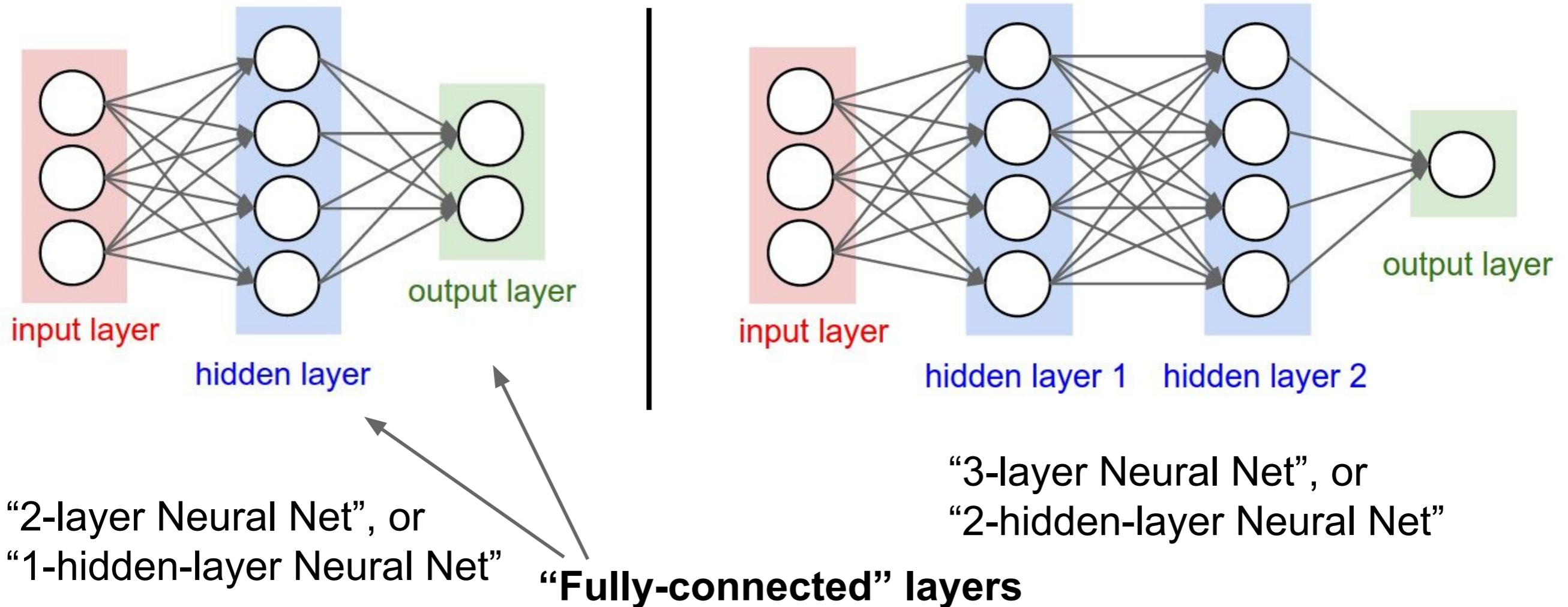
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Neural networks: Architectures

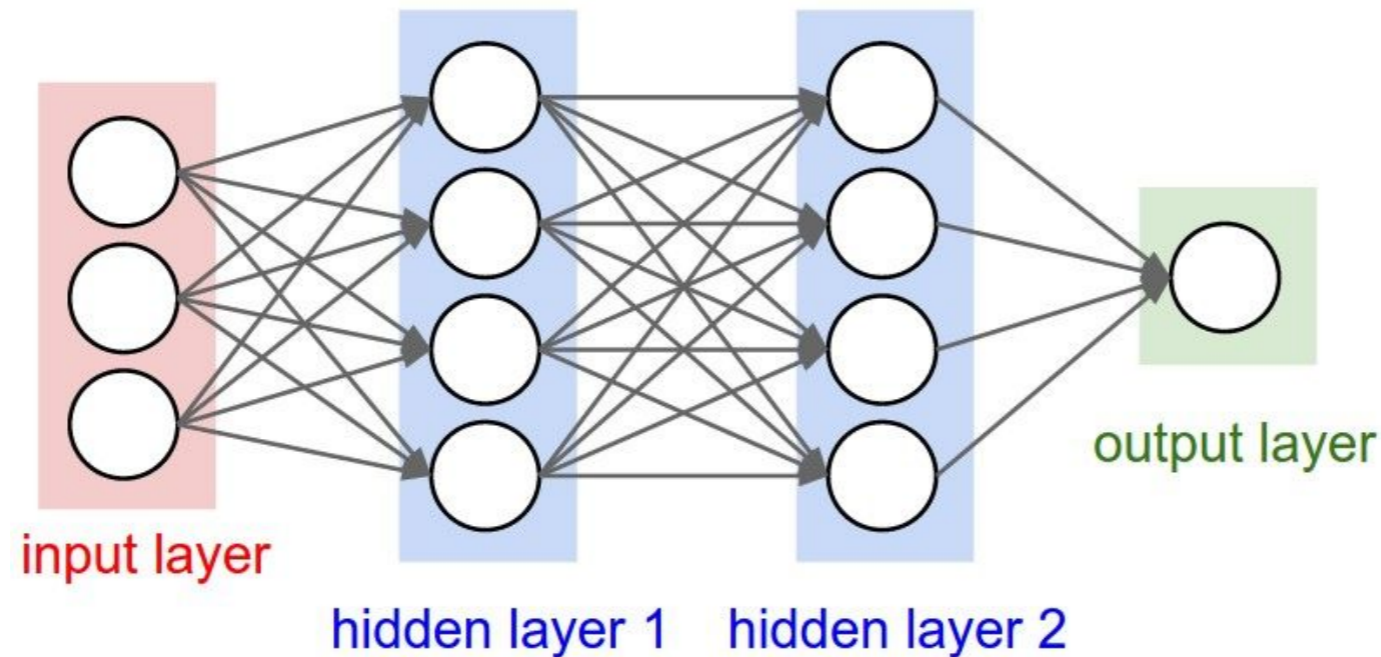


Example feed-forward computation of a neural network

```
class Neuron:  
    # ...  
    def neuron_tick(inputs):  
        """ assume inputs and weights are 1-D numpy arrays and bias is a number """  
        cell_body_sum = np.sum(inputs * self.weights) + self.bias  
        firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation function  
        return firing_rate
```

We can efficiently evaluate an entire layer of neurons.

Example feed-forward computation of a neural network



```
# forward-pass of a 3-layer neural network:  
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)  
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)  
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)  
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)  
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```

Summary

- We arrange neurons into fully-connected layers
- The abstraction of a **layer** has the nice property that it allows us to use efficient vectorized code (e.g. matrix multiplies)
- Neural networks are not really *neural*
- Next time: Convolutional Neural Networks