INT305 Machine Learning

Lecture 5

Neural Network and Back Propagation

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Neural network

Neural Network: without the brain stuff

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

Neural network

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

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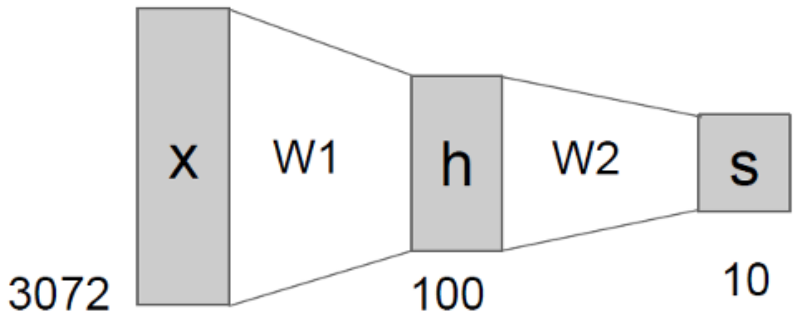


Neural network

Neural Network: without the brain stuff

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

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

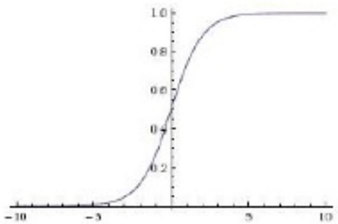
or 3-layer Neural Network:

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

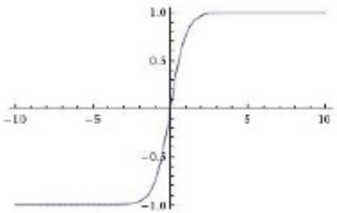
Activation functions

Activation Functions

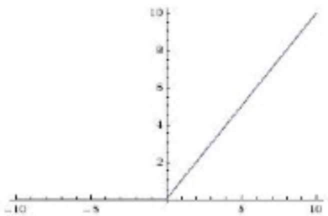
Sigmoid
$\sigma(x) = 1/(1 + e^{-x})$



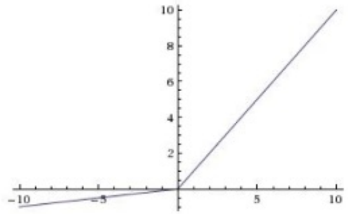
tanh $\tanh(x)$



ReLU $\max(0, x)$



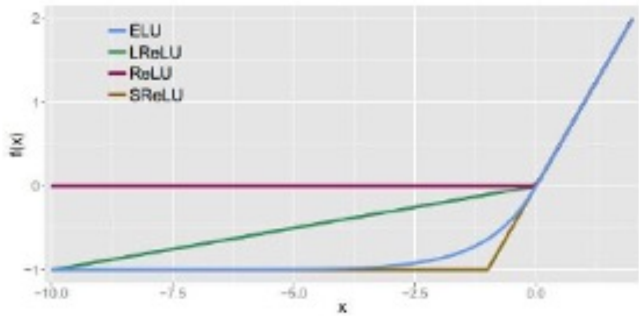
Leaky ReLU
$\max(0.1x, x)$



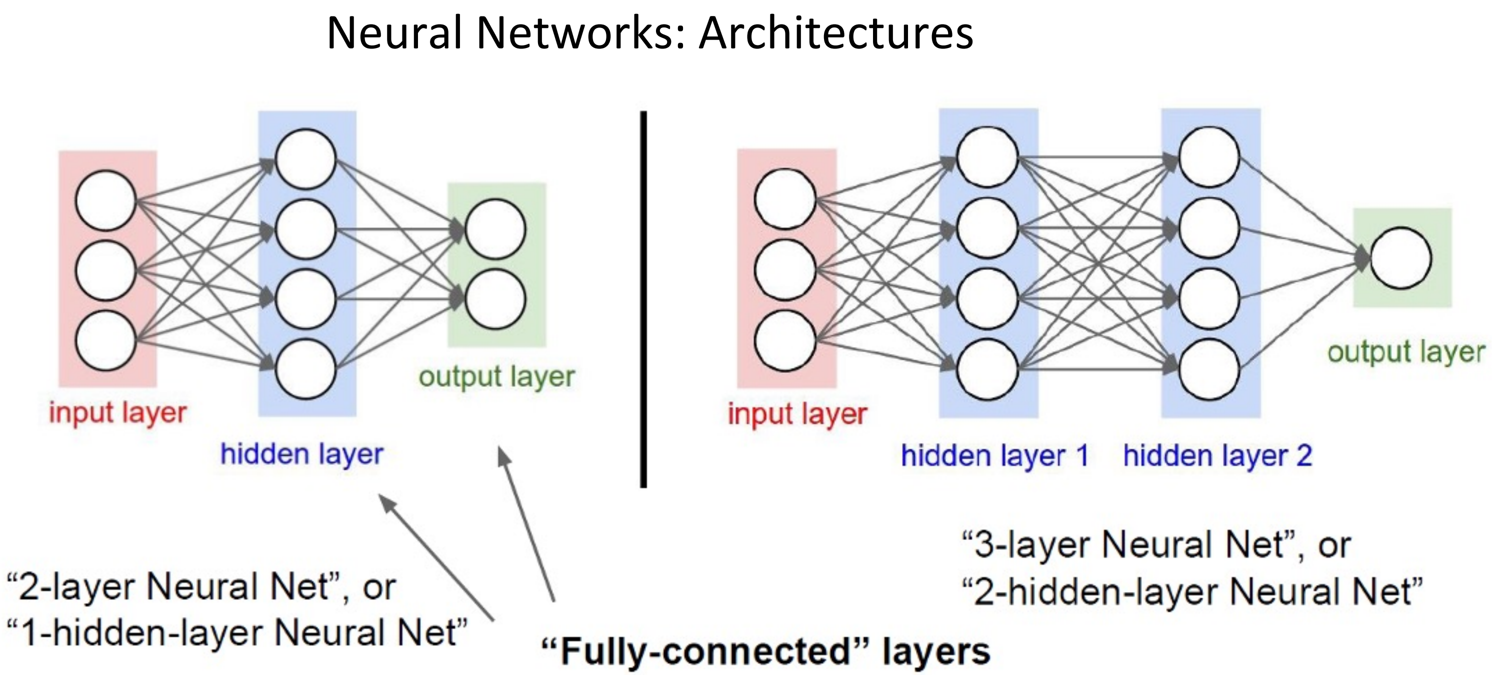
Maxout $\max(w_1^\intercal x + b_1, w_2^\intercal x + b_2)$

ELU

$$f(x) = \begin{cases} x & if\ x > 0 \\ \alpha(\exp(x) - 1) & if\ x \leq 0 \end{cases}$$

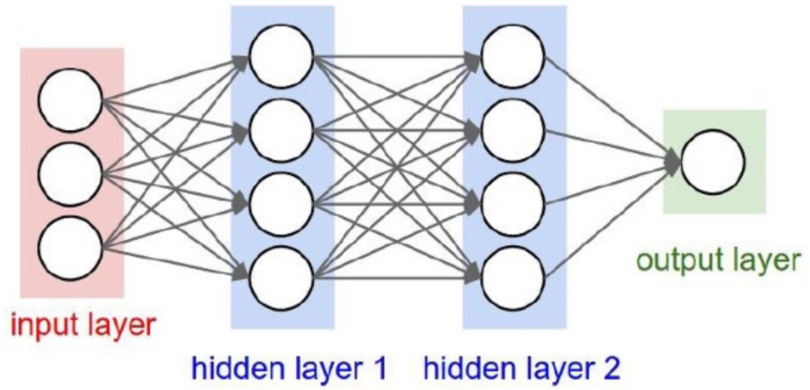


Neural network



Neural network

Example Feed-forward computation of a Neural Network




```python
# 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)
```

Gradient Descent

Where we are…

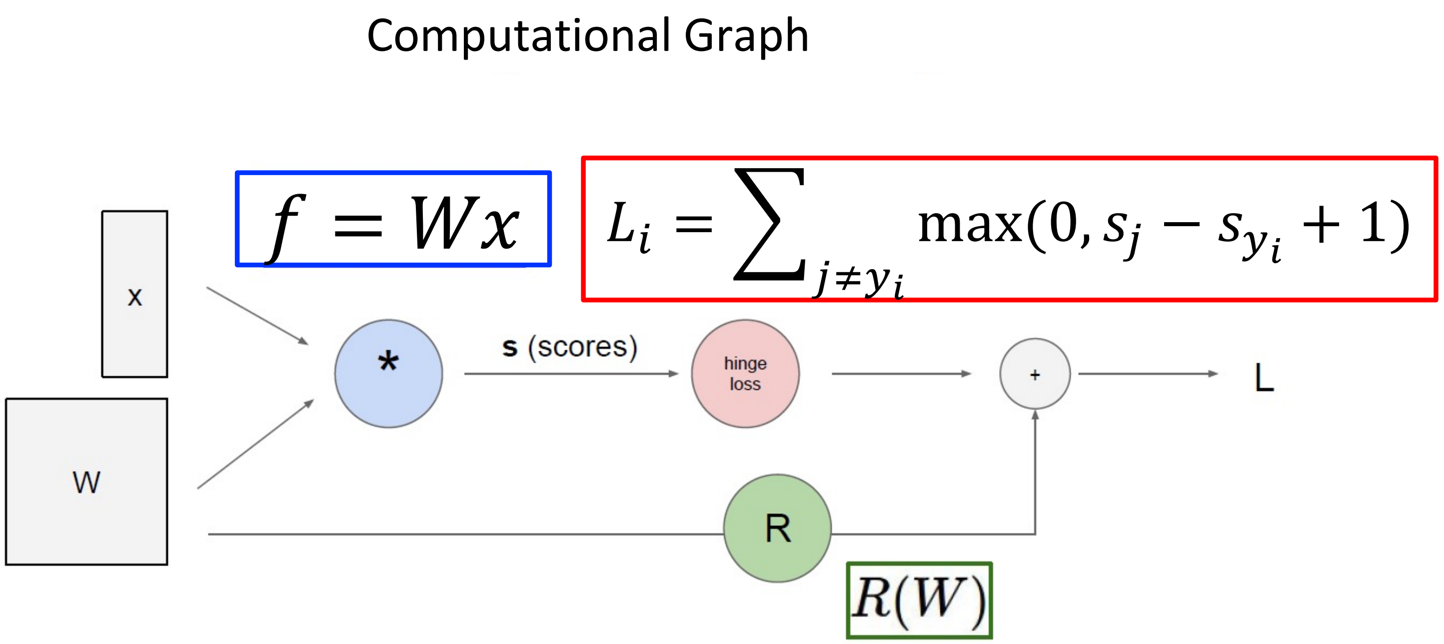
$s = f(x; W) = Wx$ scores function

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

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

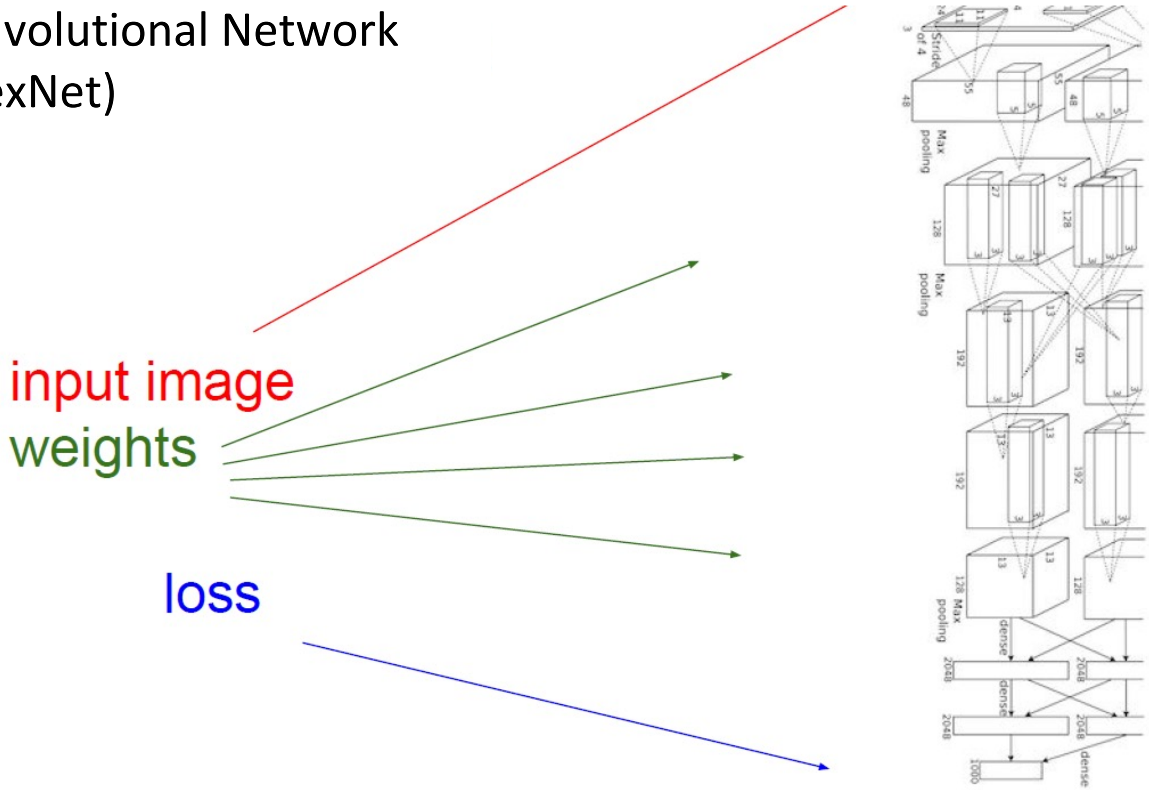
want $\boxed{\nabla_W L}$

Computational Graph



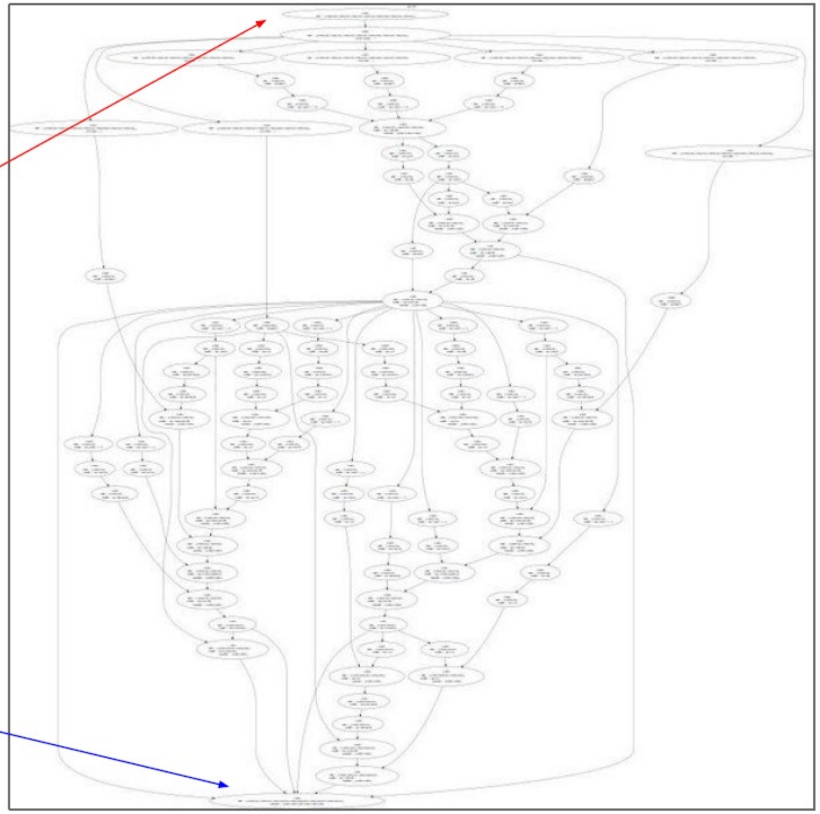
Computational Graph

Convolutional Network
(AlexNet)



Computational Graph

Neural Turing Machine



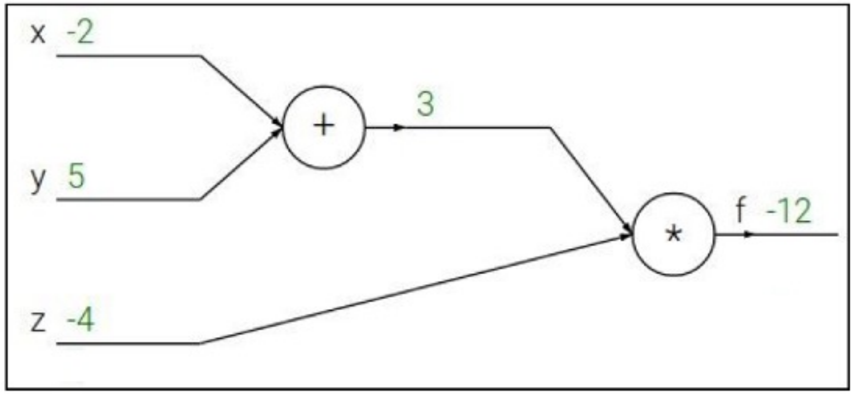
input tape

loss

Example 1

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

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



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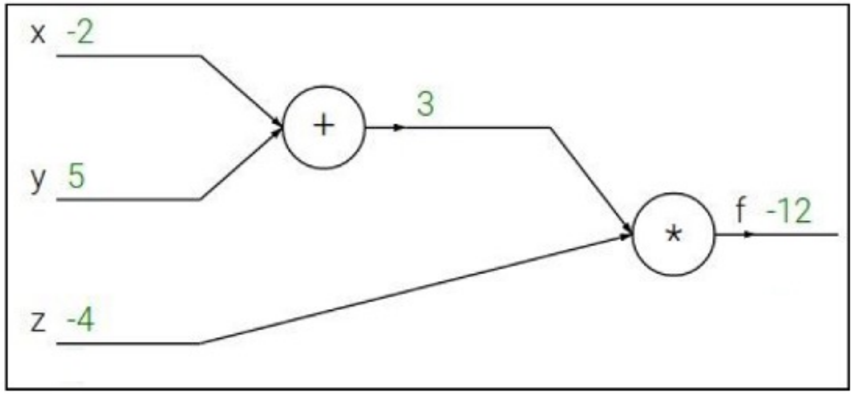

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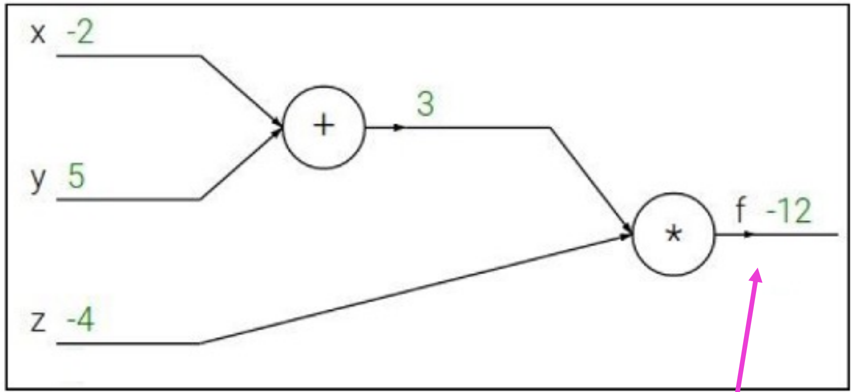

$$\boxed{\frac{\partial f}{\partial f}}$$

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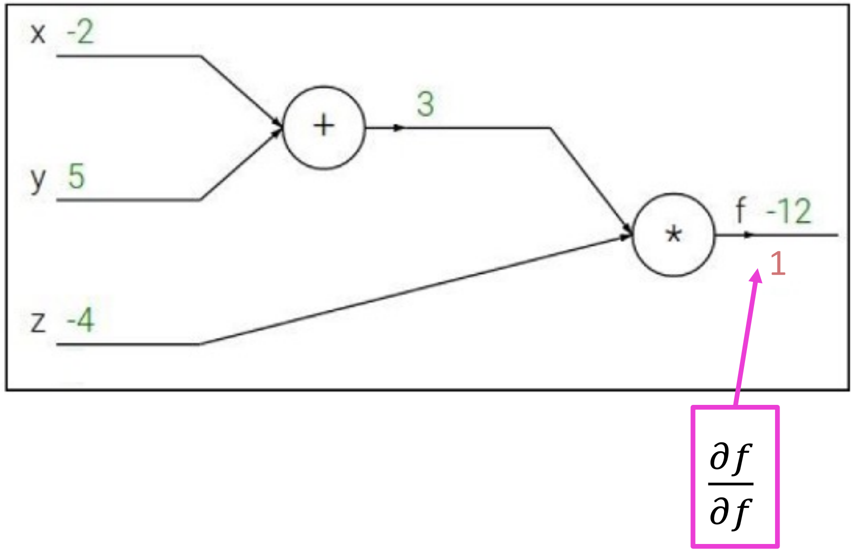

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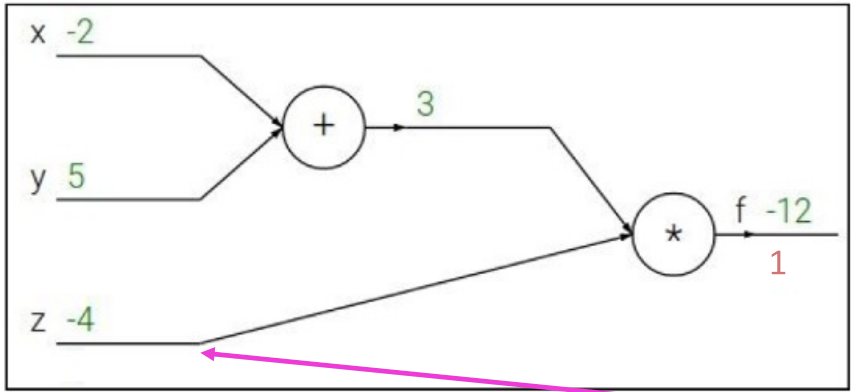

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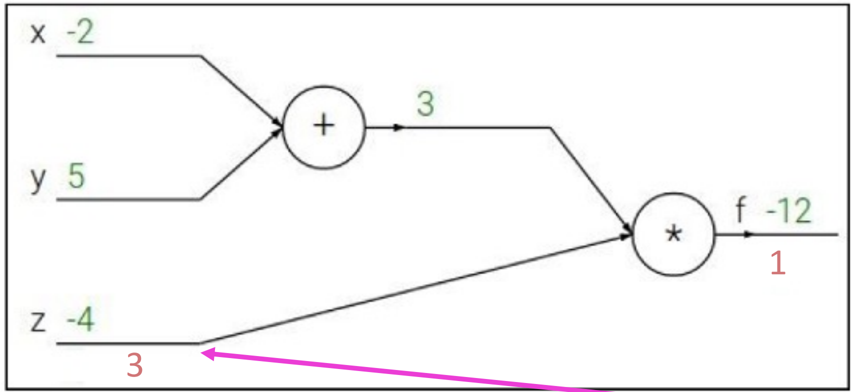

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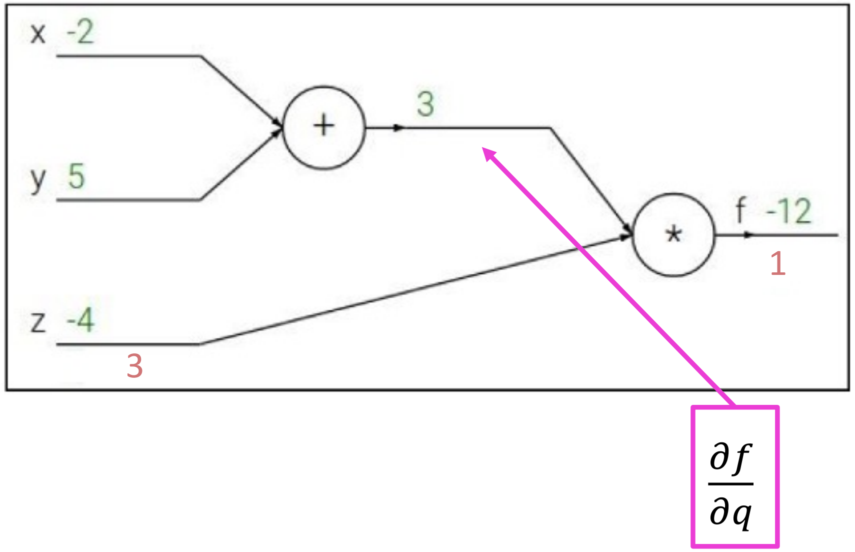

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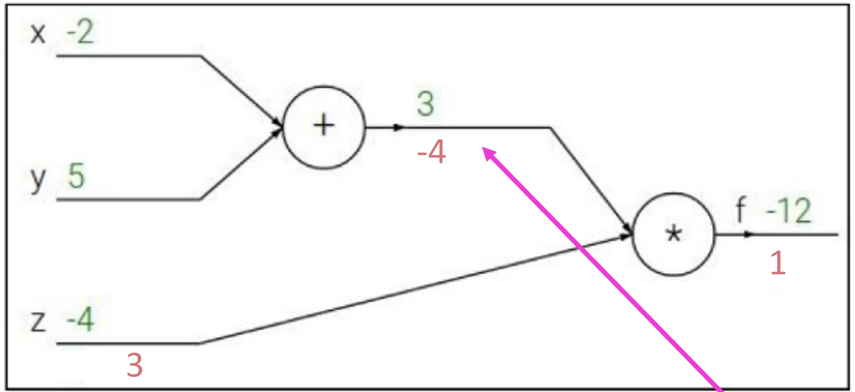

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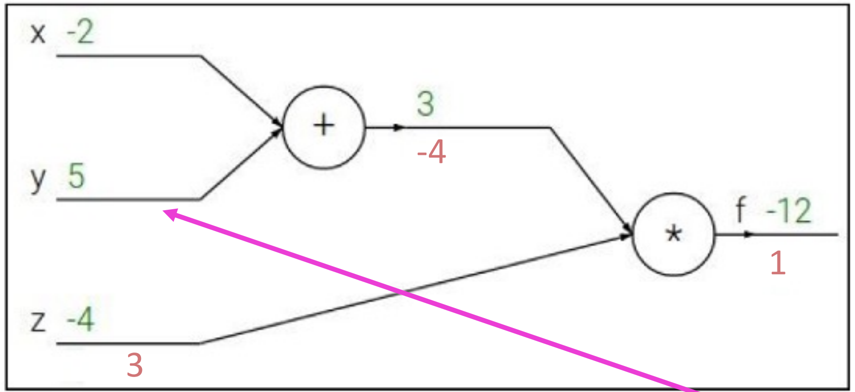

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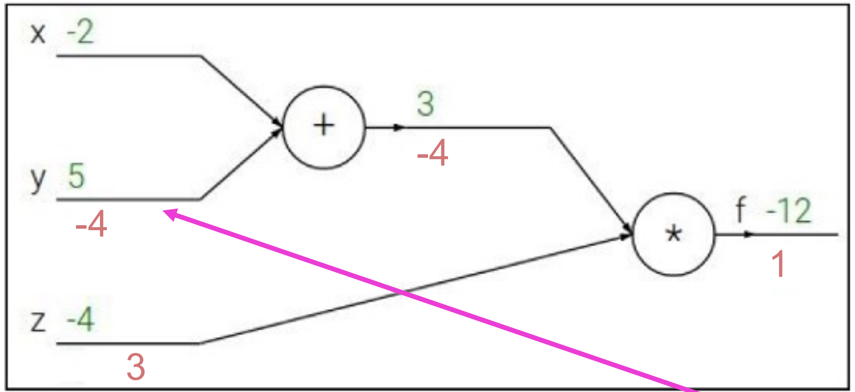

$$\frac{\partial f}{\partial y}$$

Chain rule:

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

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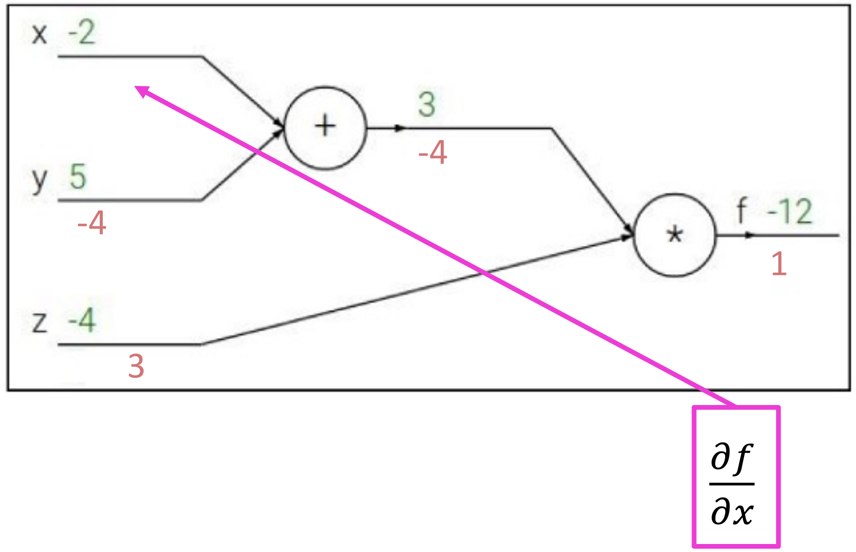

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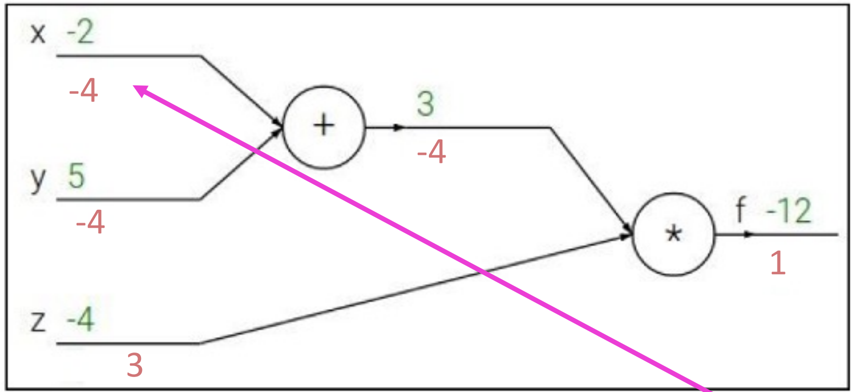

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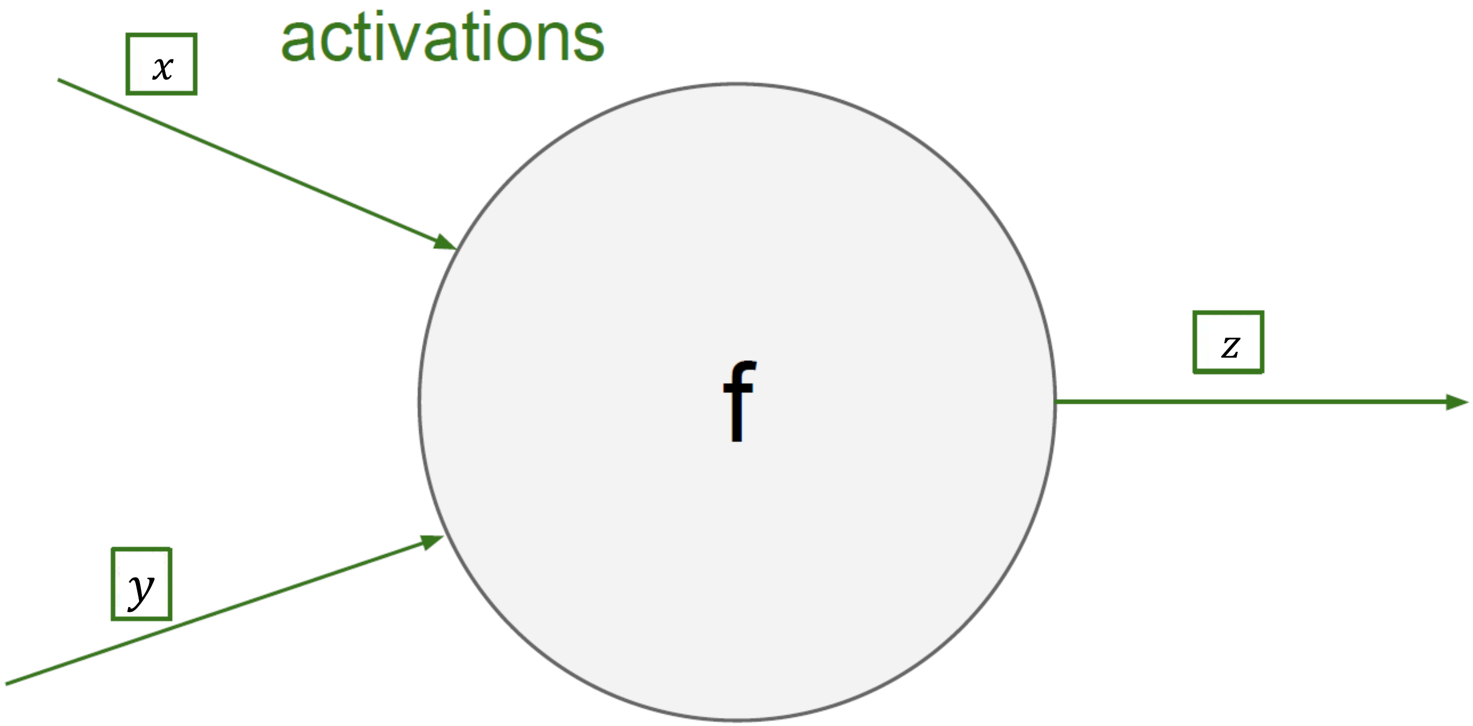
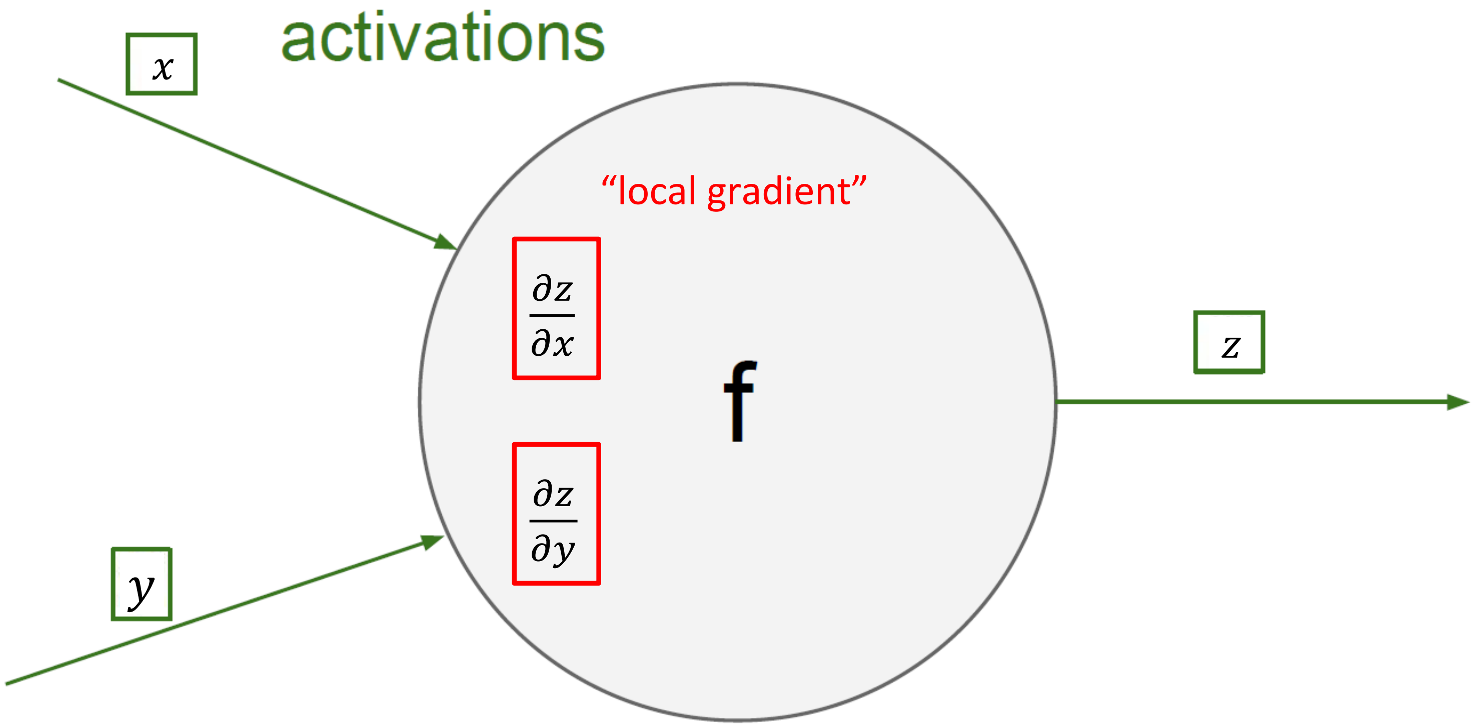
Chain rule

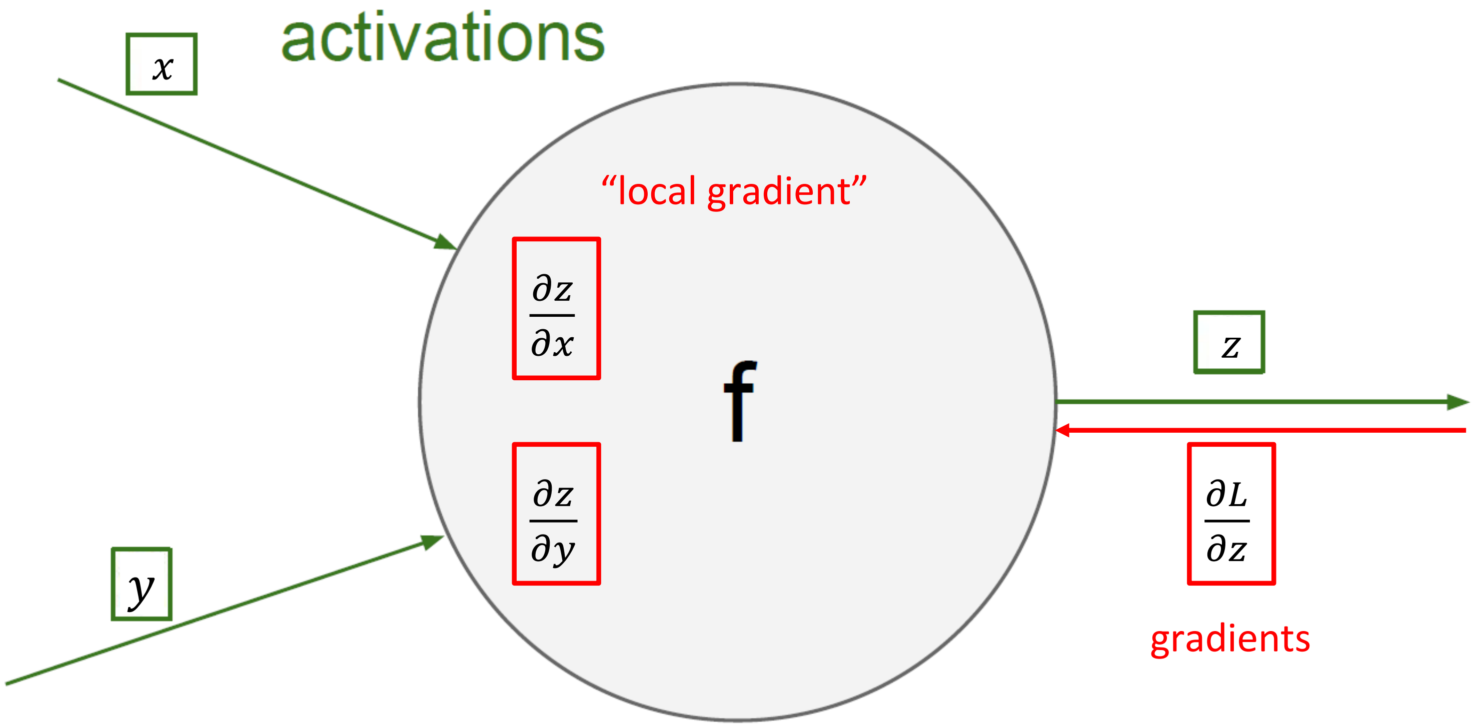


Chain rule



activations
x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
y

Chain rule



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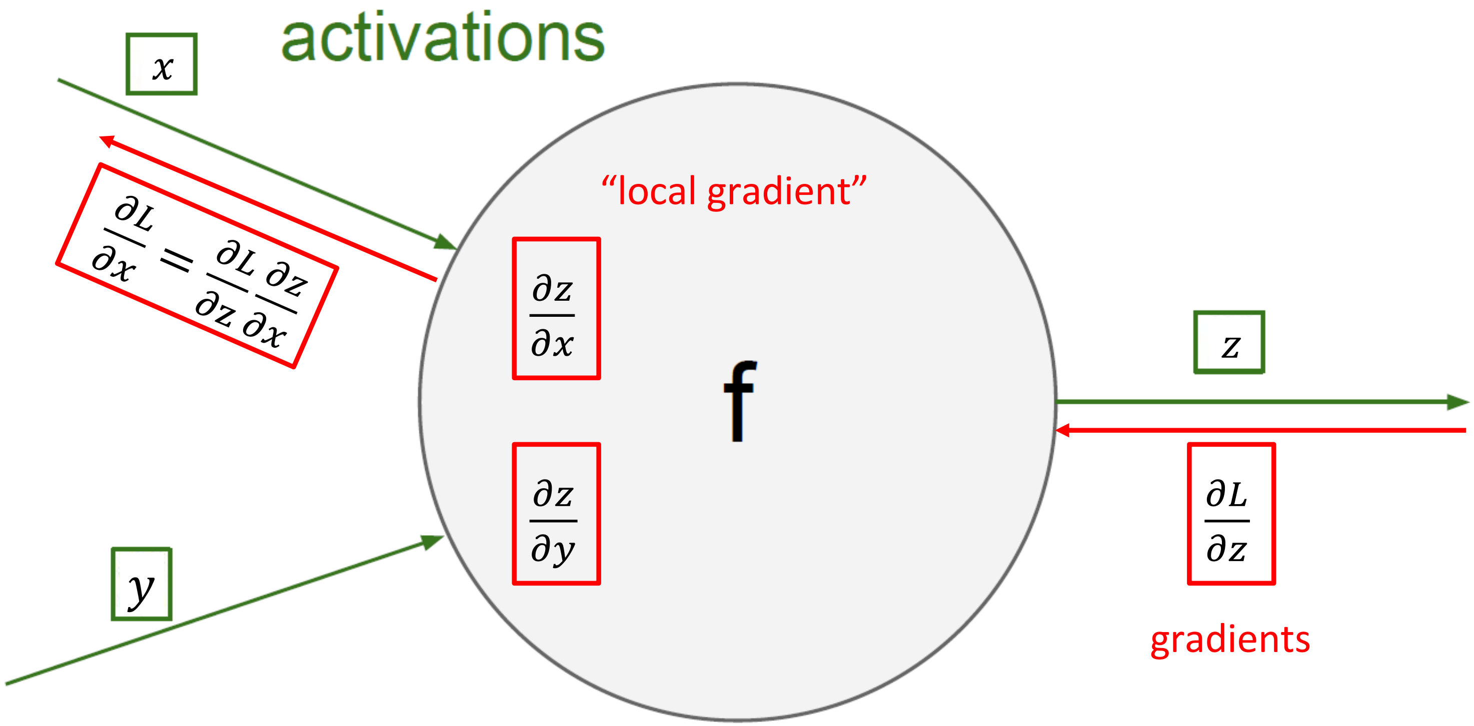
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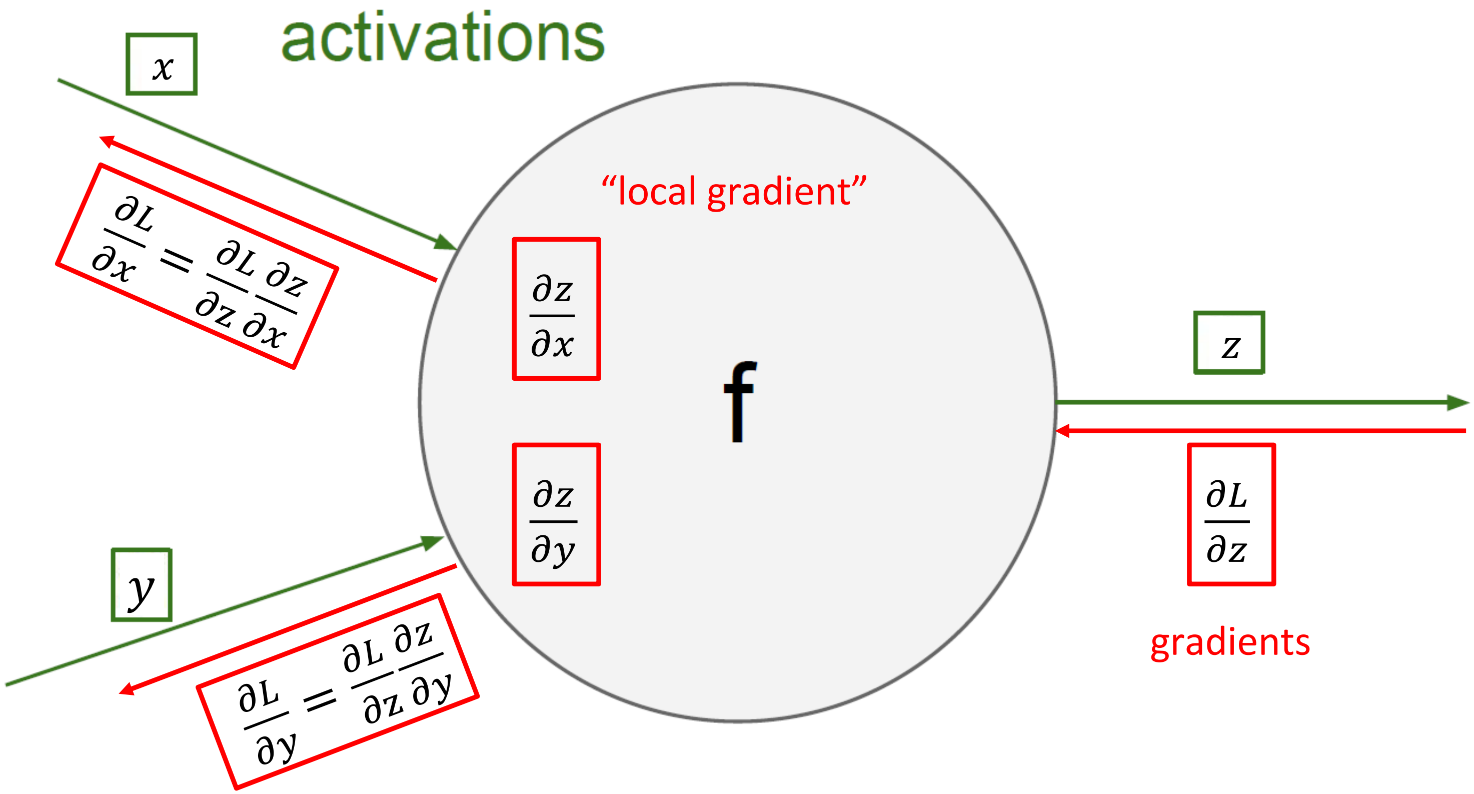

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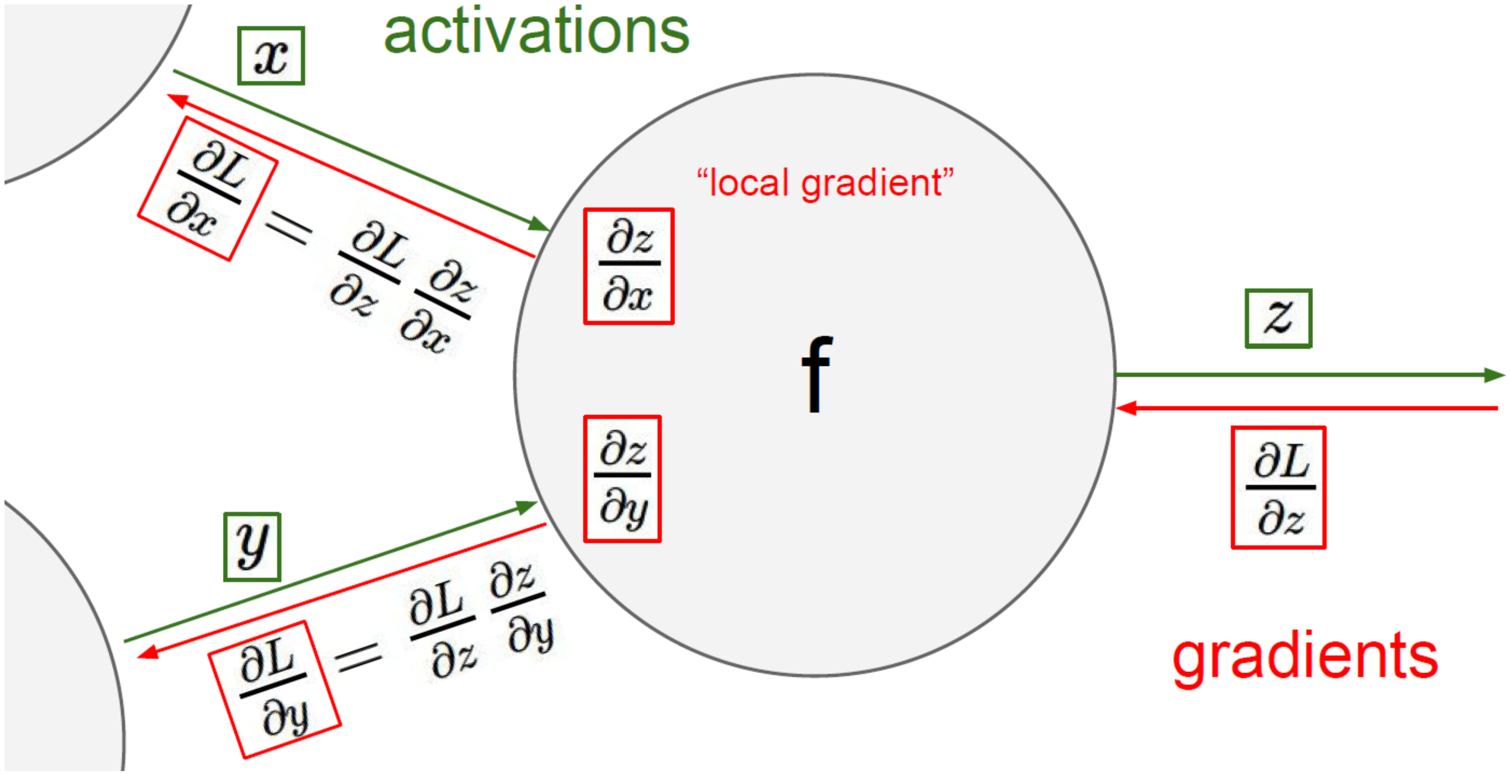

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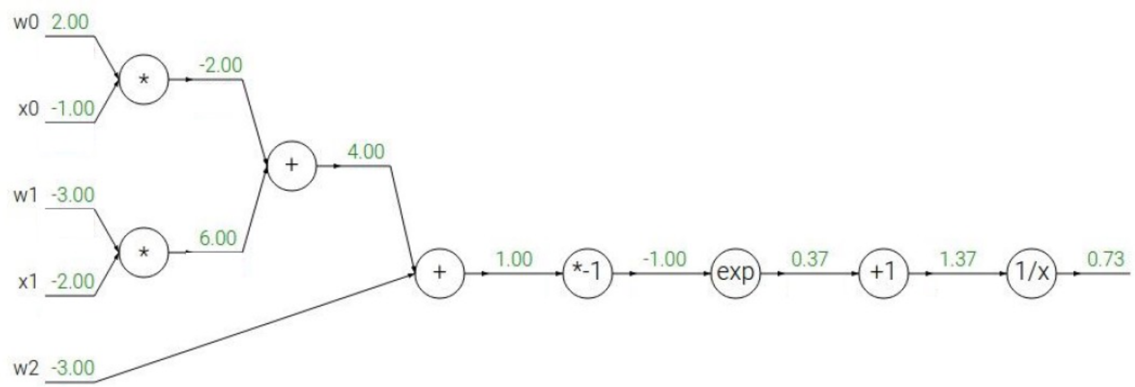
gradients

Chain rule

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



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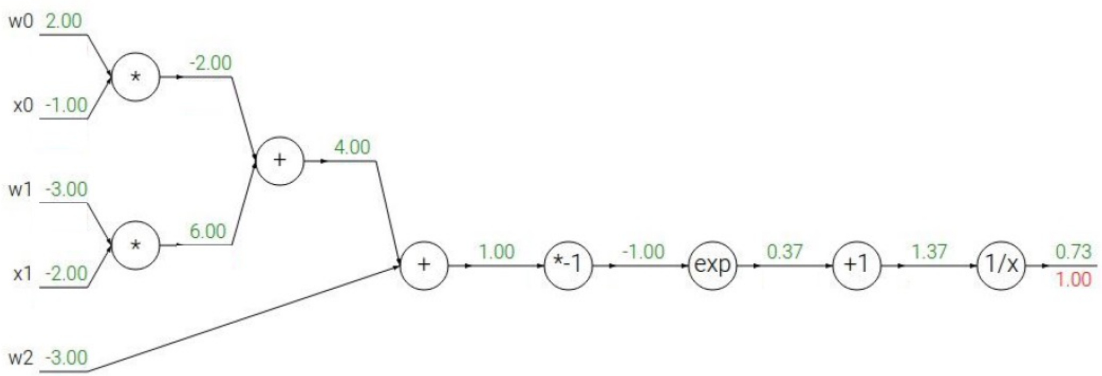

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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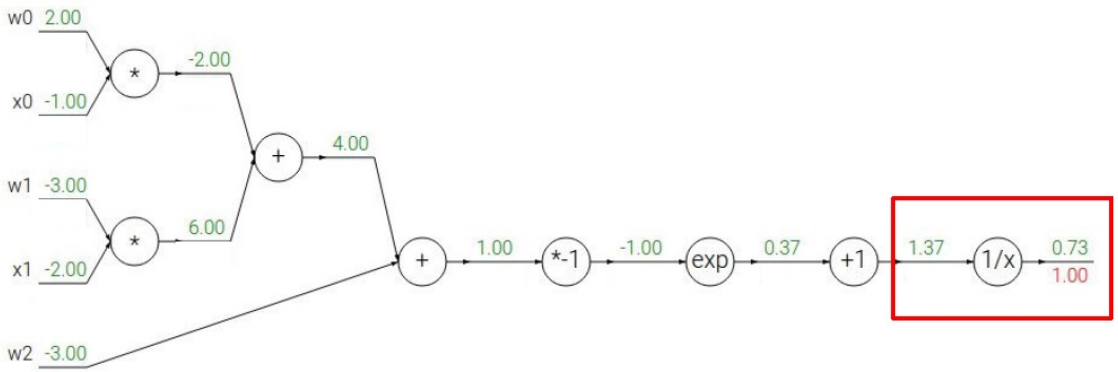

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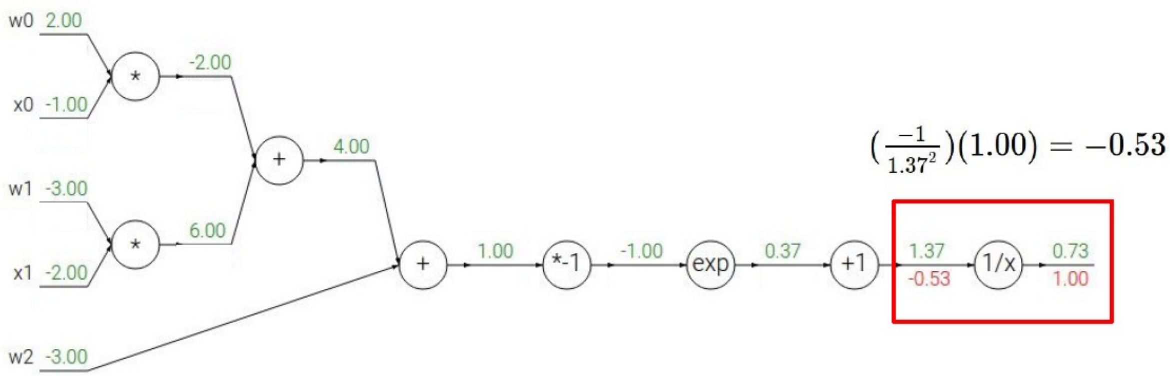

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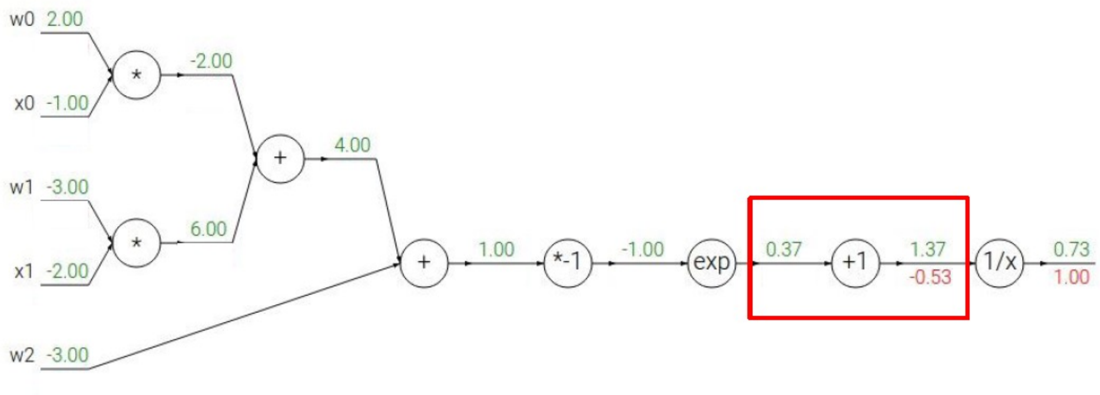

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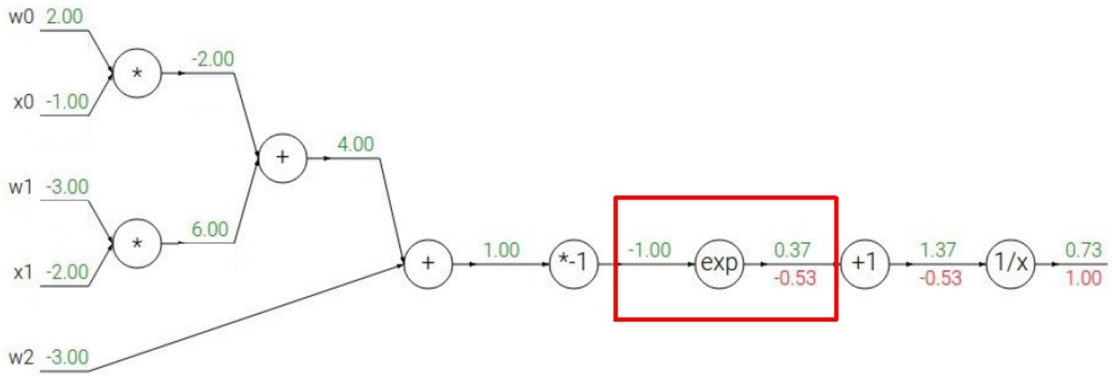

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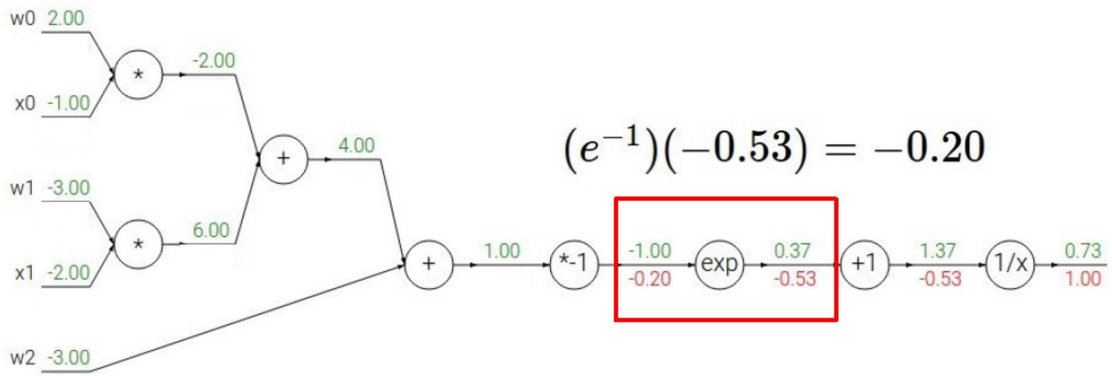

$$(e^{-1})(-0.53) = -0.20$$

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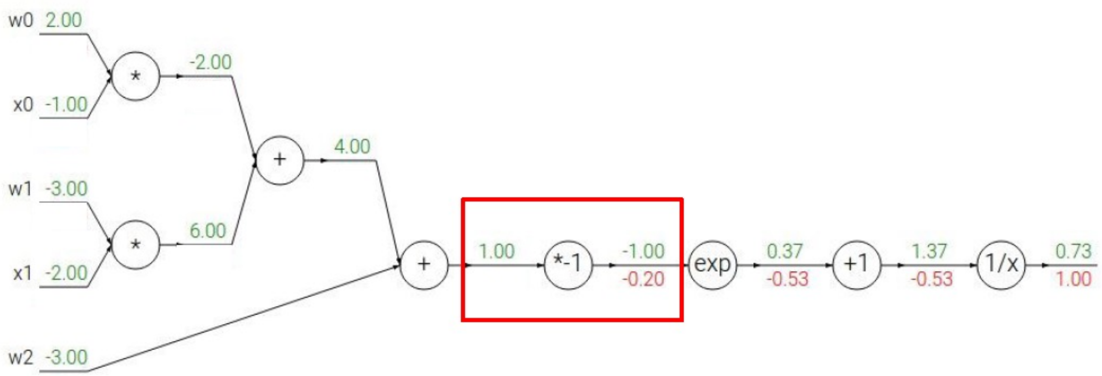

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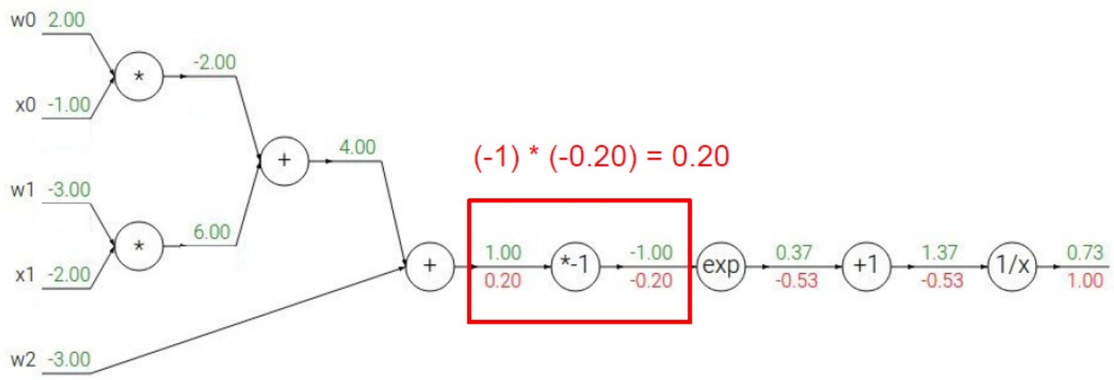

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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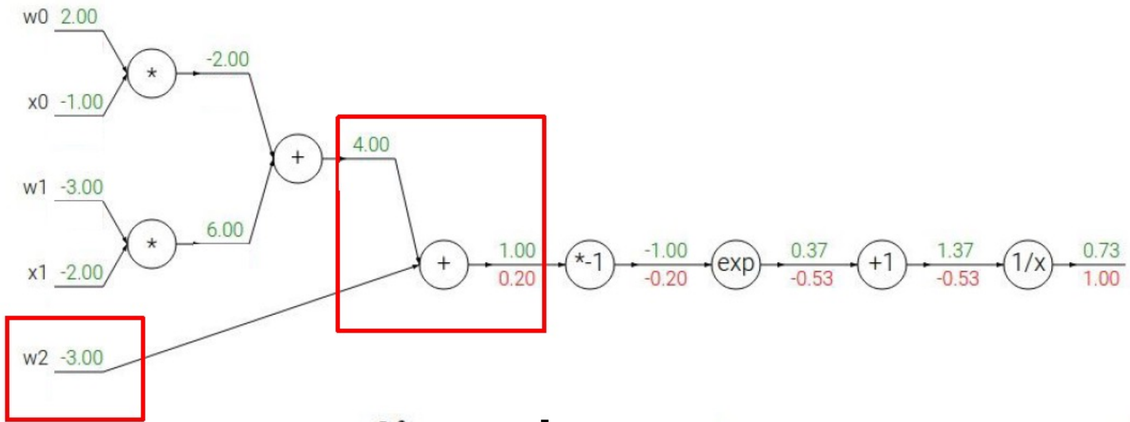

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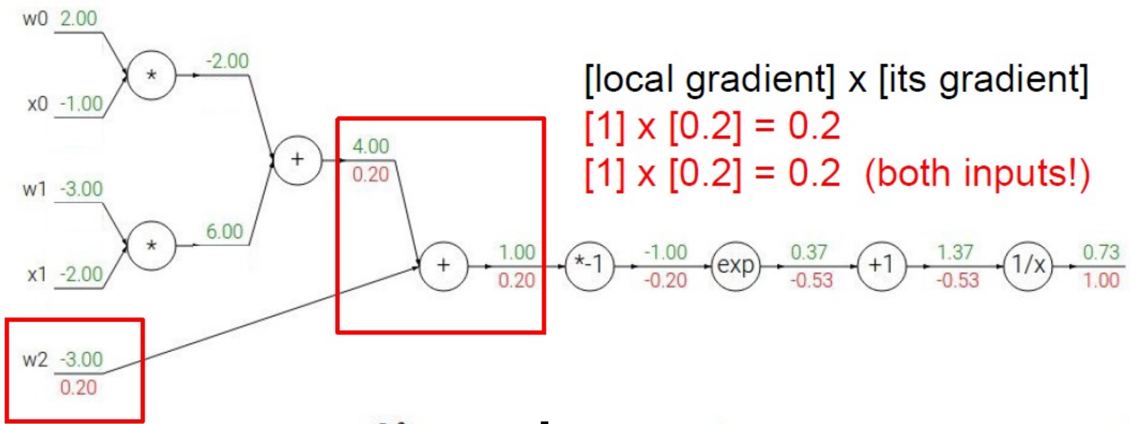

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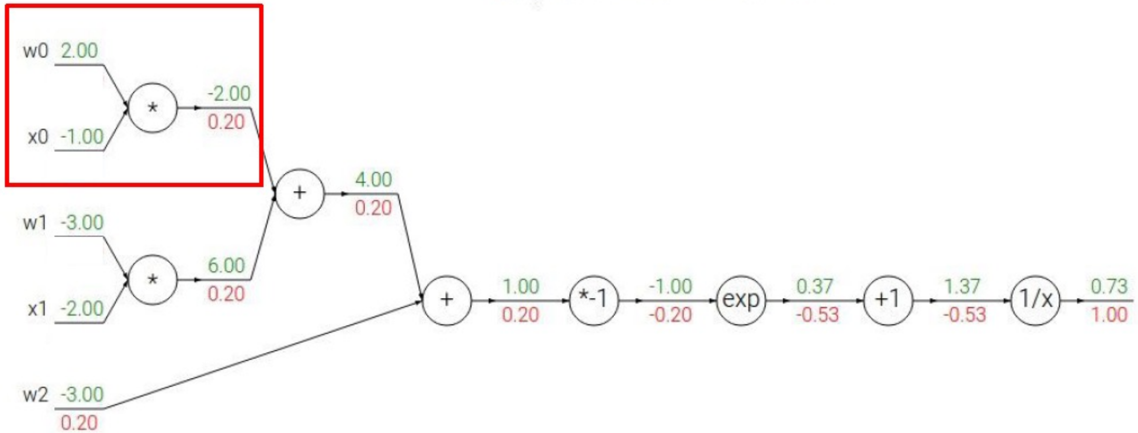

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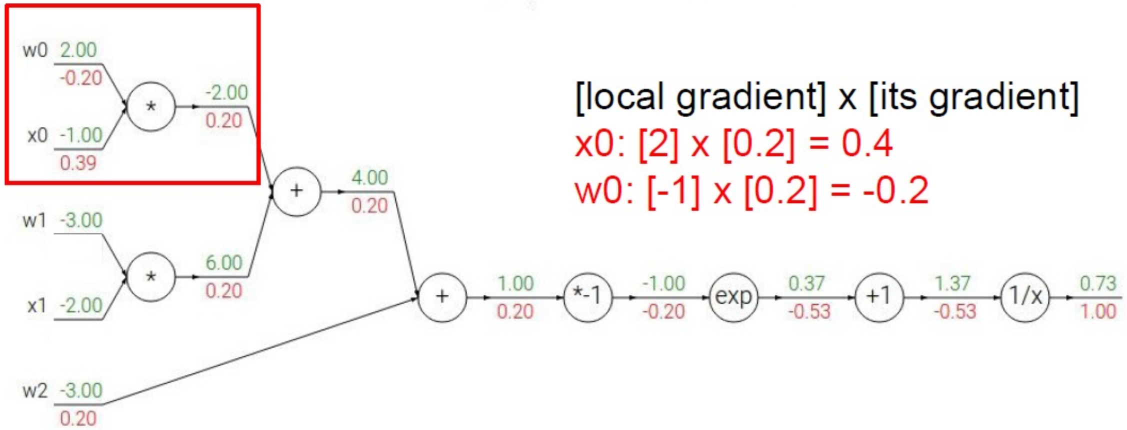

[local gradient] x [its gradient]
x0: [2] x [0.2] = 0.4
w0: [-1] x [0.2] = -0.2

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

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

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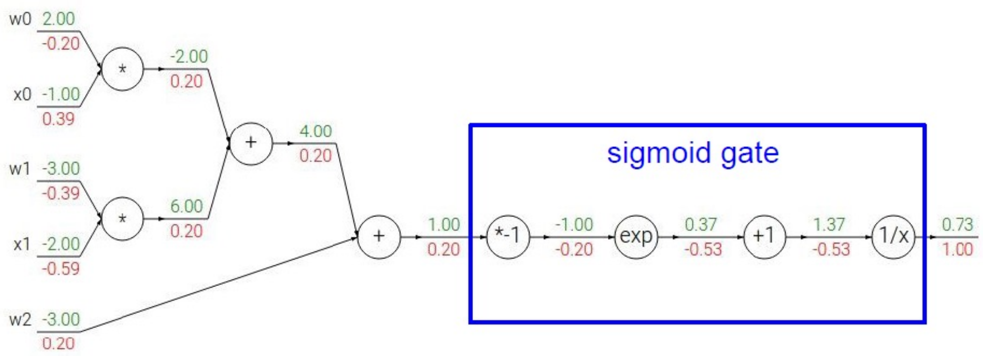
Sigmoid

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

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

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



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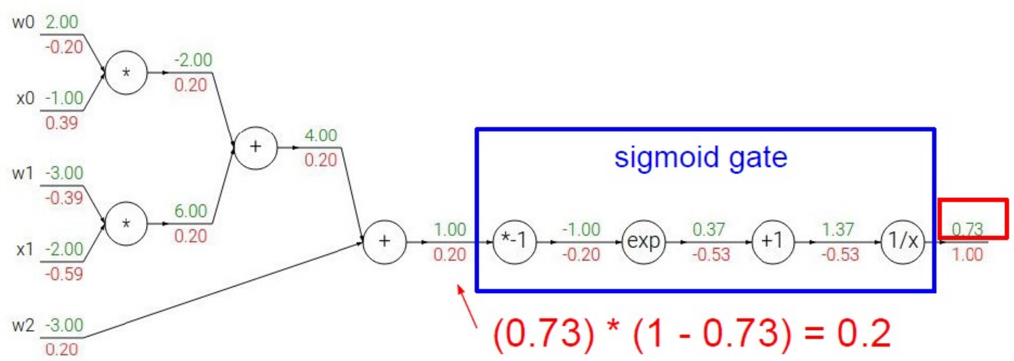


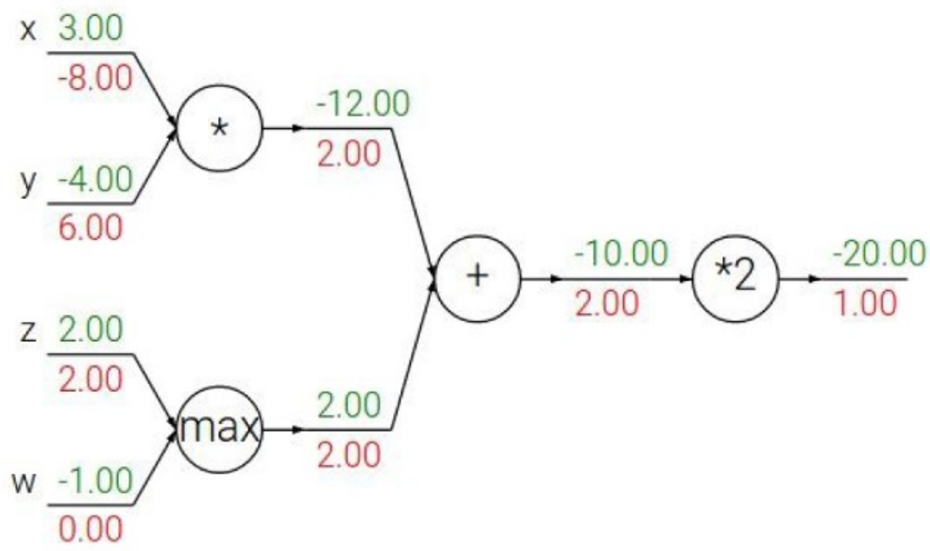
Pattern in backward flow

add gate: gradient distributor

max gate: gradient router

mul gate: gradient… “switcher”?

Patterns in backward flow



Exercise 1

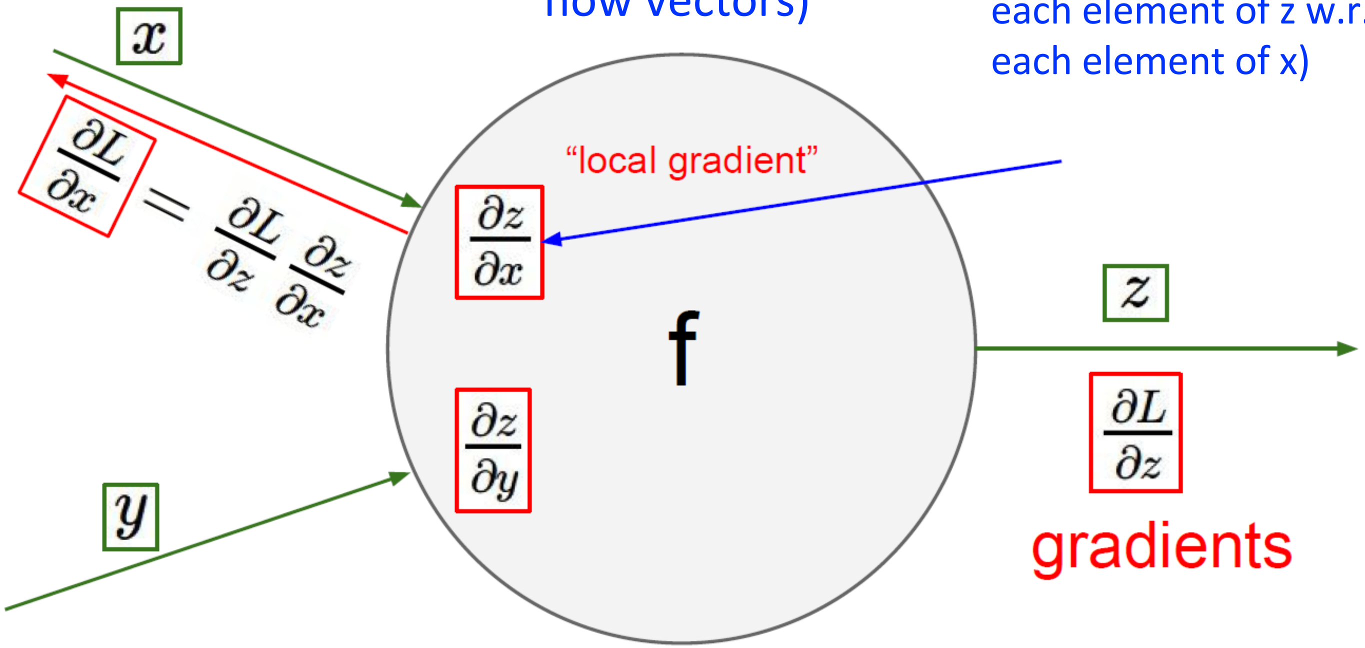
Pooling units take *n* values x_i, $\mathrm{i} \in [1, \mathrm{n}]$ and compute a scalar output whose value is invariant to permutations of the inputs.

1. The Lp-pooling module takes positive inputs and computes $\mathrm{y} = (\sum_i x_i^p)^{\frac{1}{p}}$, assuming we know that $y' = \frac{\partial L}{\partial y}$, what is $x_i' = \frac{\partial L}{\partial x_i}$?
2. The log-average module computes $\mathrm{y} = \frac{1}{\beta} \ln(\frac{1}{n} \sum_i \exp(\beta x_i))$, assuming we know that $y' = \frac{\partial L}{\partial y}$, what is $x_i' = \frac{\partial L}{\partial x_i}$?

Gradients for vector

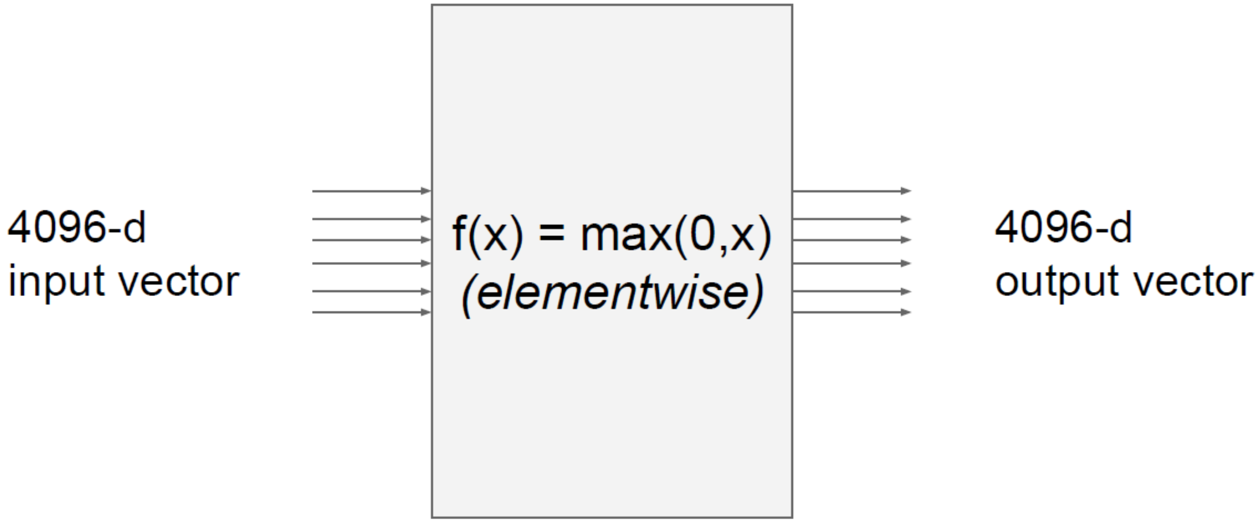
Gradients for vectorized code (x, y, z are now vectors)

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



Gradients for vector

Vectorized operation



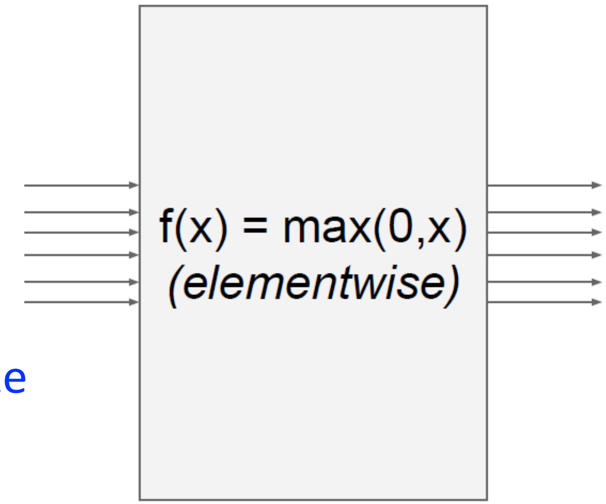
Gradients for vector

Vectorized operation

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

Jacobian matrix

4096-d
input vector



4096-d
output vector

Q: what is the size of the Jacobian matrix

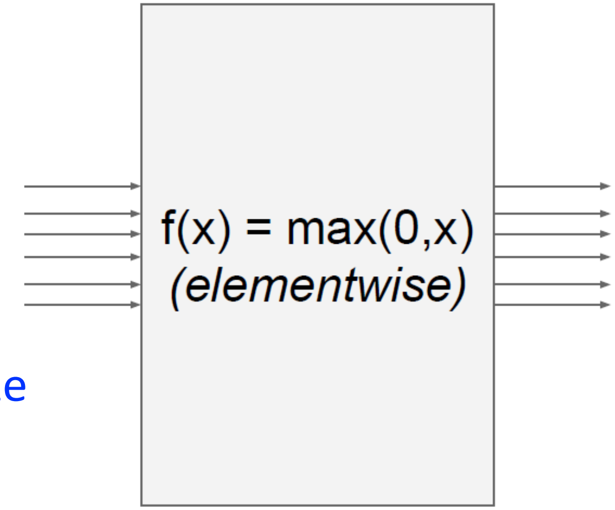
Gradients for vector

Vectorized operation

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

Jacobian matrix

4096-d
input vector



4096-d
output vector

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

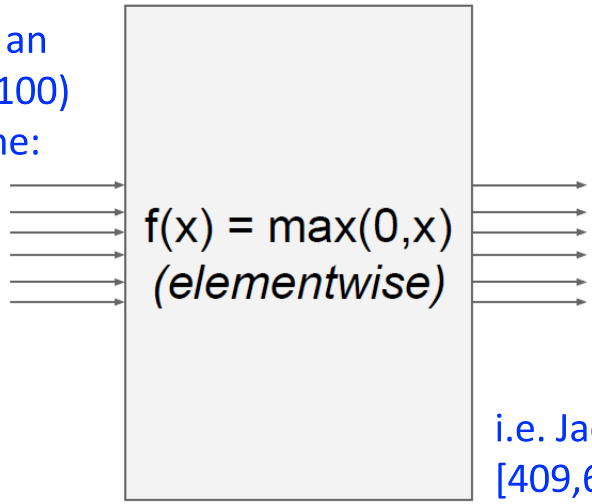
Q2: what does it look like?

Gradients for vector

Vectorized operation

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

100 4096-d input vectors



100 4096-d output vectors

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

Gradients for vector

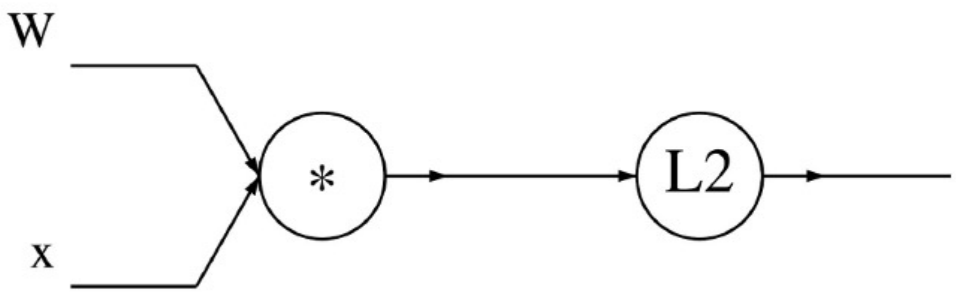
A vectorized example: $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$

Gradients for vector

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

Gradients for vector

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

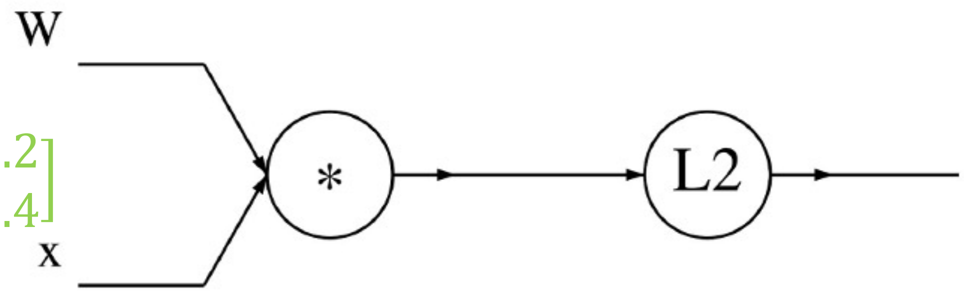


Gradients for vector

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

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

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



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

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

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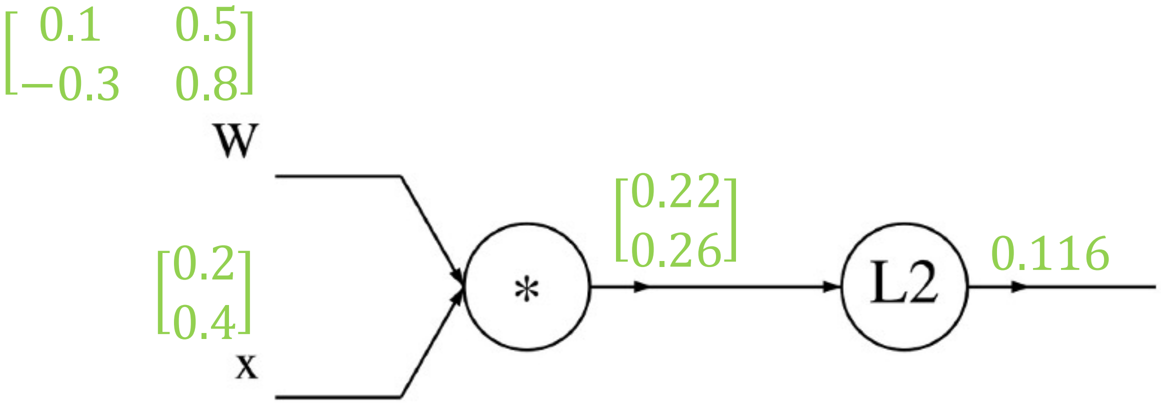

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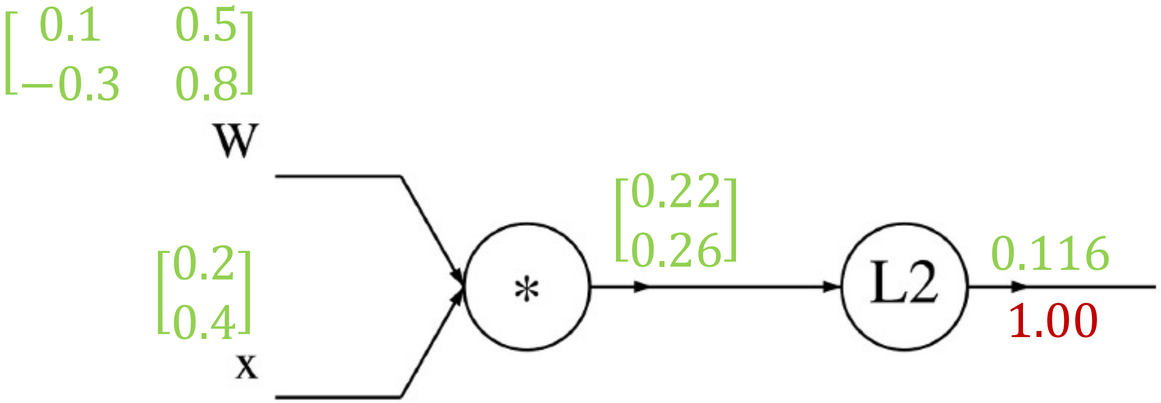

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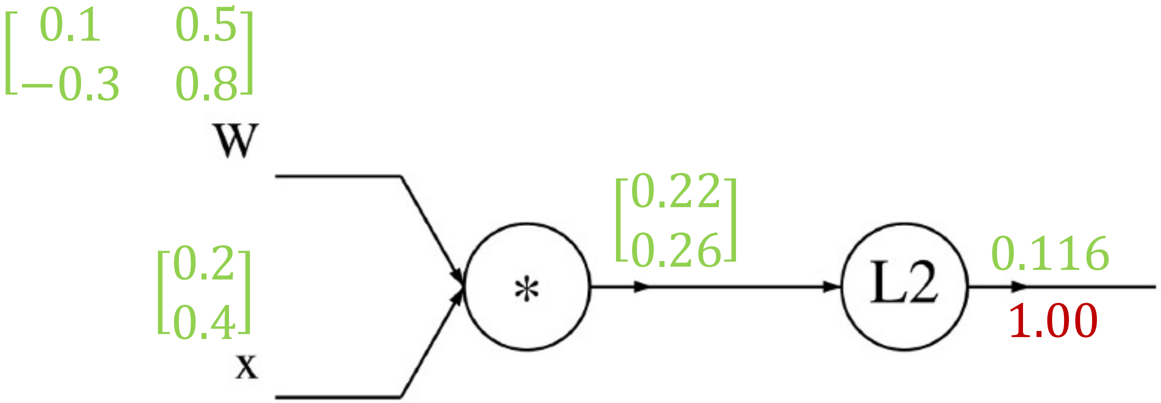

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$$\frac{\partial f}{\partial q_i} = 2q_i$$

$$\boxed{\nabla_q f = 2q}$$

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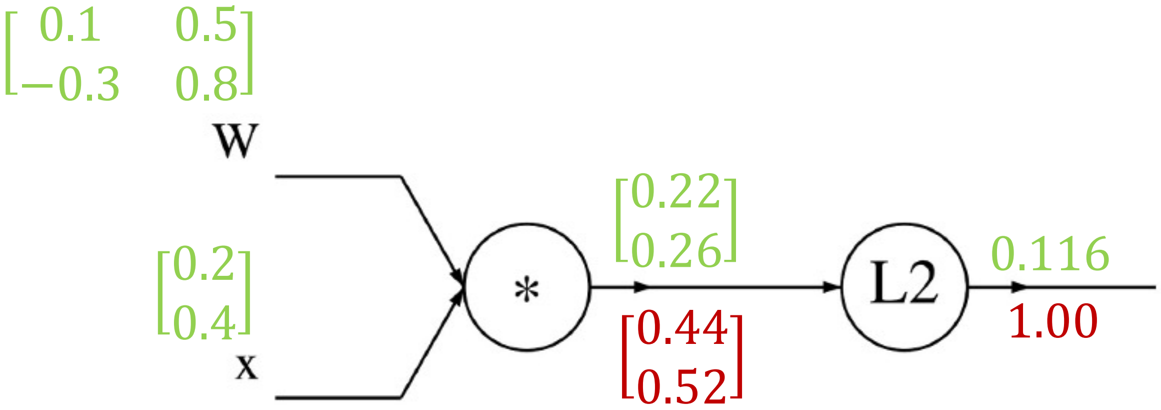

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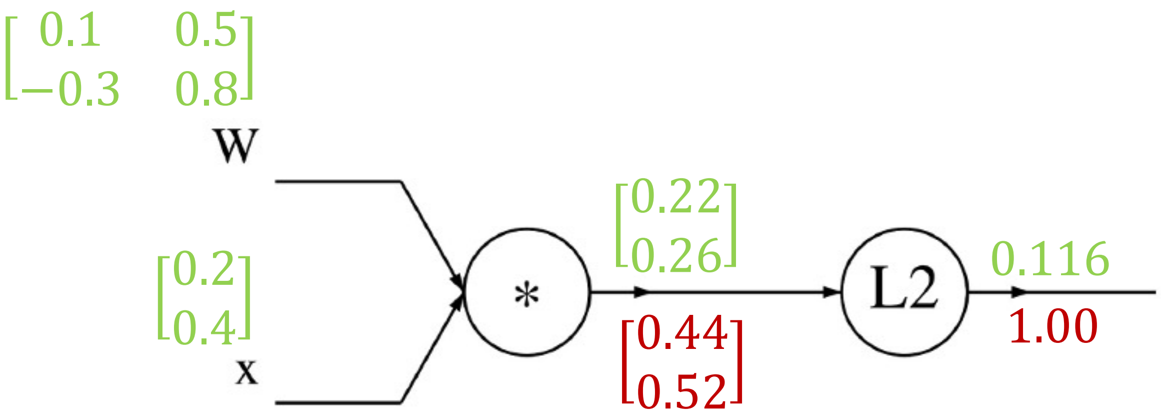

$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

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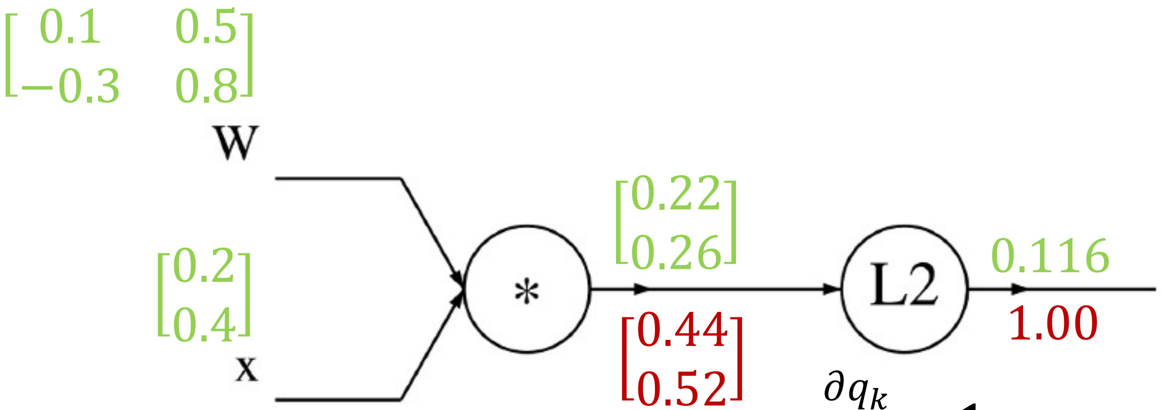

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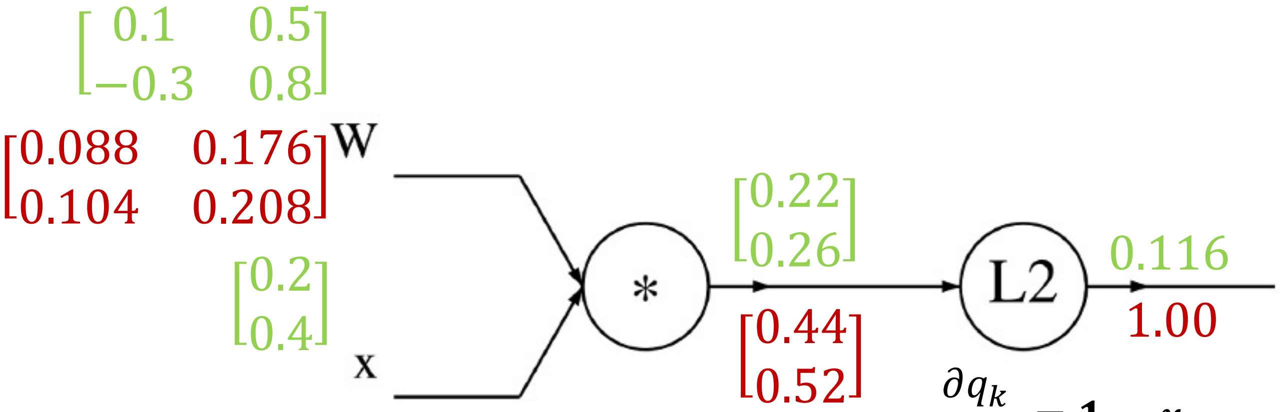

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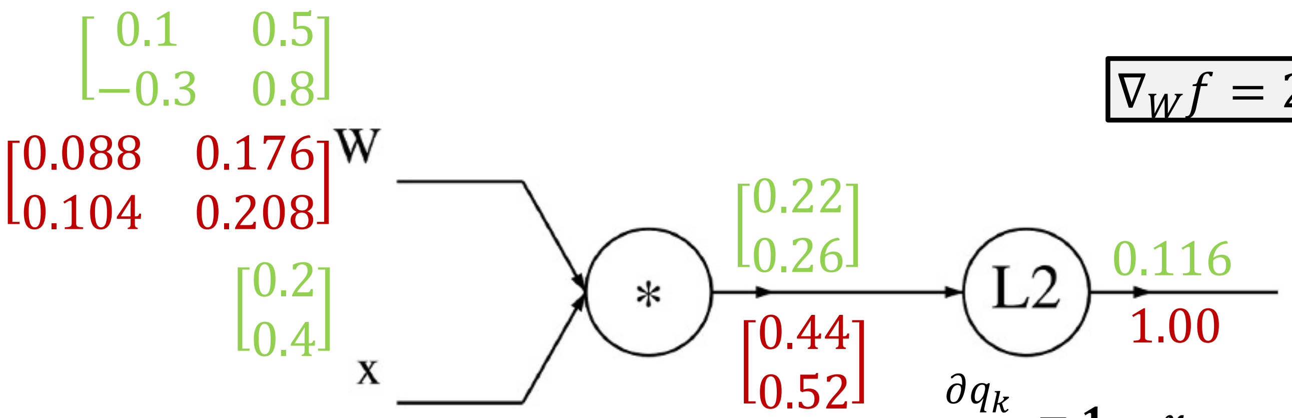

$$\boxed{\nabla_W f = 2q \cdot x^\top}$$

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Gradients for vector

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

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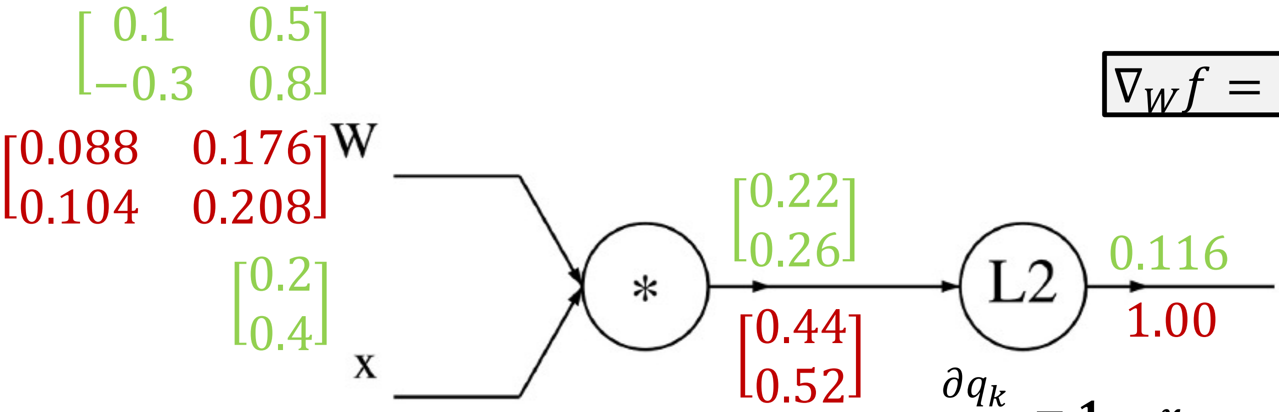

Always check: The gradient with respect to a variable should have the same shape as the variable

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

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

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Gradients for vector

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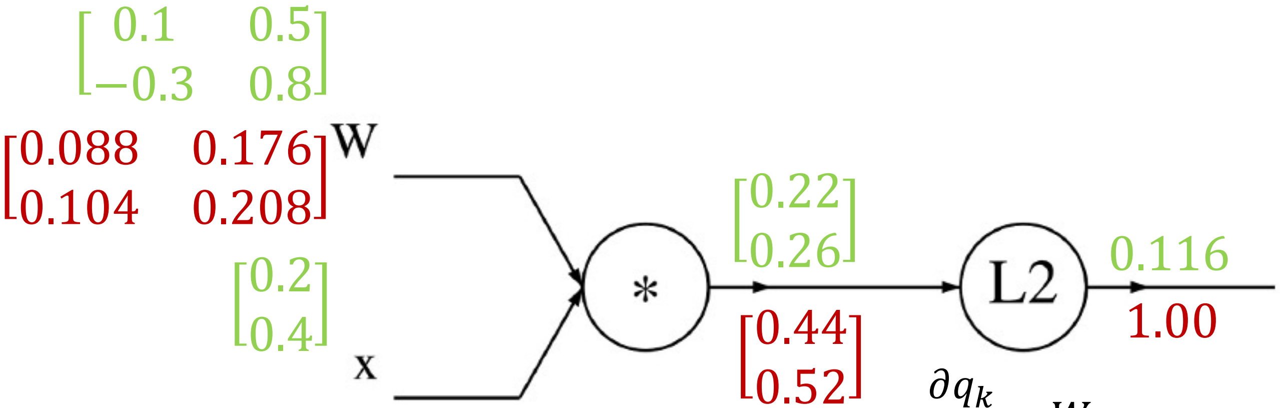

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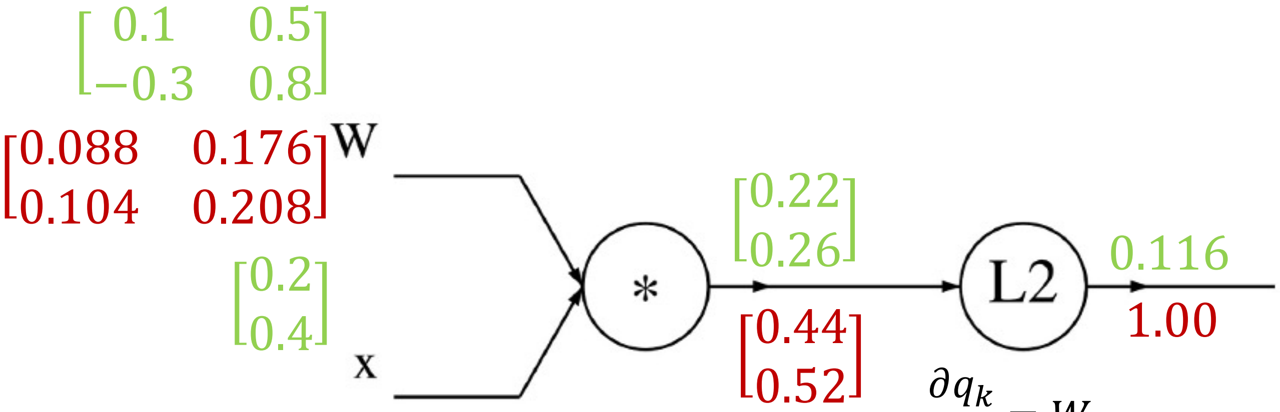

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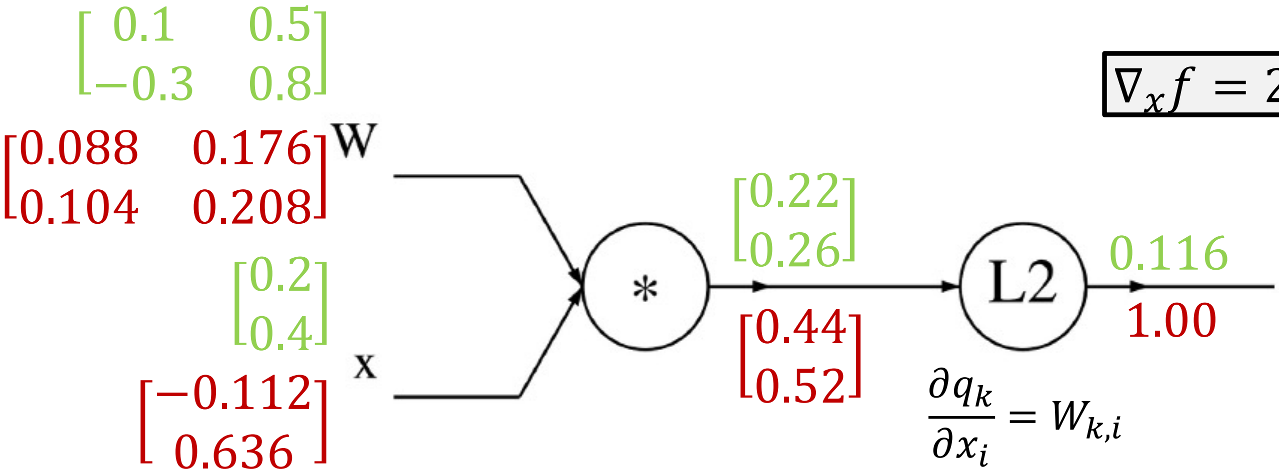
Gradients for vector

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

$$\boxed{\nabla_x f = 2W^\top \cdot q}$$



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