# COMP/EECE 7/8740 Neural Networks

Topics:

- Computational Graph
- How to compute the gradients during back-prop.?
- Notation + example

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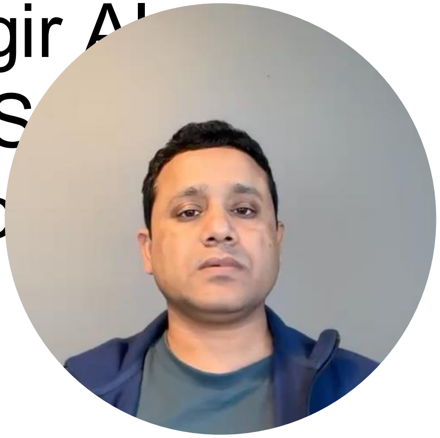
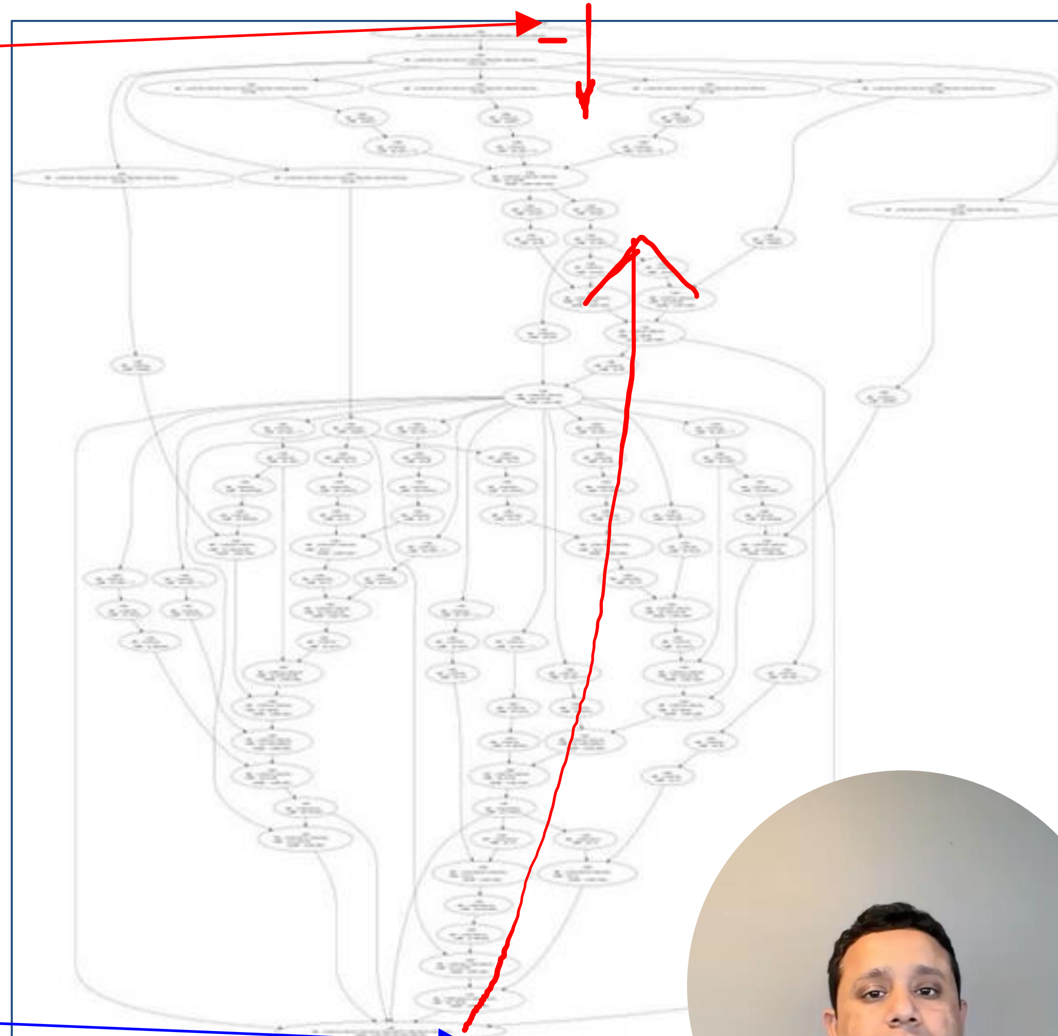


# Neural Turing Machine (NTM)

inputs

A hybrid AI architecture that combines **a neural network (controller)** with external, addressable memory resources. Proposed by Google DeepMind in 2014.

- NTM allows neural networks to **store, read, and write data**, improving memory capabilities for tasks like **sorting, copying, and associative recall**.



loss

Loss

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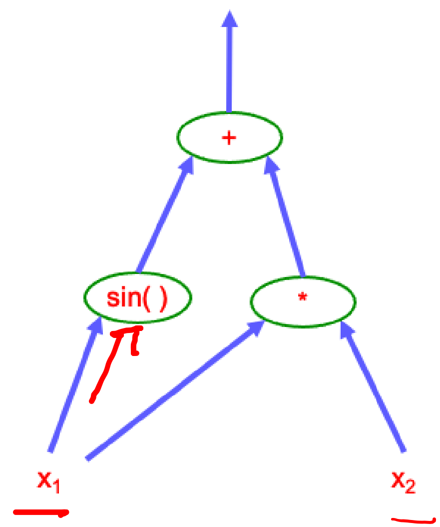
Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

# Computational Graphs

- **A computational graph** is a way to represent a math function in the language of graph theory. Recall the premise of **graph** theory:
  - Nodes are connected by edges, and
  - Everything in the **graph** is either a node or an edge.

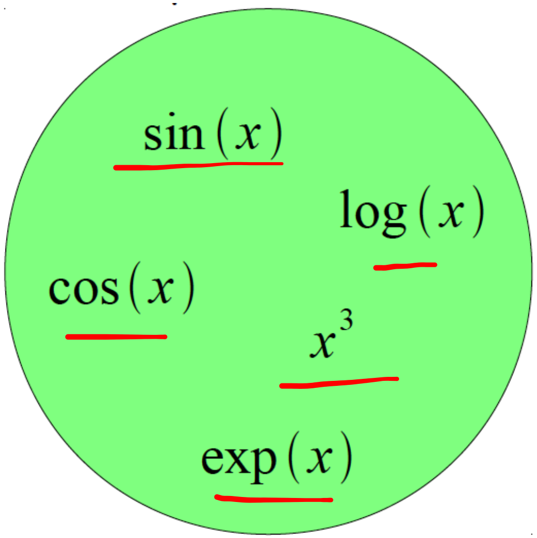
**Example**

$$f(x_1, x_2) = x_1 x_2 + \sin(x_1)$$



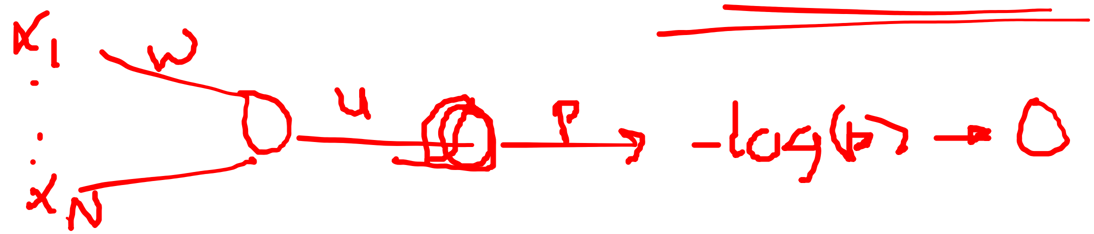

# Logistic Regression as a Cascade

Given a library of simple functions



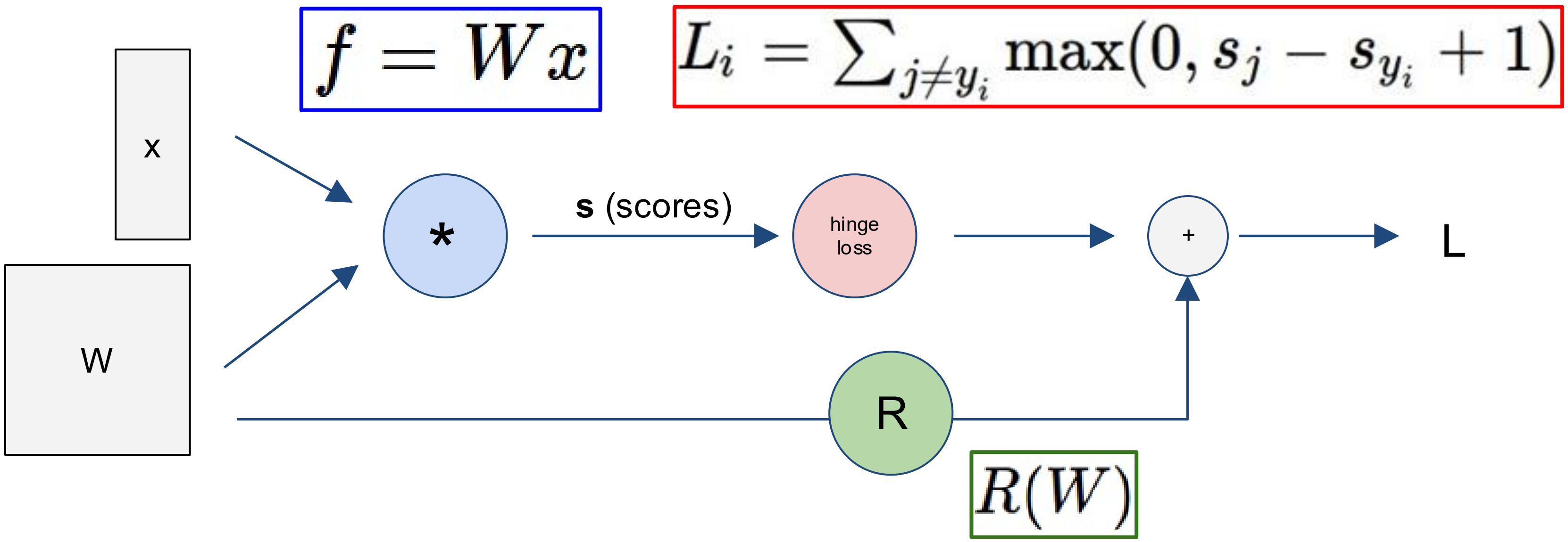

Compose into a complicate function

$$-\log\left(\frac{1}{1+e^{-\mathbf{w}^{\mathsf{T}}\mathbf{x}}}\right)$$




$$\boxed{\mathbf{w}^{\mathsf{T}}\mathbf{x}} \xrightarrow{u} \boxed{\frac{1}{1+e^{-u}}} \xrightarrow{p} \boxed{-\log(p)}$$

# Computational Graph and NNs



# Backpropagation: a simple example

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

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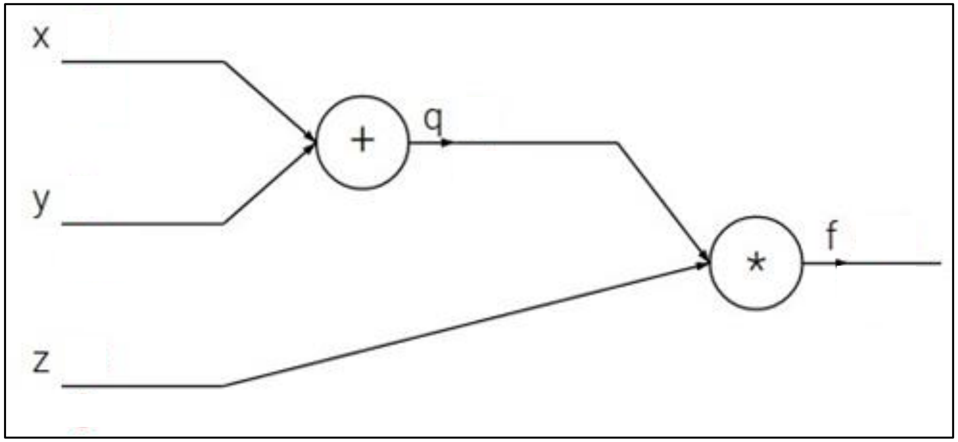

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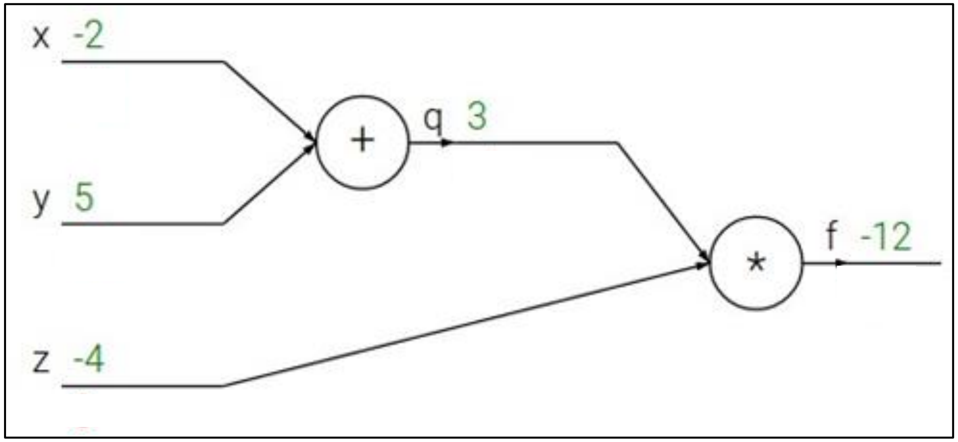
e.g. x = -2, y = 5, z = -4



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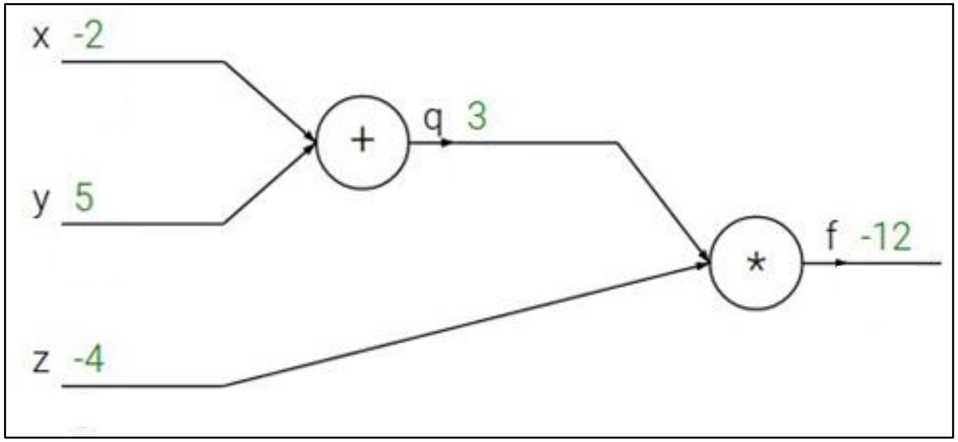


Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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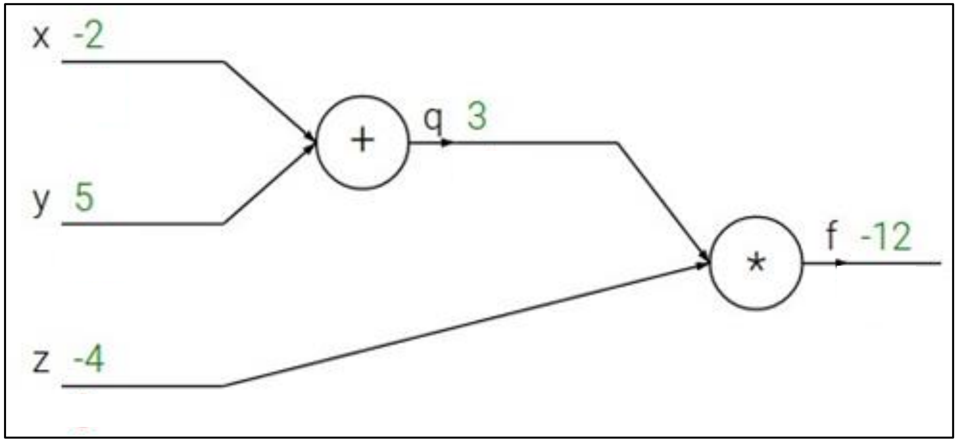


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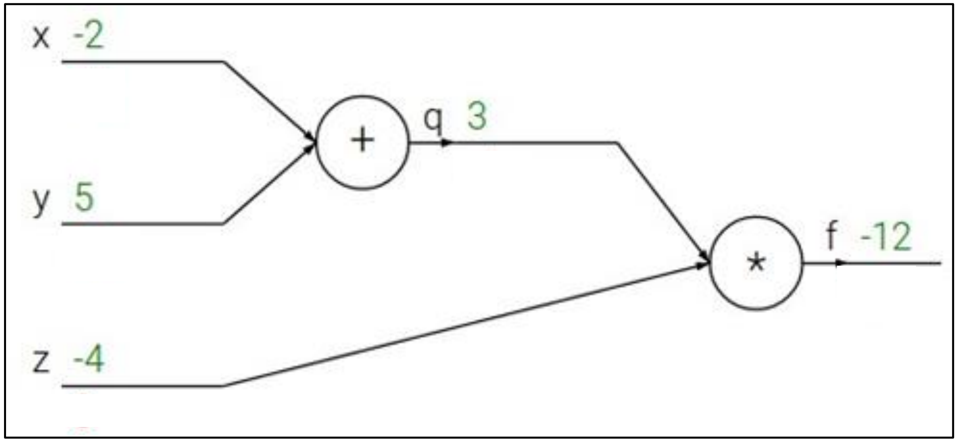

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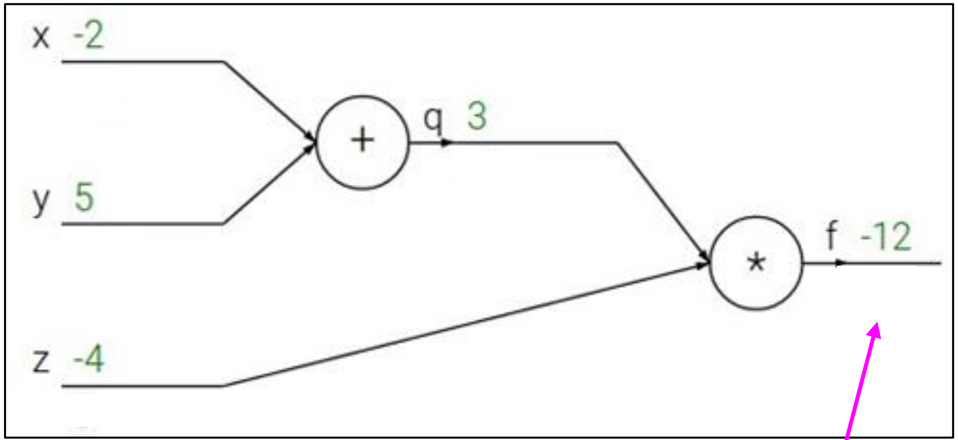


$$\frac{\partial f}{\partial f}$$

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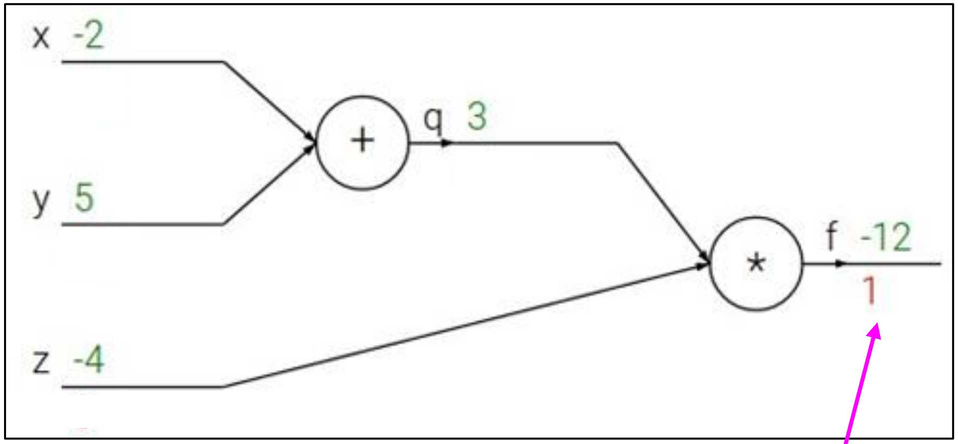


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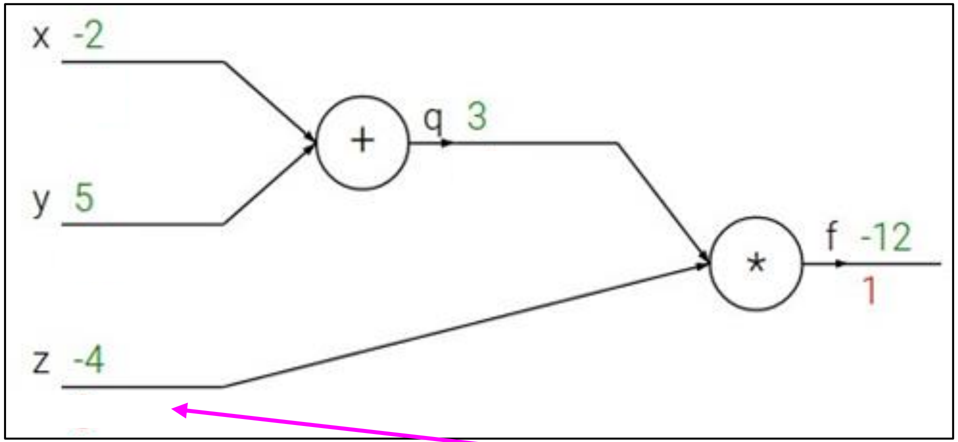


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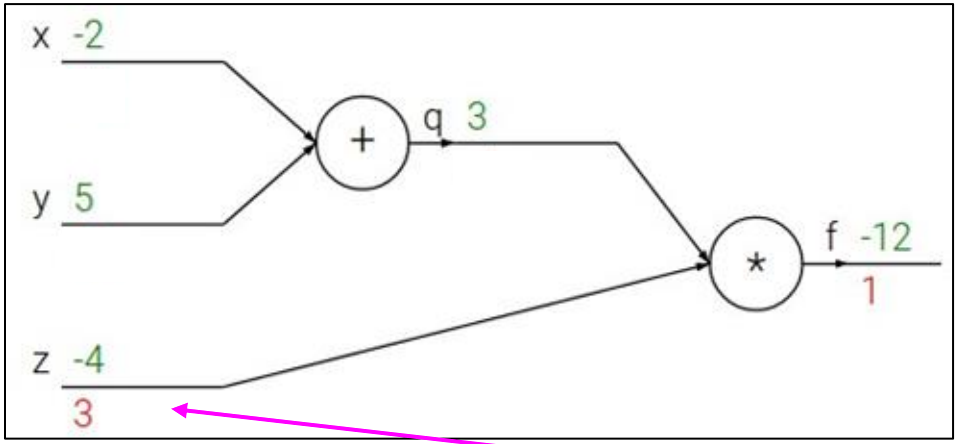


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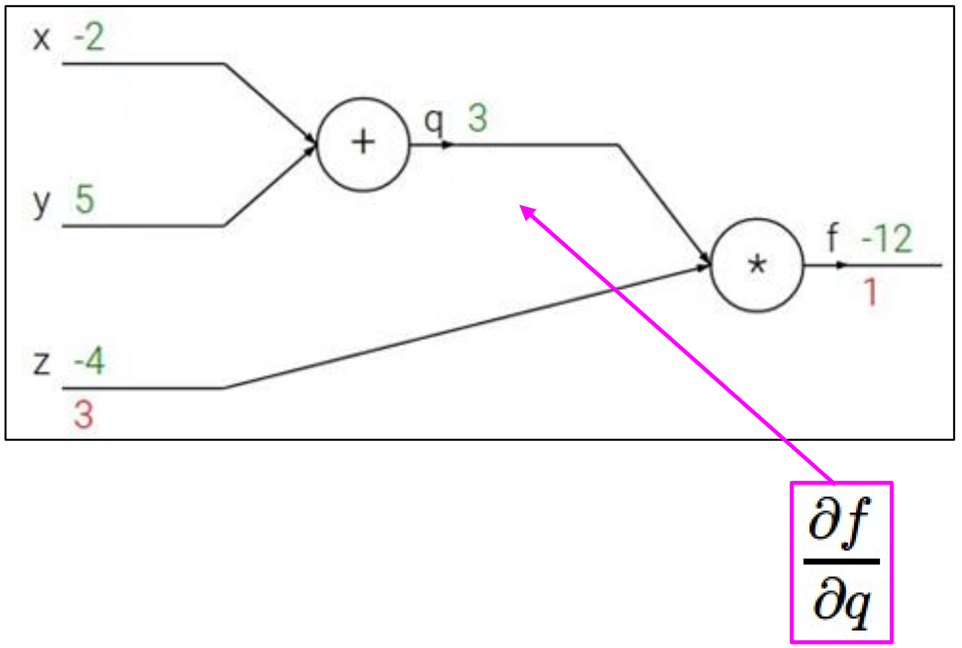

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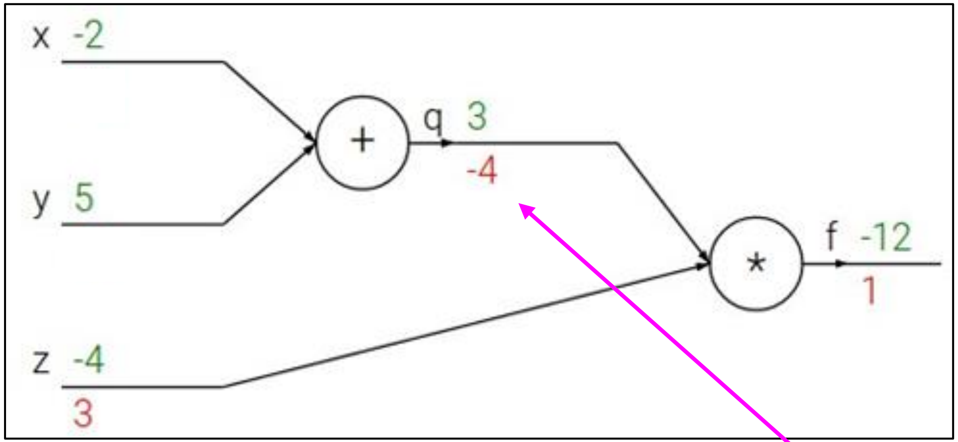


$$\boxed{\frac{\partial f}{\partial q}}$$

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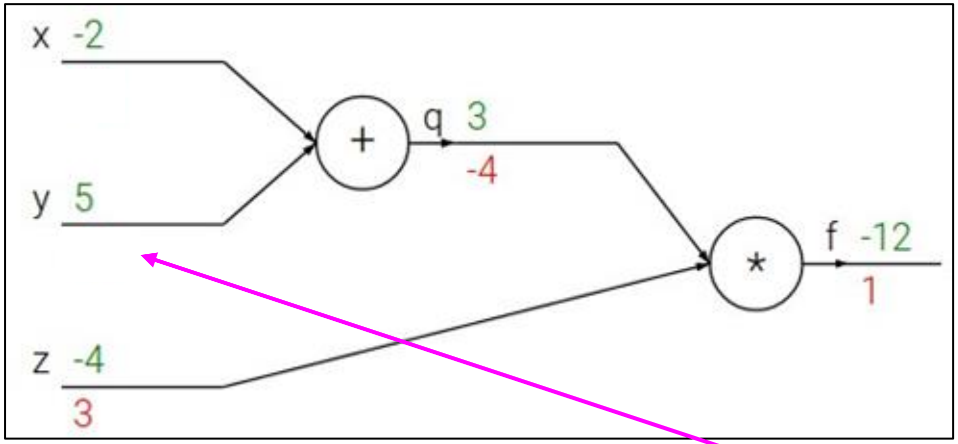



$$\frac{\partial f}{\partial y}$$

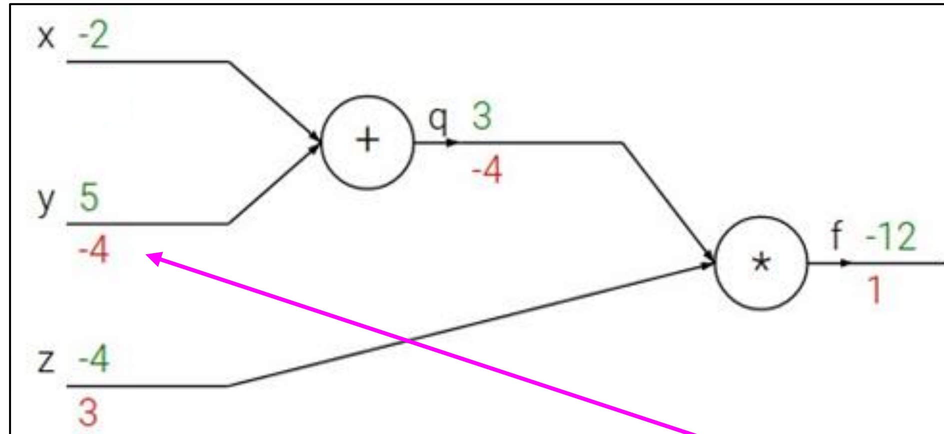
Chain rule:

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

Upstream gradient

Local gradient

# Backpropagation: a simple example

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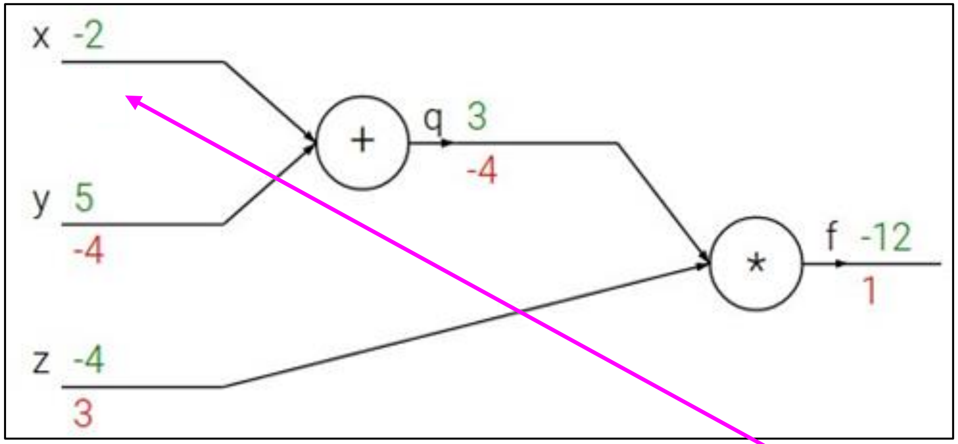


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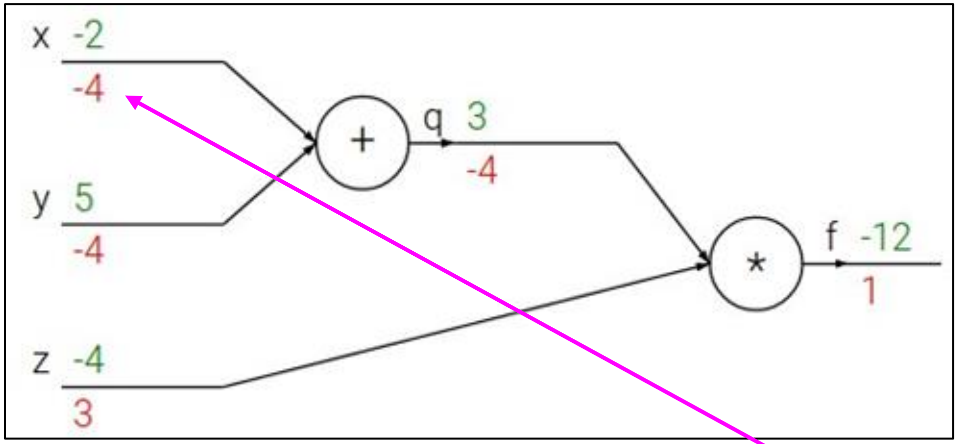


$$\frac{\partial f}{\partial x}$$

Chain rule:

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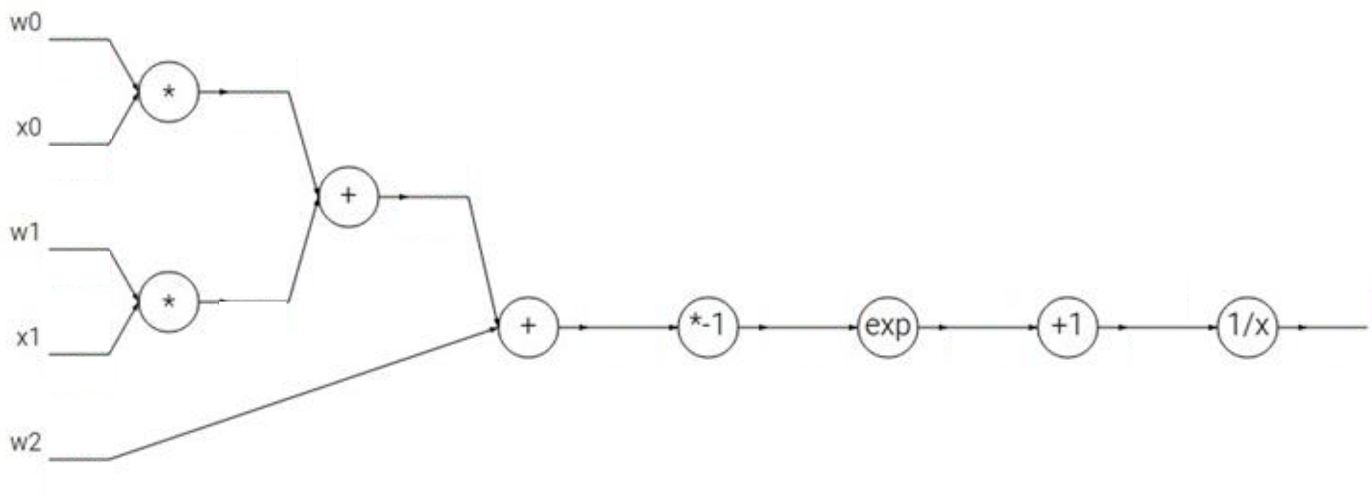
Upstream gradient

Local gradient

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



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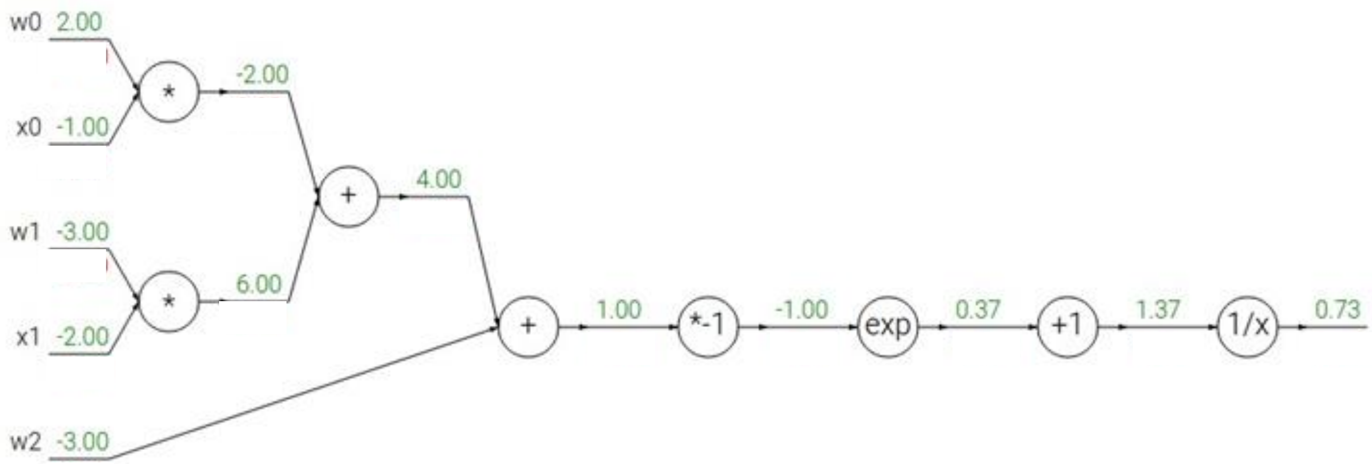

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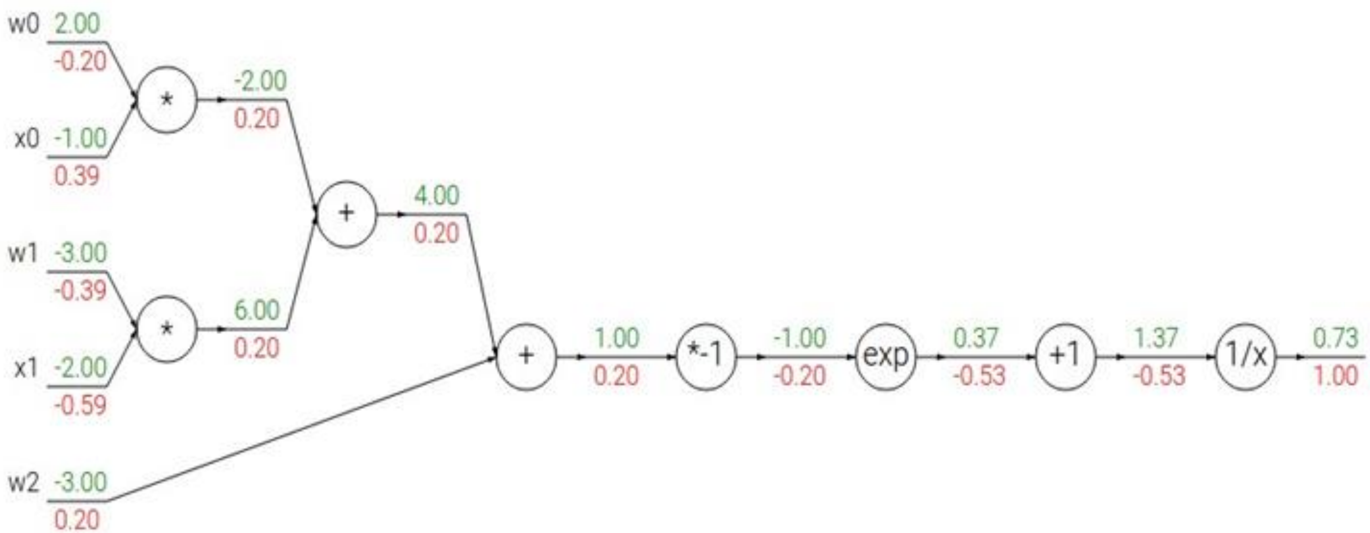


| | | | | | |
|---|---|---|---|---|---|
| $f(x) = e^x$ | $\rightarrow$ | $\frac{df}{dx} = e^x$ | $f(x) = \frac{1}{x}$ | $\rightarrow$ | $\frac{df}{dx} = -1/x^2$ |
| $f_a(x) = ax$ | $\rightarrow$ | $\frac{df}{dx} = a$ | $f_c(x) = c + x$ | $\rightarrow$ | $\frac{df}{dx} = 1$ |

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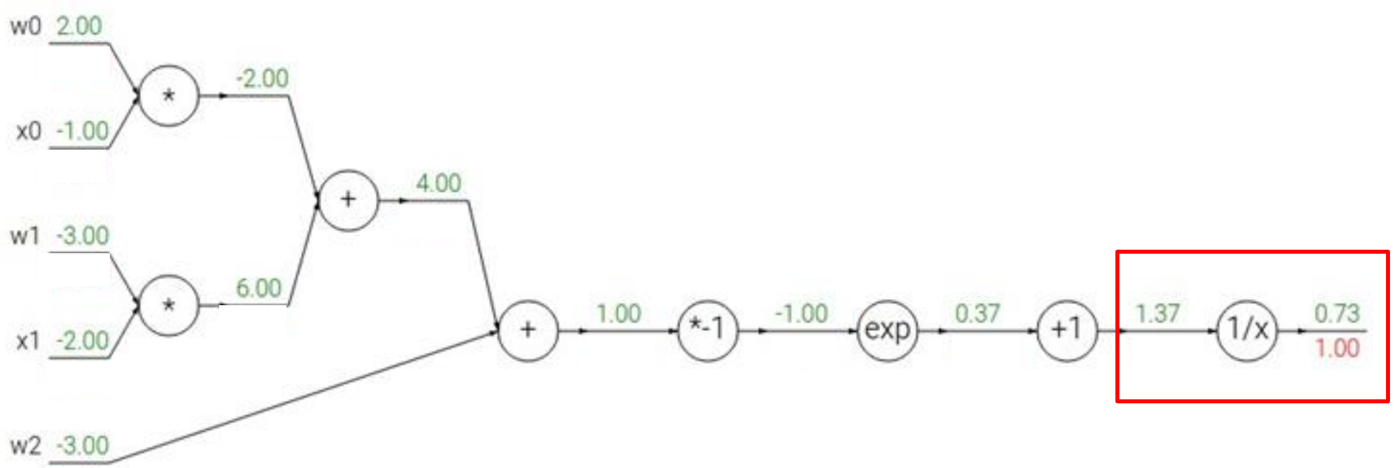


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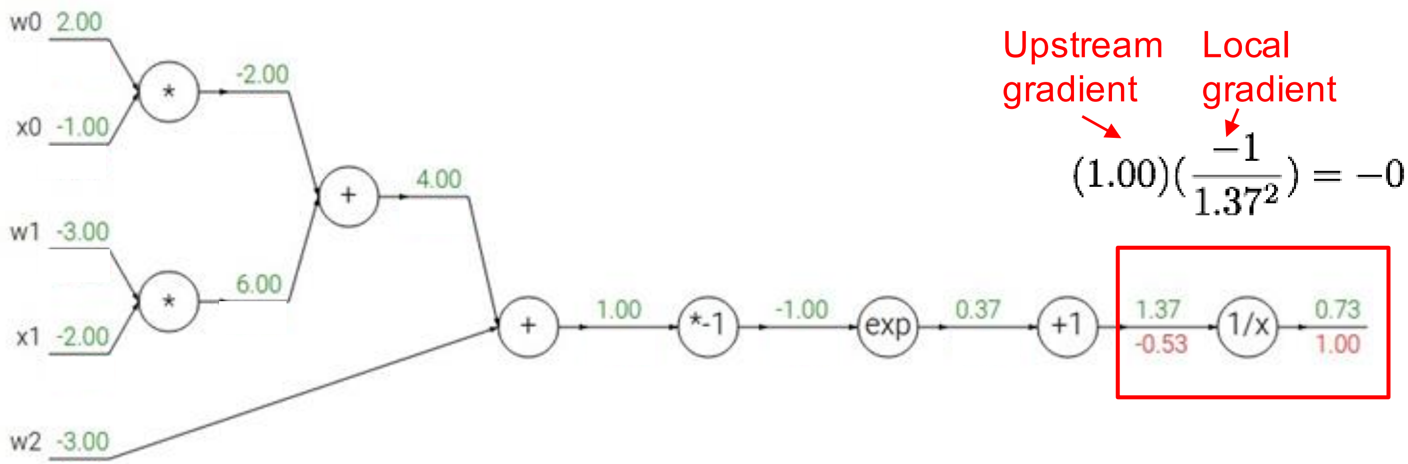


$$(1.00)\left(\frac{-1}{1.37^2}\right) = -0.53$$

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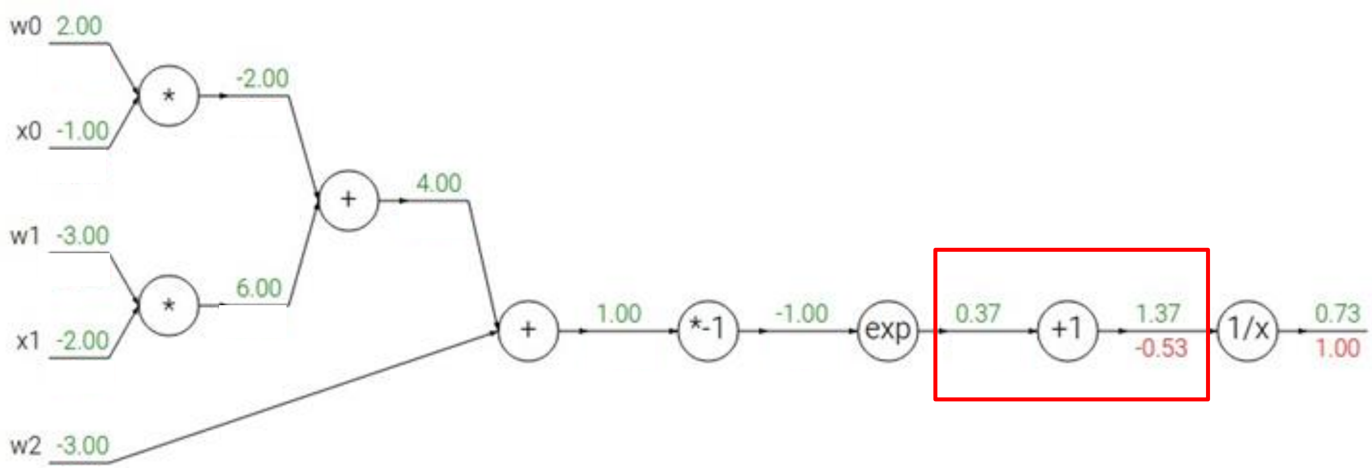


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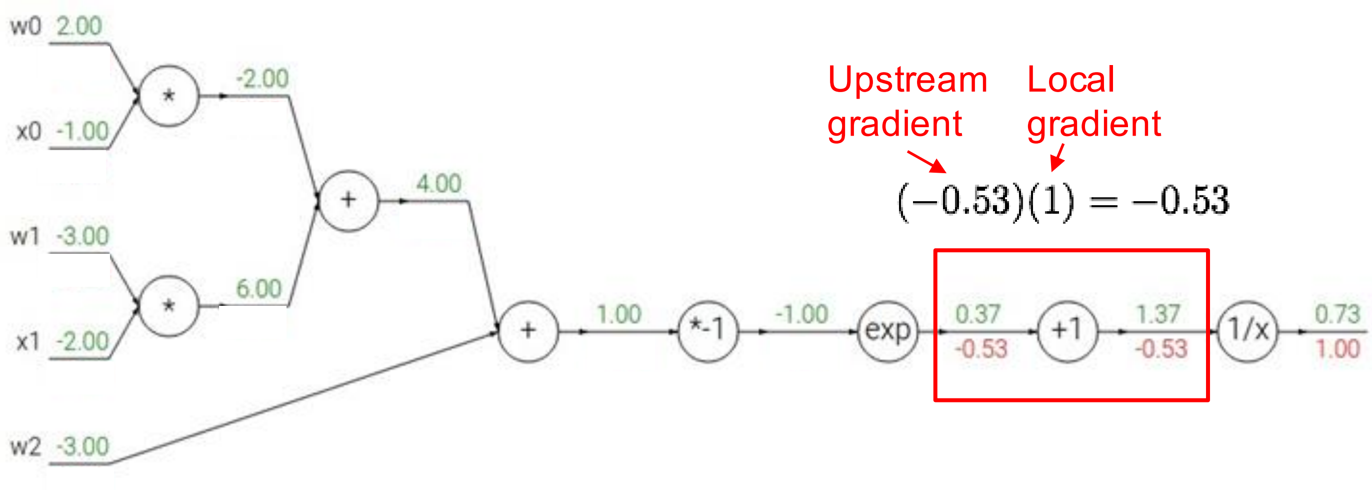


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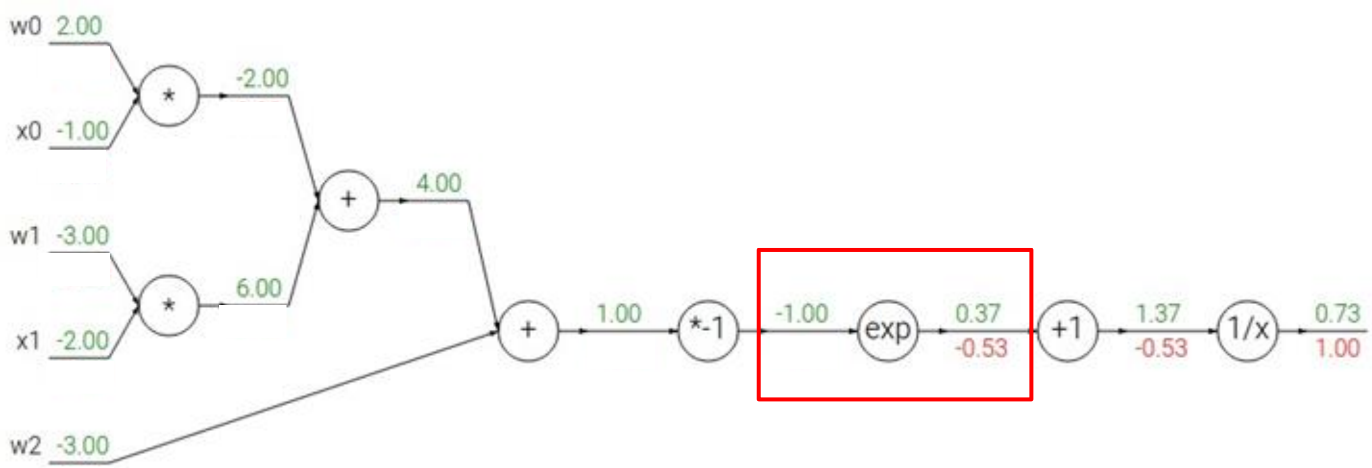


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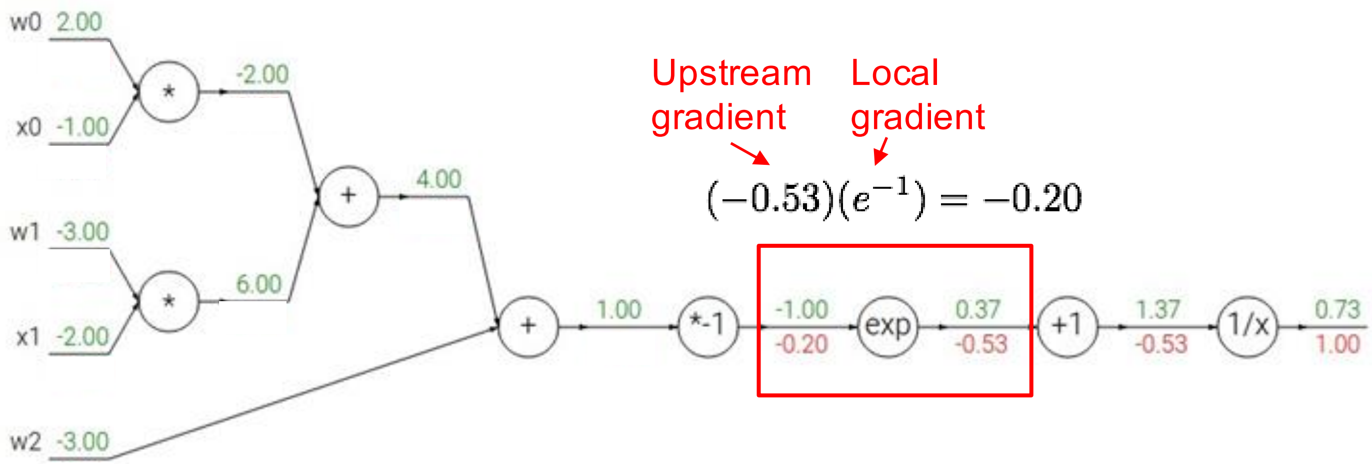


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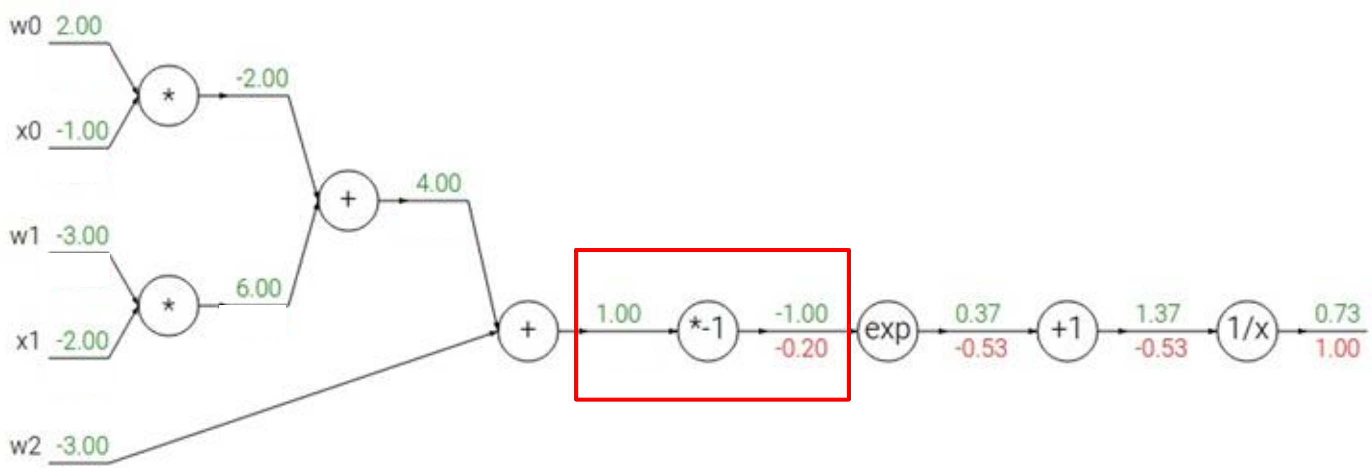


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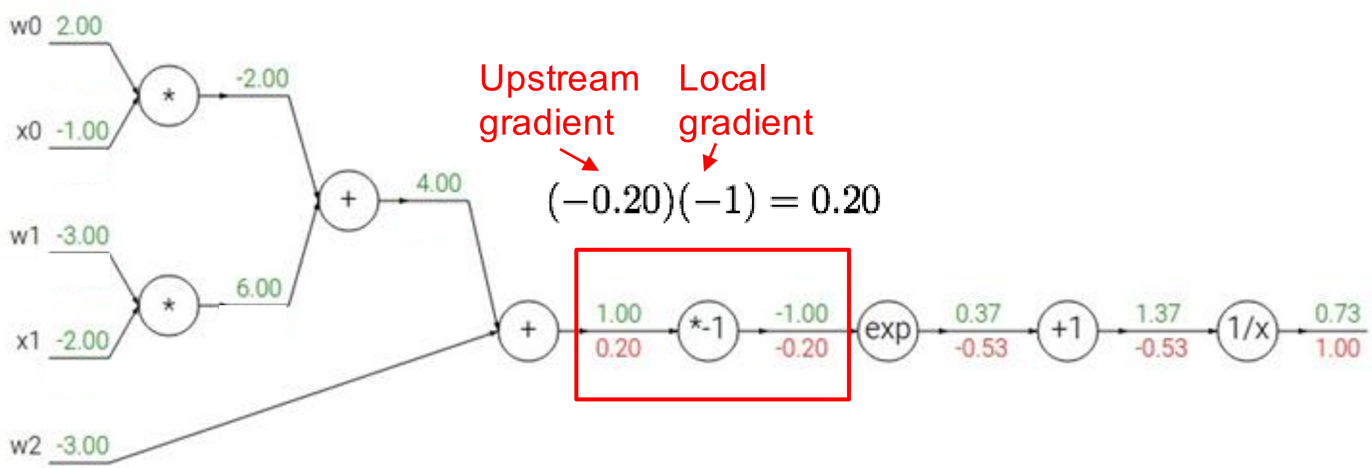


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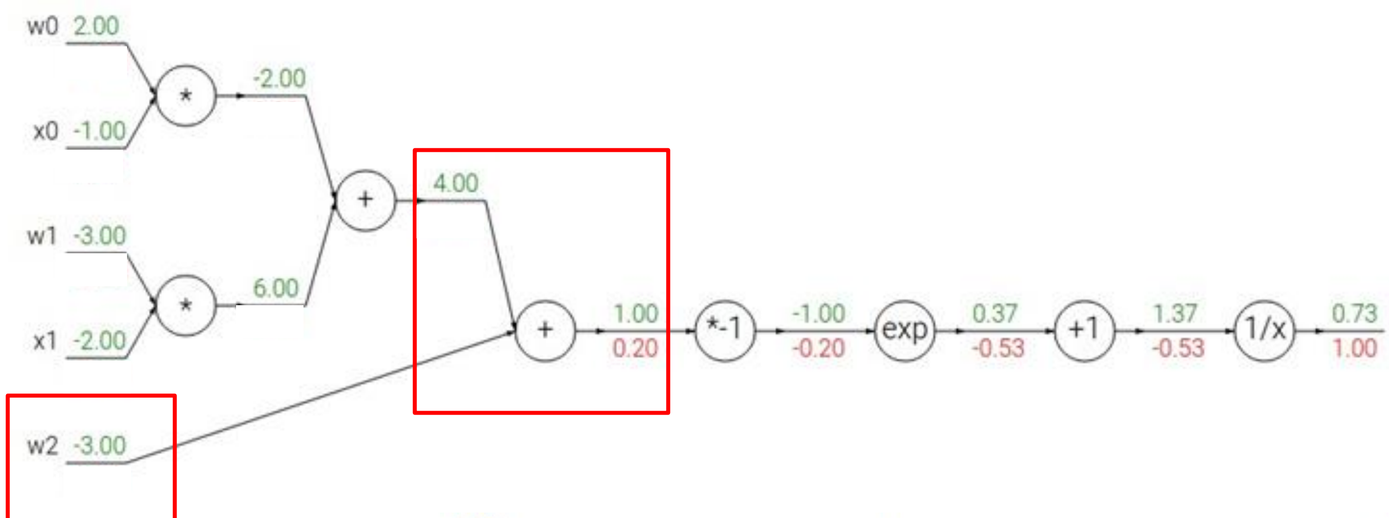


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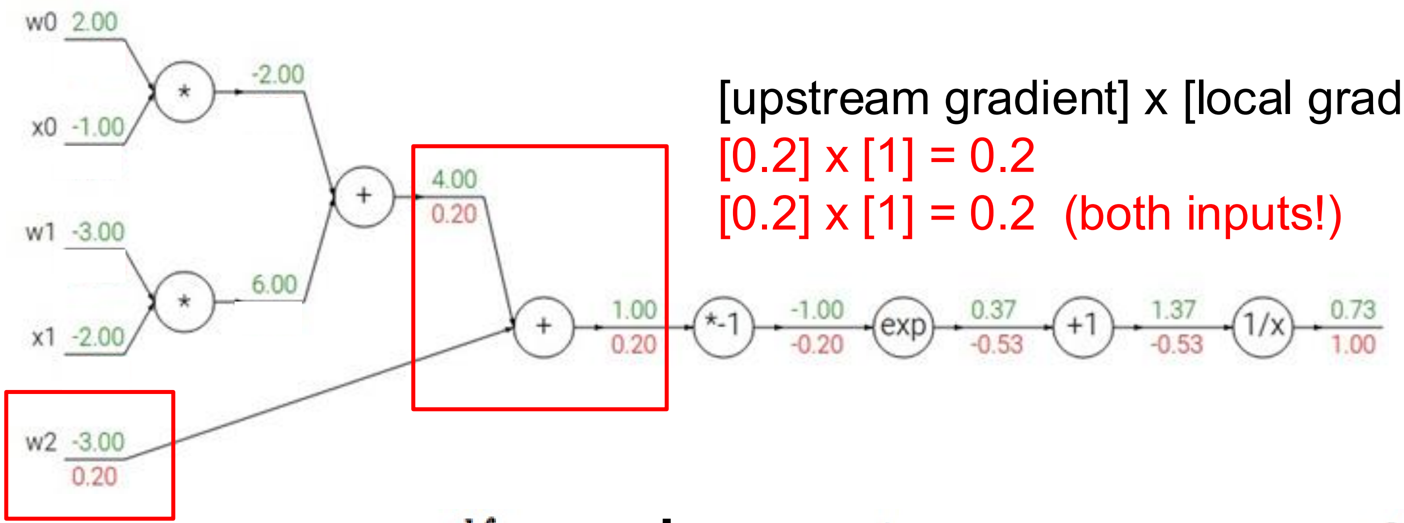


[upstream gradient] x [local gradient]

[0.2] x [1] = 0.2

[0.2] x [1] = 0.2 (both inputs!)

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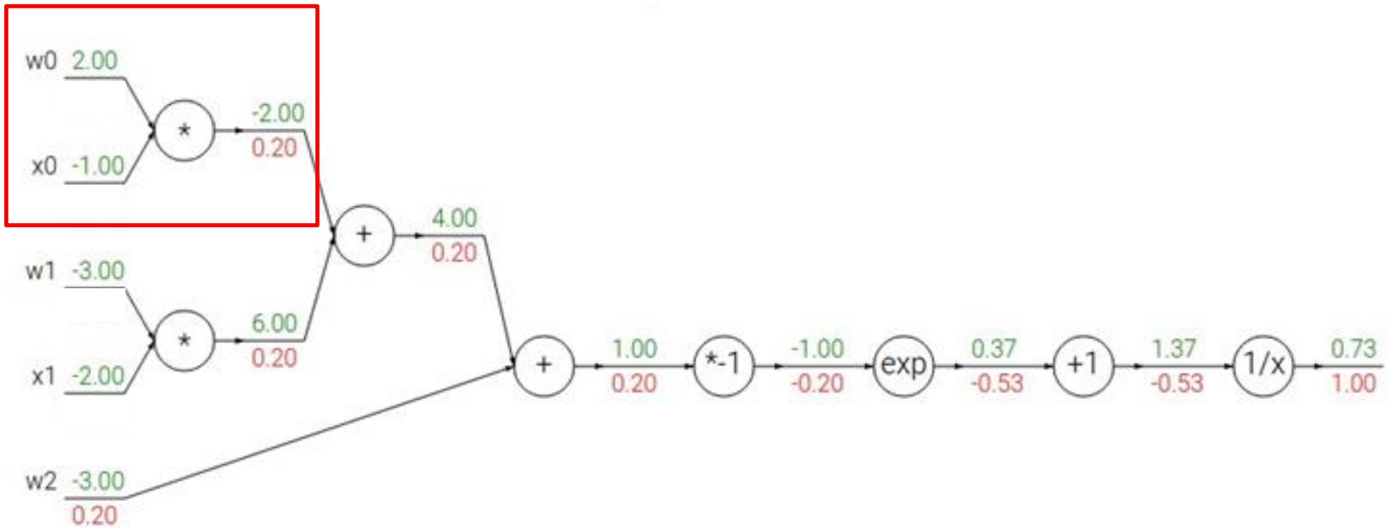
# Example:

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




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

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

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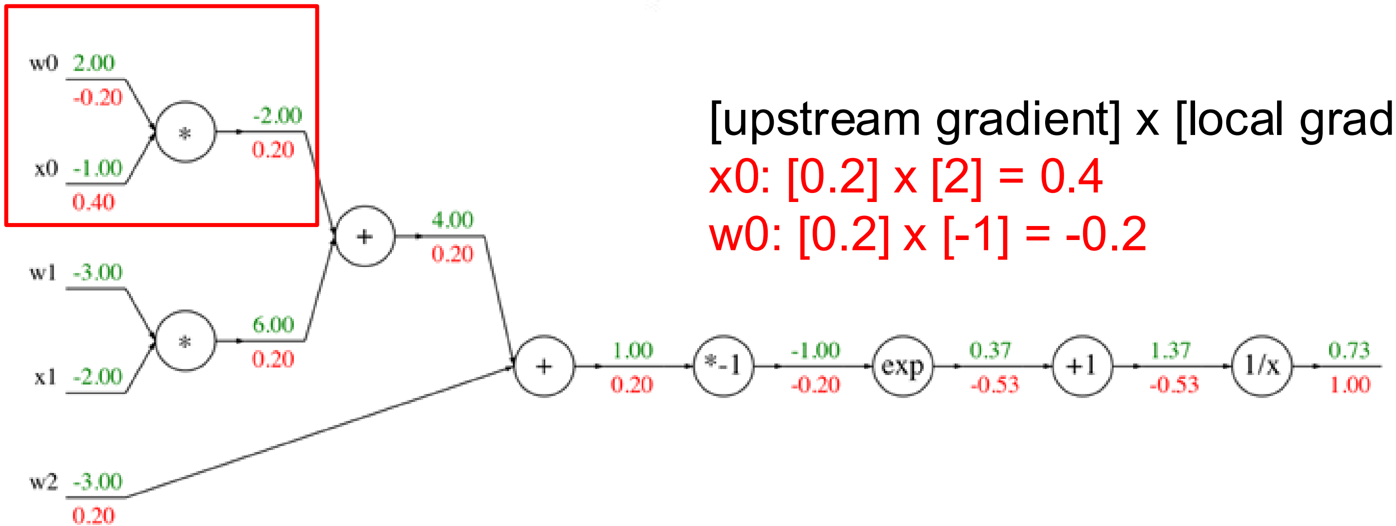


[upstream gradient] x [local gradient]
x0: [0.2] x [2] = 0.4
w0: [0.2] x [-1] = -0.2

| | |
|---|---|
| $f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$ | $f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$ |
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# Example:

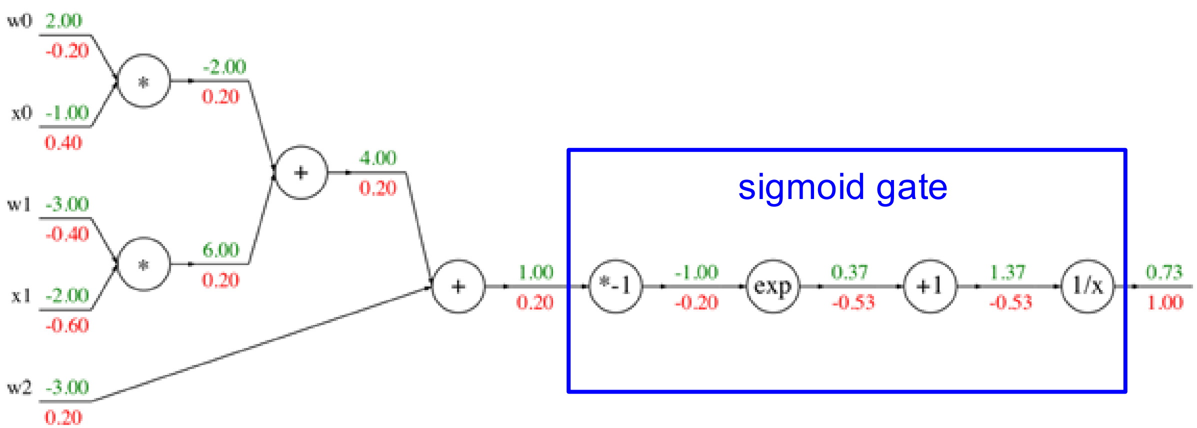
$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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

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

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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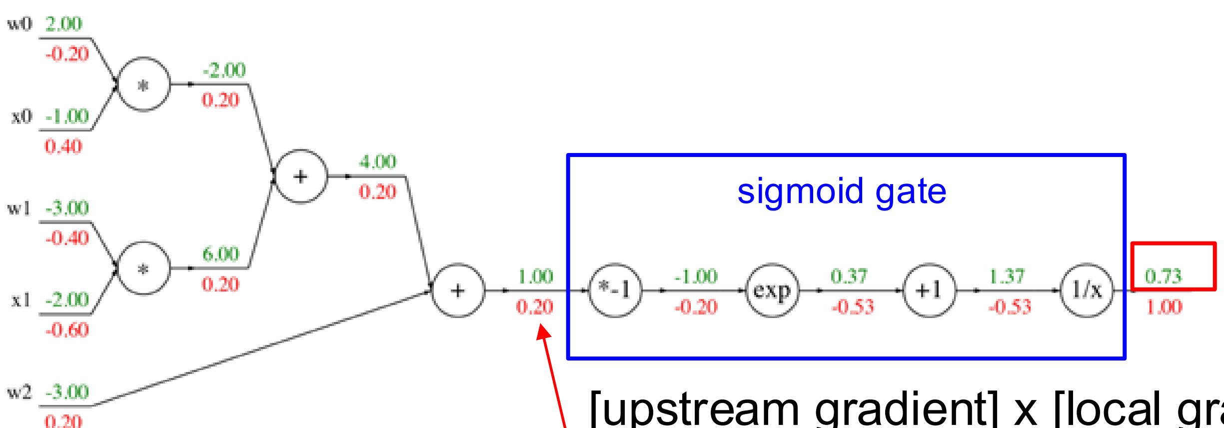
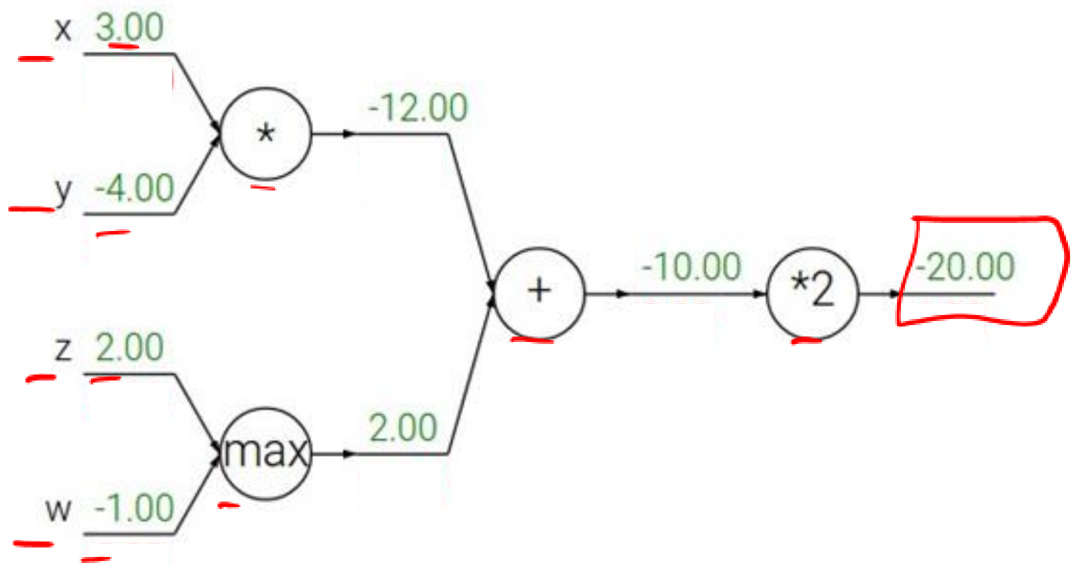



[upstream gradient] x [local gradient]

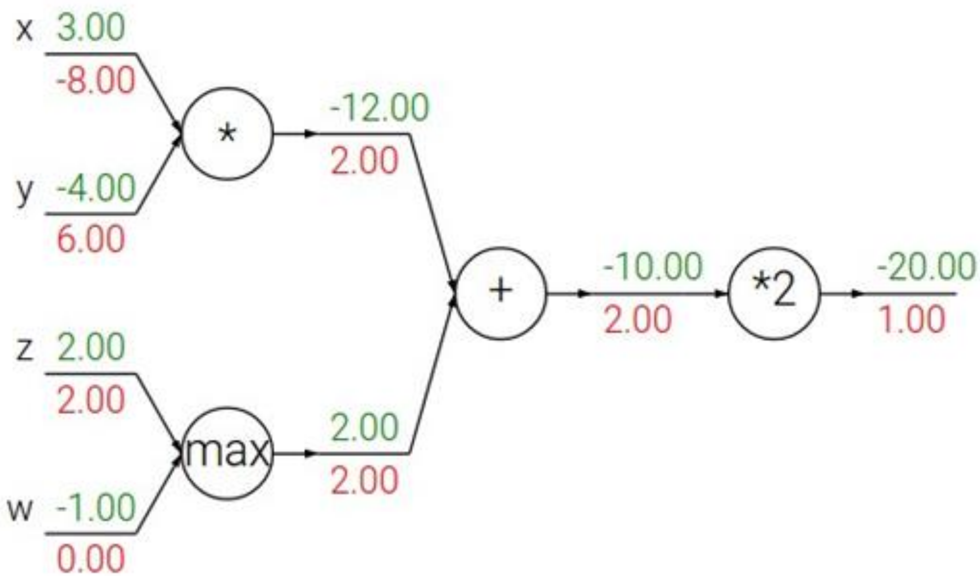
[1.00] x [(1 - 0.73) (0.73)]= 0.2

# Patterns in backward flow

$f(\cdot \cdot\cdot)$
$= 2(xy + \max\{z, w\})$



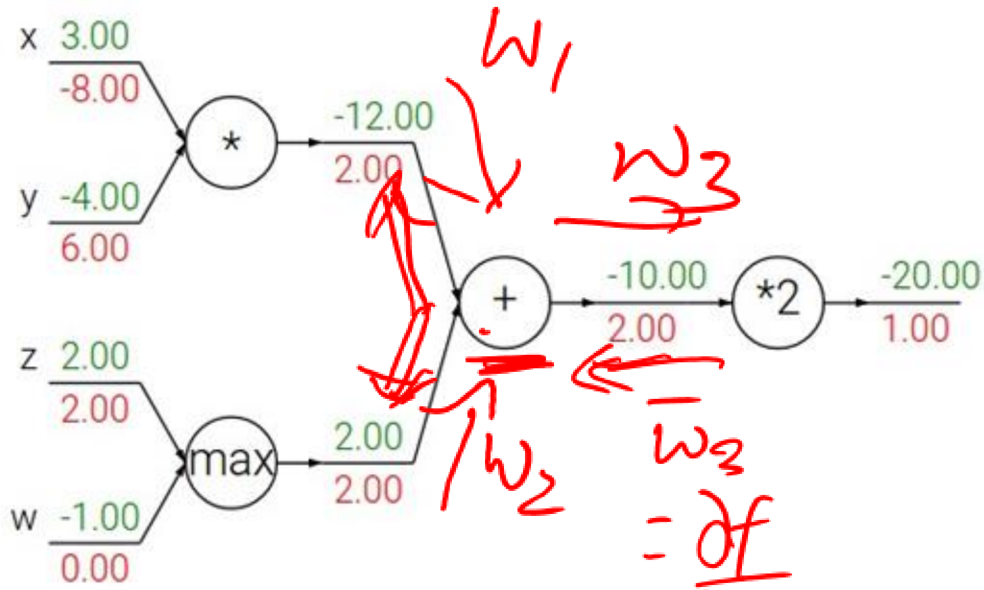
# Patterns in backward flow




Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

# Patterns in backward flow

**add** gate: gradient distributor




$w_3 = \frac{\partial f}{\partial w_3}$

$w_3 = w_1 + w_2$

$\frac{\partial w_3}{\partial w_1} = 1$

$\boxed{\frac{\partial f}{\partial w_1}} = \boxed{\frac{\partial f}{\partial w_3}} \cdot \boxed{\cancel{\frac{\partial w_3}{\partial w_1}}}$

# Patterns in backward flow

$w_2 = \max\{z, w\}$

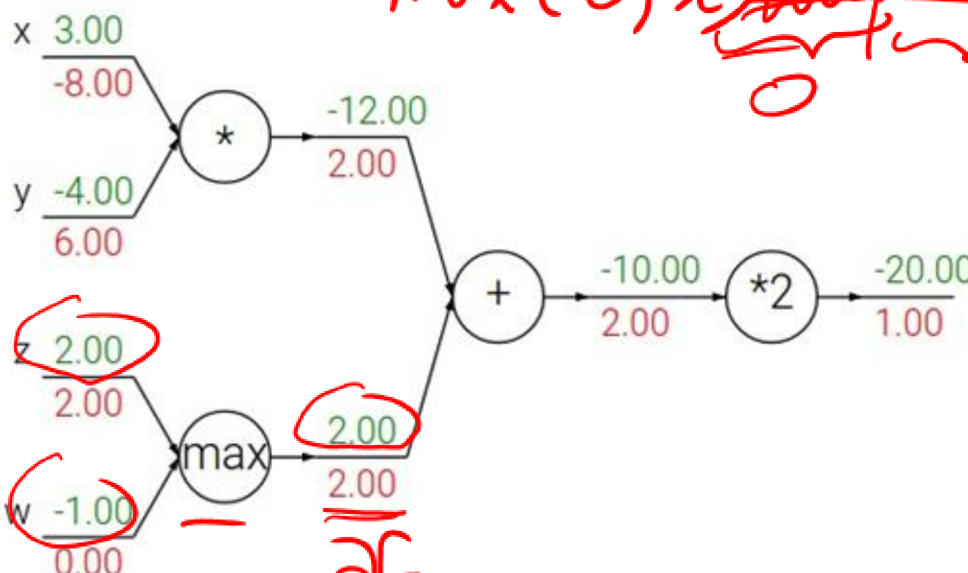
$\max(0, x)$

**add** gate: gradient distributor

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

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

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

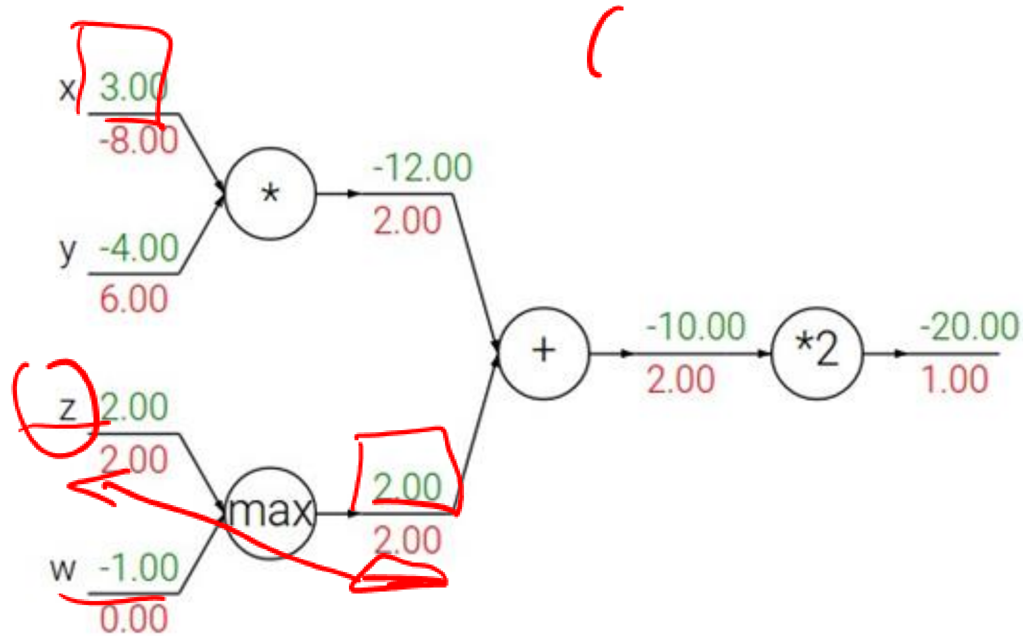



$\frac{\partial f}{\partial w_2}$

# Patterns in backward flow

**add** gate: gradient distributor

**max** gate: gradient router

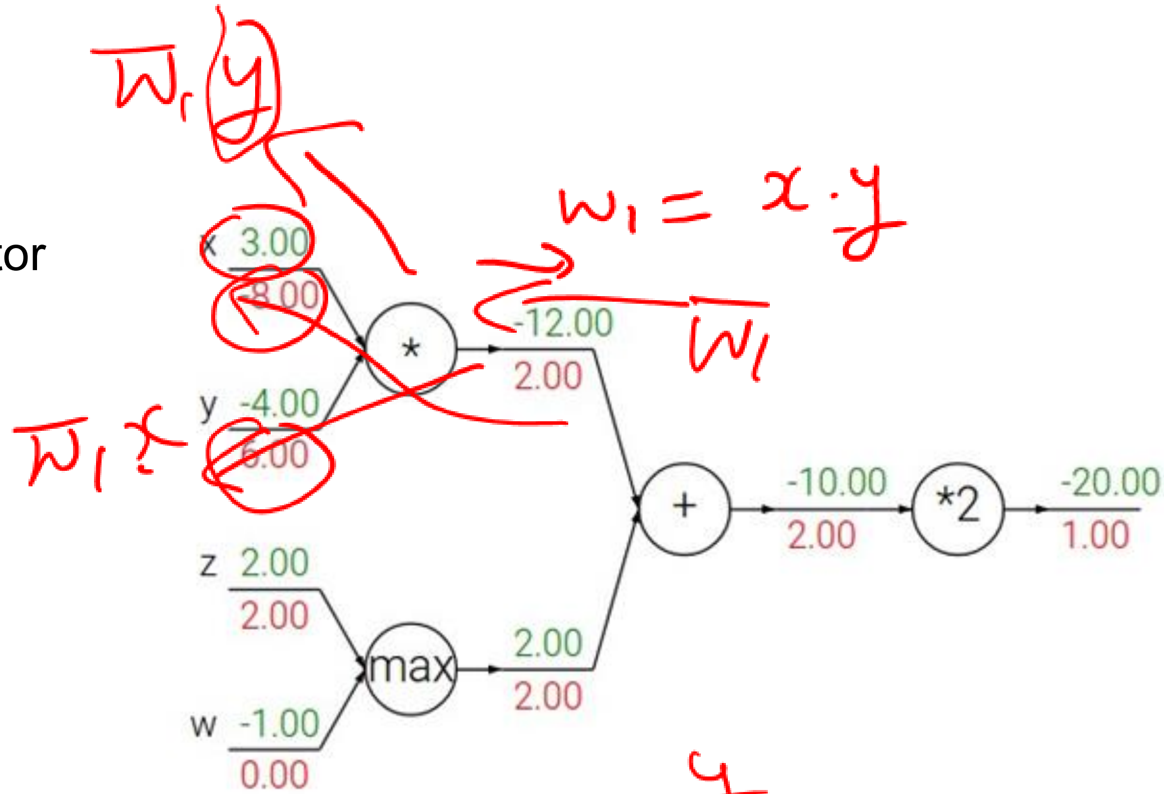


# Patterns in backward flow

**add** gate: gradient distributor

**max** gate: gradient router

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



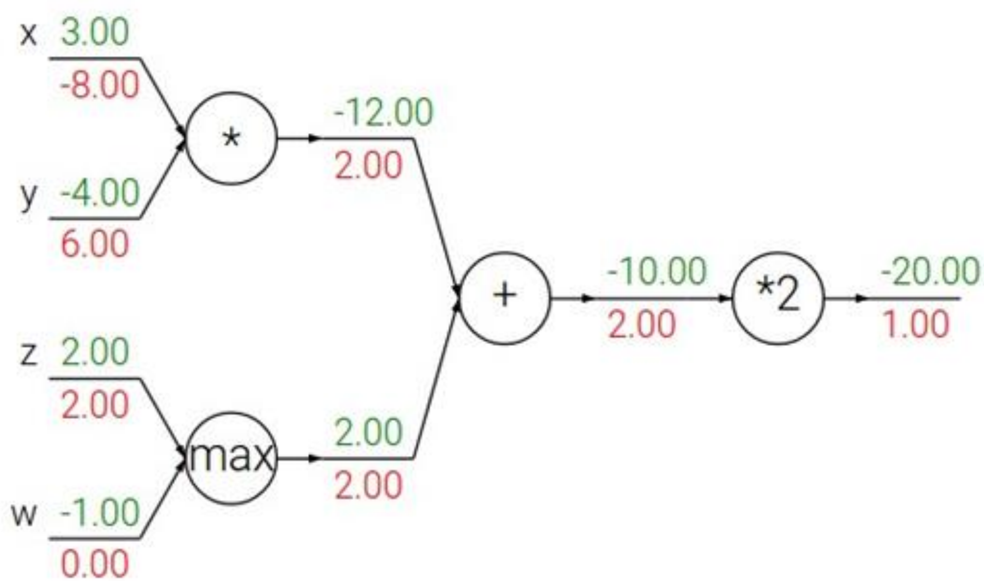

$$\frac{\partial f}{\partial x} = \boxed{\frac{\partial f}{\partial w_1}}\ \overbrace{\boxed{\frac{\partial w_1}{\partial x}}}^{y}$$

# Patterns in backward flow

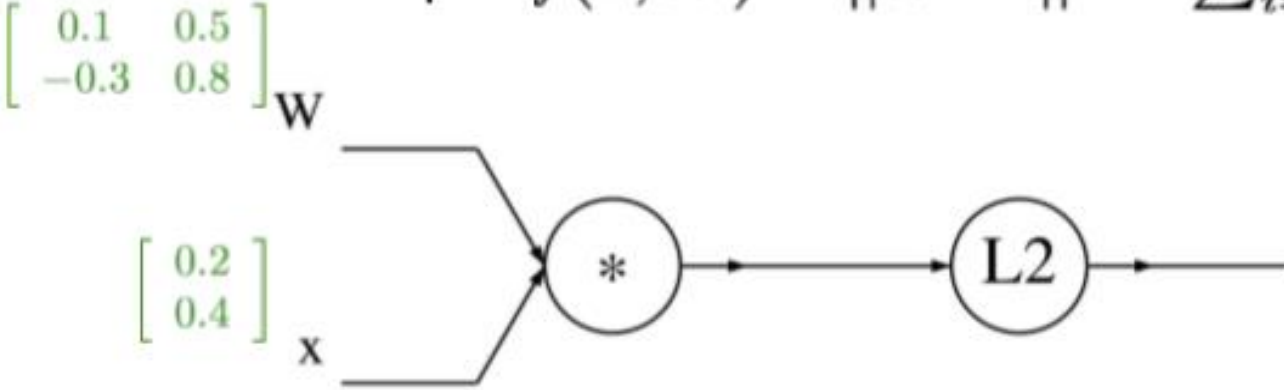
**add** gate: gradient distributor

**max** gate: gradient router

**mul** gate: gradient switcher



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




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

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



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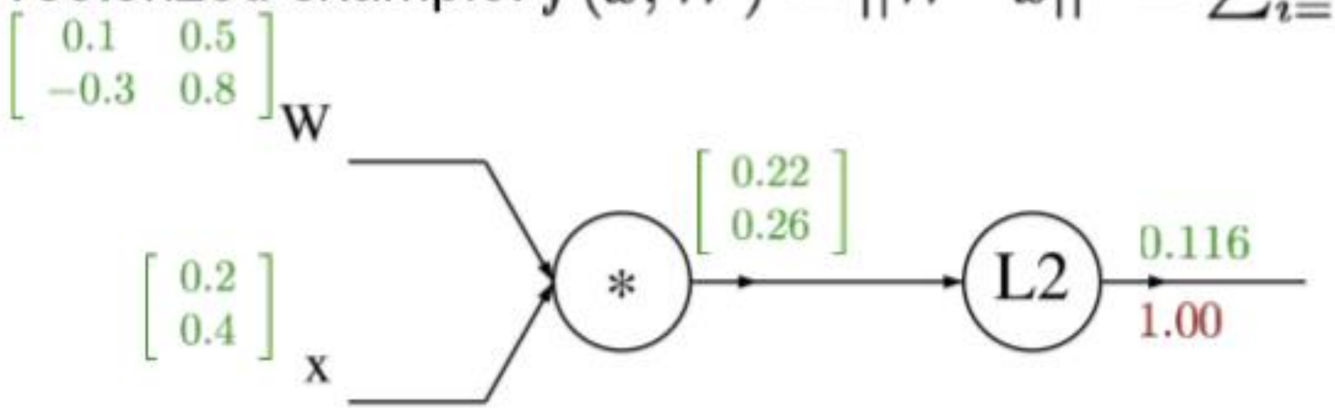


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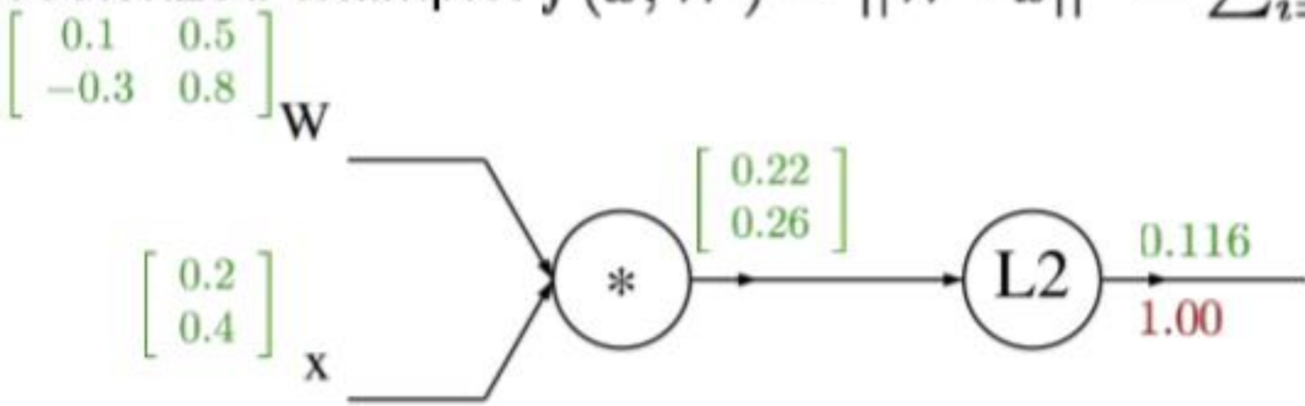


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$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

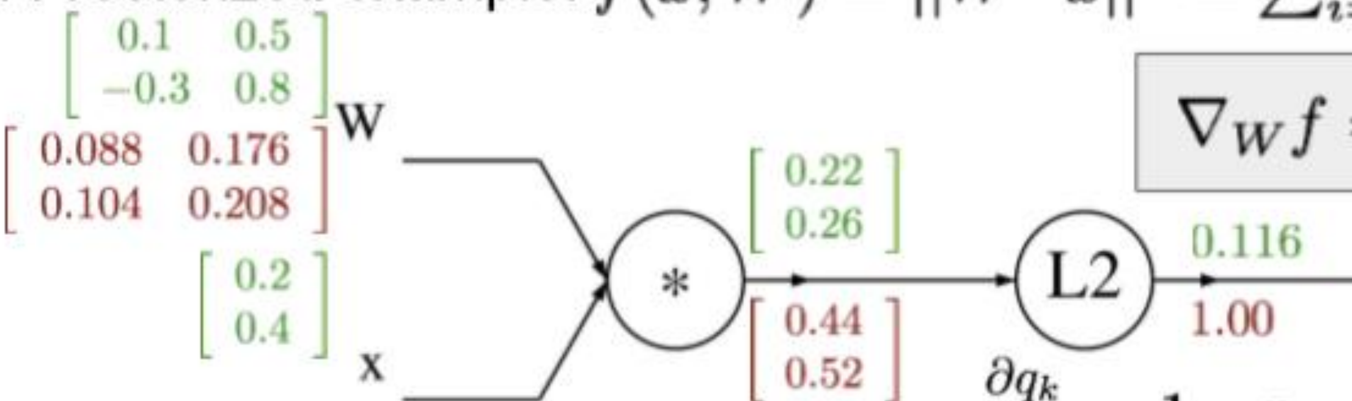
$$\frac{\partial f}{\partial q_i} = 2q_i$$

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



Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

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




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

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

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

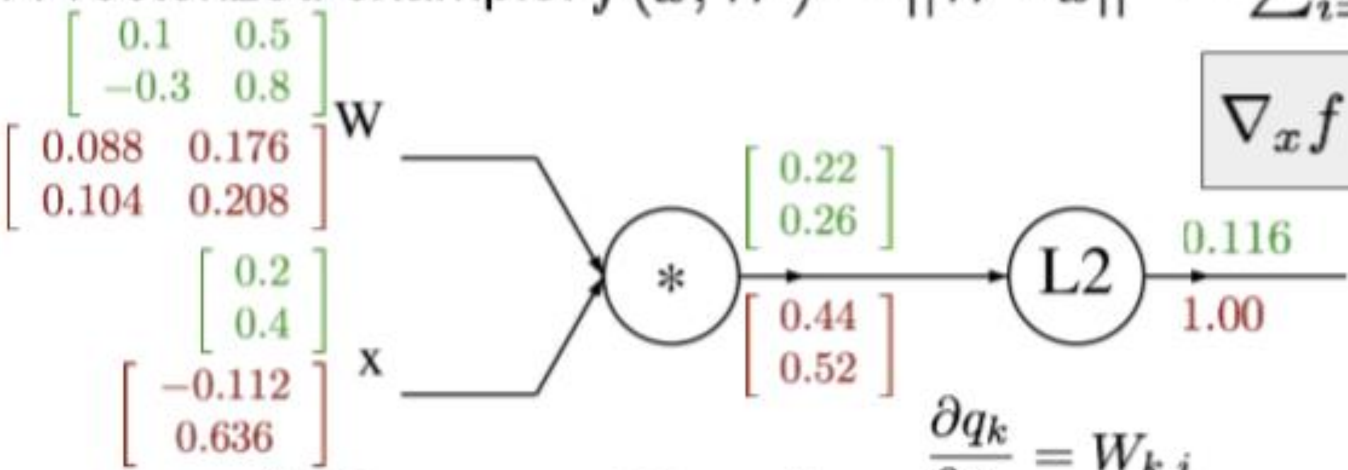
$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

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



Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

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




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

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

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

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

$$\frac{\partial f}{\partial x_i} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i}$$

$$= \sum_k 2 q_k W_{k,i}$$



Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

# Summary

- Learned computational graphs (CG) and efficient gradient computing methods
- How to calculate the gradient during back-propagation using CG
- Notations & examples

- What is next ?
  - Fully connected neural networks (NNs) to convolutional networks