COMP/EECE 7/8740 Neural Networks

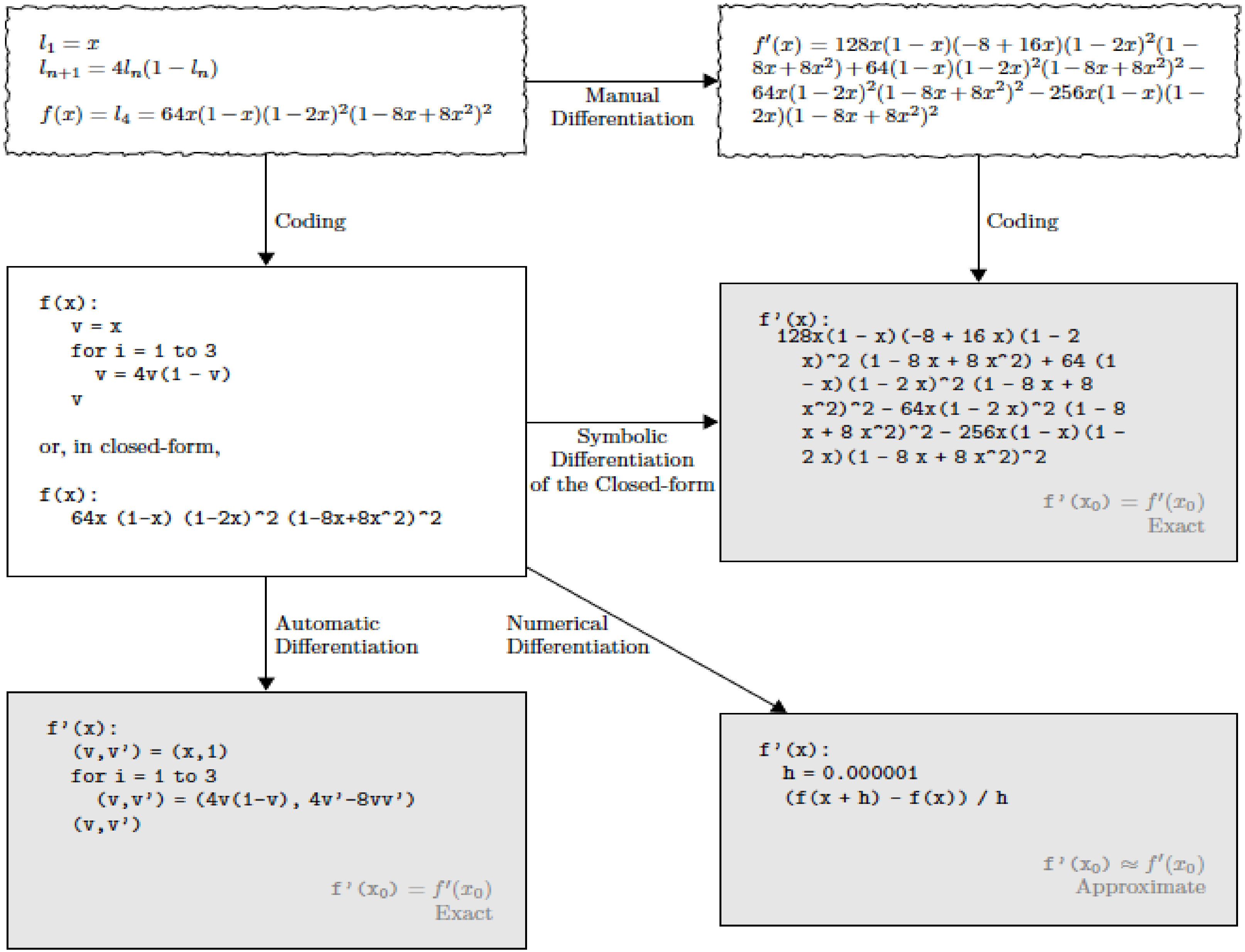
Topics:

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

Md Zahangir Alom
Department of Computer Science
University of Memphis, TN

How do we compute gradients?

- Analytic or “Manual” Differentiation
- Symbolic Differentiation
- Numerical Differentiation
- Automatic Differentiation (AD)
  - Forward mode AD
  - Reverse mode AD
    - aka “backpropagation”


$l_1 = x$
$l_{n+1} = 4l_n(1 - l_n)$
$f(x) = l_4 = 64x(1-x)(1-2x)^2(1-8x+8x^2)^2$
Manual
Differentiation
$f'(x) = 128x(1-x)(-8+16x)(1-2x)^2(1-8x+8x^2)+64(1-x)(1-2x)^2(1-8x+8x^2)^2-64x(1-2x)^2(1-8x+8x^2)^2-256x(1-x)(1-2x)(1-8x+8x^2)^2$
Coding
Coding
f(x):
v = x
for i = 1 to 3
v = 4v(1 - v)
v
or, in closed-form,
f(x):
64x (1-x) (1-2x)^2 (1-8x+8x^2)^2
Symbolic
Differentiation
of the Closed-form
f'(x):
128x(1 - x)(-8 + 16 x)(1 - 2 x)^2 (1 - 8 x + 8 x^2) + 64 (1 - x)(1 - 2 x)^2 (1 - 8 x + 8 x^2)^2 - 64x(1 - 2 x)^2 (1 - 8 x + 8 x^2)^2 - 256x(1 - x)(1 - 2 x)(1 - 8 x + 8 x^2)^2
f'(x$_0$) = $f'(x_0)$
Exact
Automatic
Differentiation
Numerical
Differentiation
f'(x):
(v,v') = (x,1)
for i = 1 to 3
(v,v') = (4v(1-v), 4v'-8vv')
(v,v')
f'(x$_0$) = $f'(x_0)$
Exact
f'(x):
h = 0.000001
(f(x + h) - f(x)) / h
f'(x$_0$) ≈ $f'(x_0)$
Approximate

current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]

loss 1.25347

gradient dW:

[?,
?,
?,
?,
?,
?,
?,
?,
?,…]

current W:	**W + h** (first dim)**:**	**gradient dW:**
[0.34,	[0.34 + **0.0001**,	[?,
-1.11,	-1.11,	?,
0.78,	0.78,	?,
0.12,	0.12,	?,
0.55,	0.55,	?,
2.81,	2.81,	?,
-3.1,	-3.1,	?,
-1.5,	-1.5,	?,
0.33,…]	0.33,…]	?,…]
loss 1.25347	**loss 1.25322**	

current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]

loss 1.25347

W + h (first dim)**:**

[0.34 + **0.0001**,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]

loss 1.25322

gradient dW:

[**-2.5**,
?,
?,

(1.25322 - 1.25347)/0.0001
= -2.5

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

?,
?,…]

current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

W + h (second dim)**:**

[0.34,
-1.11 + **0.0001**,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25353

gradient dW:

[-2.5,
?,
?,
?,
?,
?,
?,
?,
?,…]

current W:	**W + h** (second dim)**:**	**gradient dW:**
[0.34,	[0.34,	[-2.5,
-1.11,	-1.11 + **0.0001**,	**0.6**,
0.78,	0.78,	?,
0.12,	0.12,	?,
0.55,	0.55,	
2.81,	2.81,	
-3.1,	-3.1,	
-1.5,	-1.5,	
0.33,…]	0.33,…]	?,…]
loss 1.25347	**loss 1.25353**	

(1.25353 - 1.25347)/0.0001
= 0.6

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

current W:	**W + h** (third dim)**:**	**gradient dW:**
[0.34,	[0.34,	[-2.5,
-1.11,	-1.11,	0.6,
0.78,	0.78 + **0.0001**,	?,
0.12,	0.12,	?,
0.55,	0.55,	?,
2.81,	2.81,	?,
-3.1,	-3.1,	?,
-1.5,	-1.5,	?,
0.33,…]	0.33,…]	?,…]
loss 1.25347	**loss 1.25347**	

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

current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

W + h (third dim)**:**

[0.34,
-1.11,
0.78 + **0.0001**,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

gradient dW:

[-2.5,
0.6,
0,
?,

(1.25347 - 1.25347)/0.0001
= 0

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

?,…]

Numerical vs Analytic Gradients

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

- **Numerical gradient**: slow :(, approximate :(, easy to write :)
- **Analytic gradient**: fast :), exact :), error-prone :(

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

This is called a **gradient check.**

Neural Turing Machine

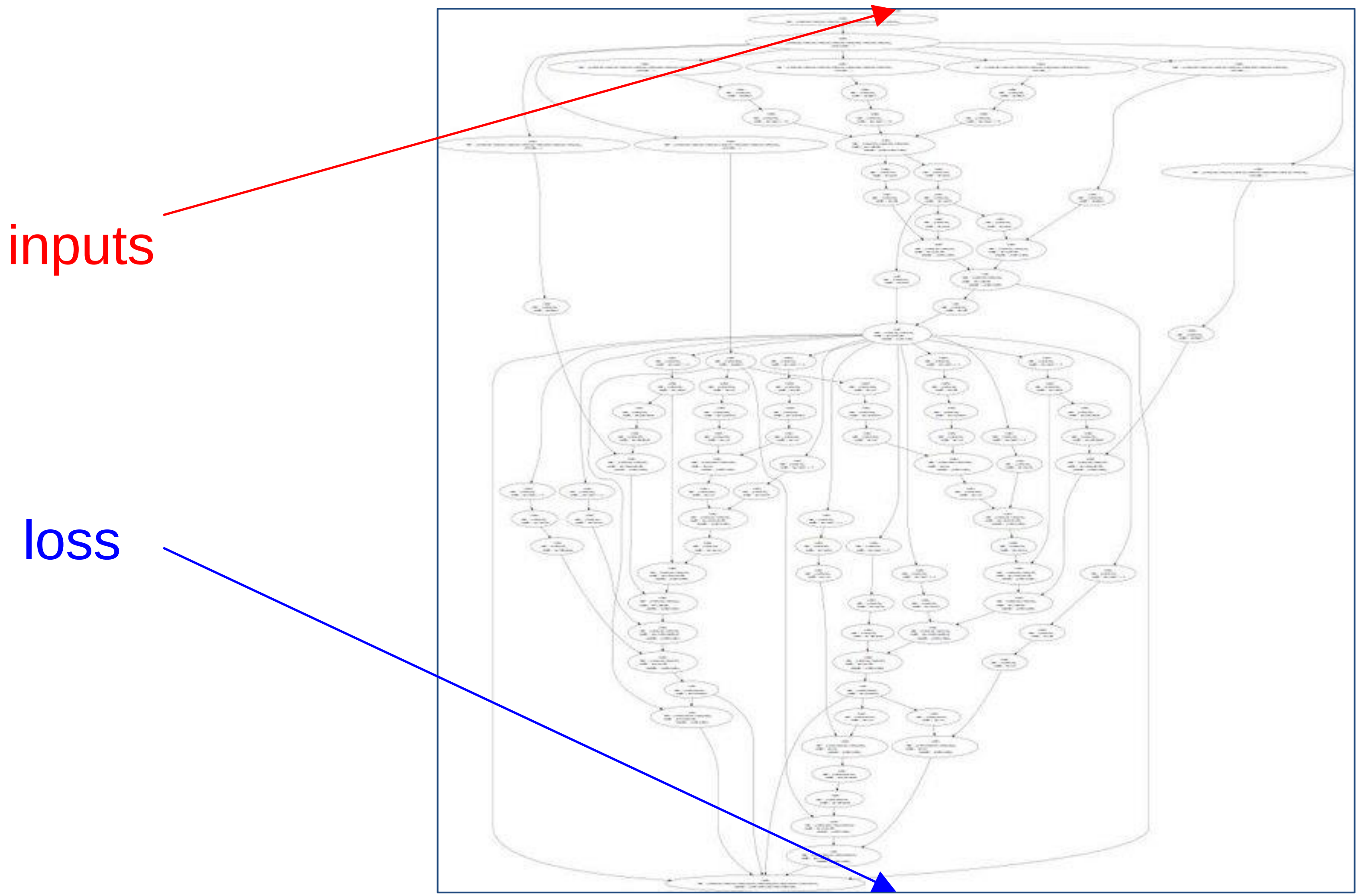


Figure reproduced with permission from a [Twitter post]() by Andrej Karpathy.

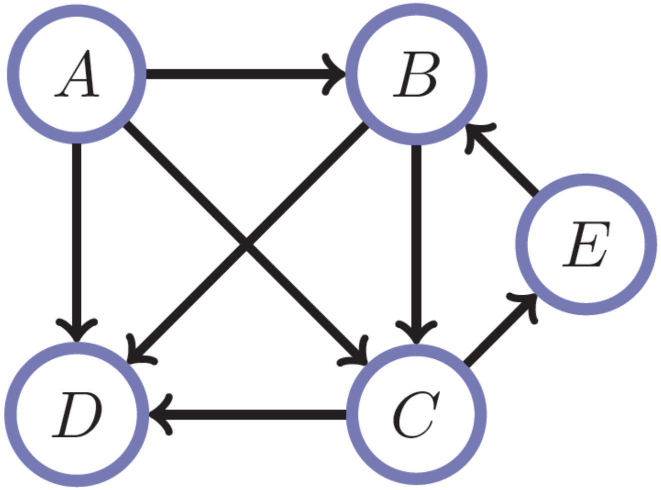
Computational Graphs

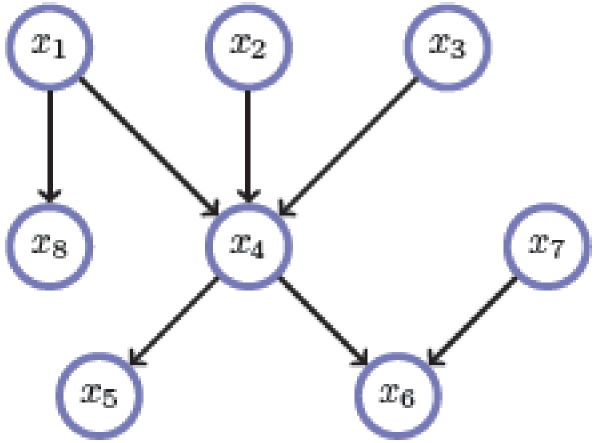
- **A computational graph** is a way to represent a math function in the language of graph theory. Recall the premise of **graph** theory:
  - Nodes are connected by edges, and
  - Everything in the **graph** is either a node or an edge.

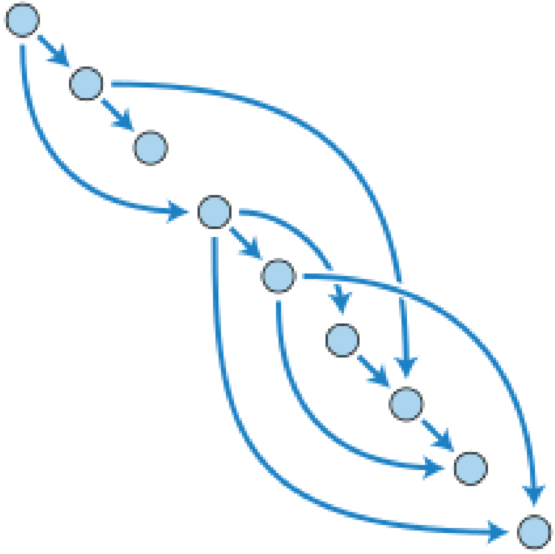
- In computational graph
  - Nodes are either input values or functions for combining values.
  - Edges receive their weights as the data flows through the graph.
    - Outbound edges from an input node are weighted with that input value
    - outbound nodes from a function node are weighted by combining the weights of the inbound edges using the specified function.

Directed Acyclic Graphs (DAGs)

- Exactly what the name suggests
  - Directed edges
  - No (directed) cycles
  - Underlying undirected cycles okay

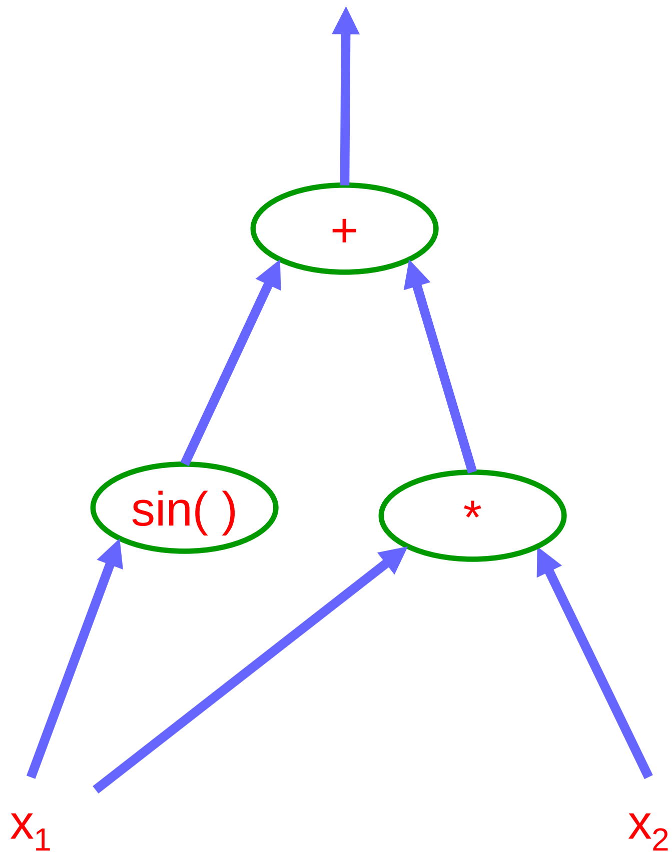






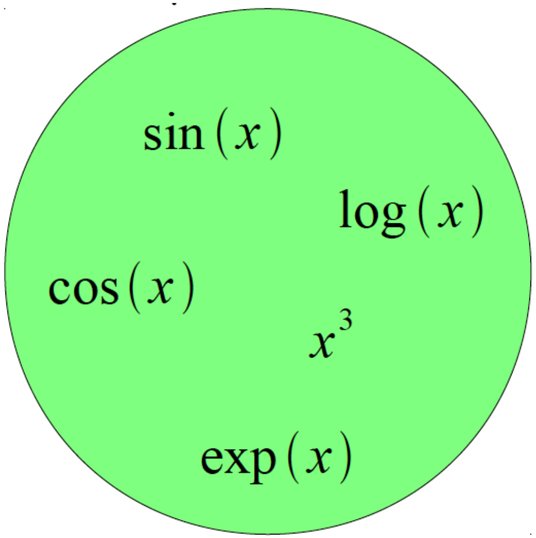
Example

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



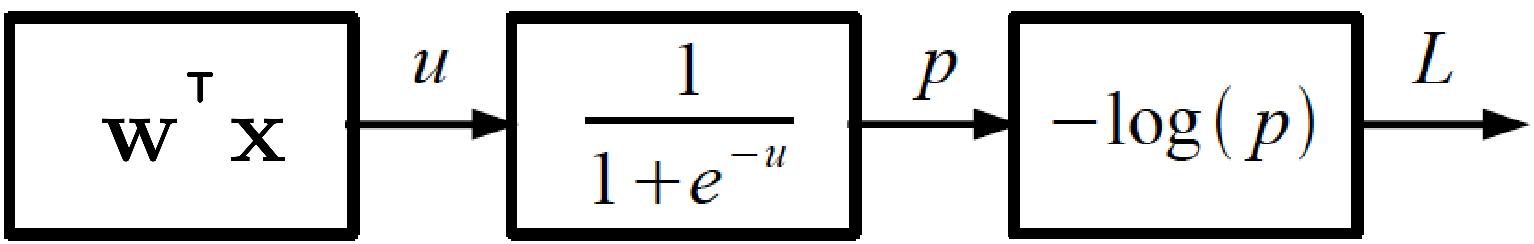
Logistic Regression as a Cascade

Given a library of simple functions

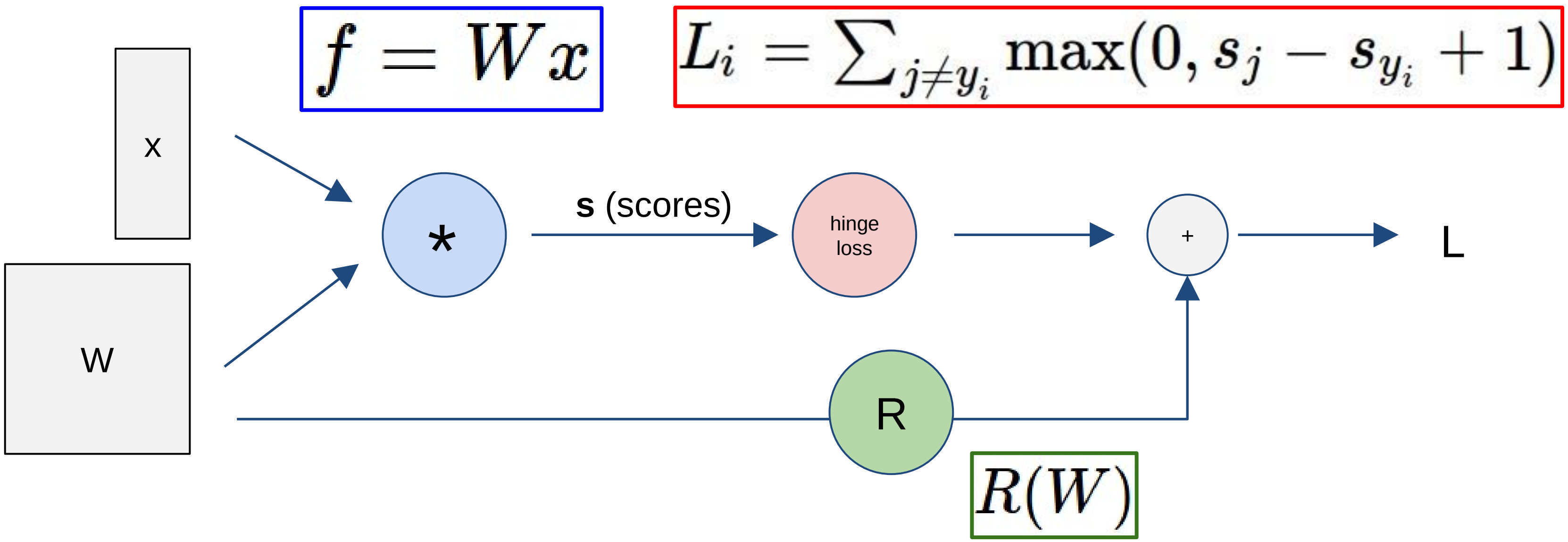


Compose into a complicate function

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

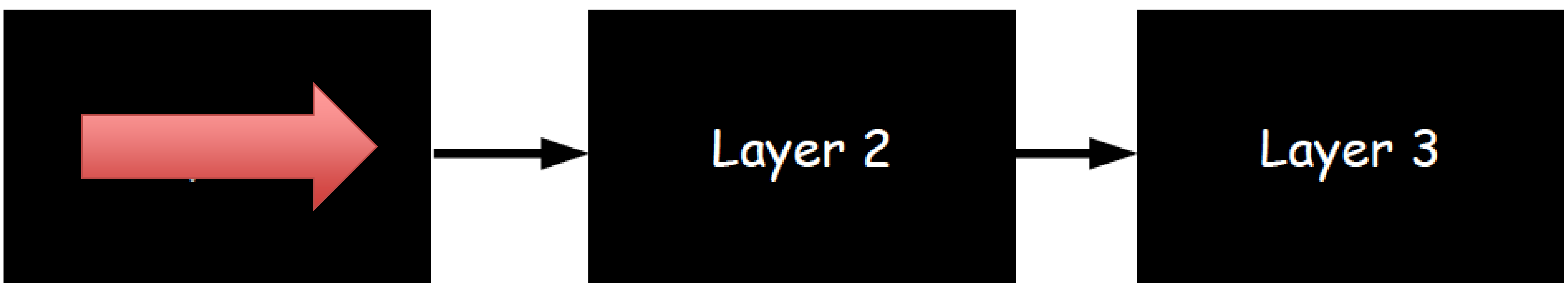


Computational Graph and NNs



Neural Network Training

- Step 1: Compute Loss on mini-batch [F-Pass]



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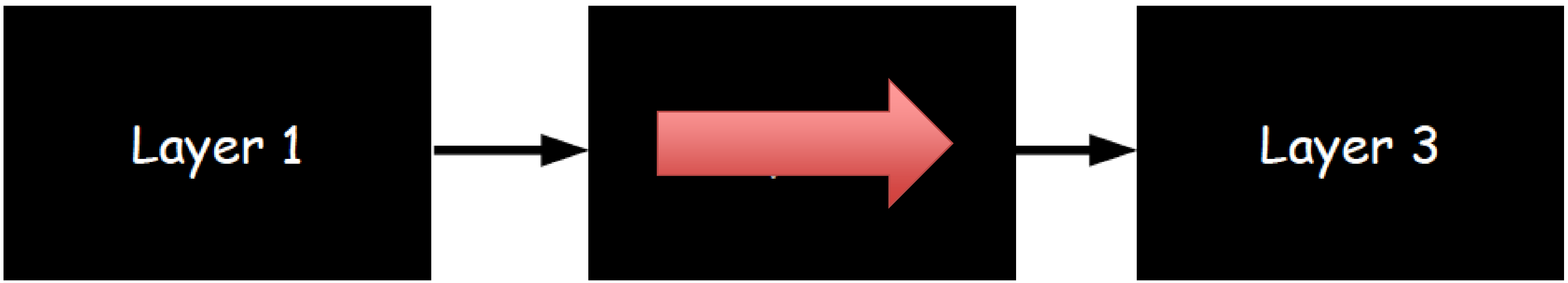

Neural Network Training

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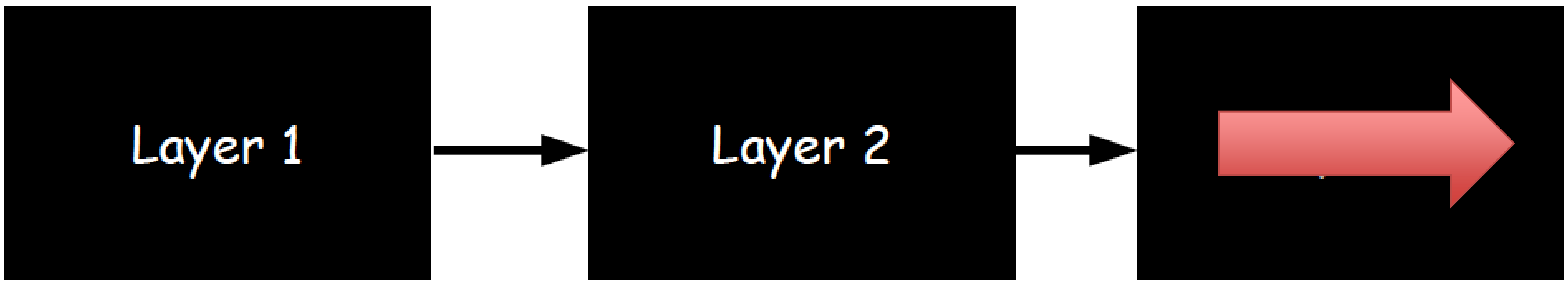
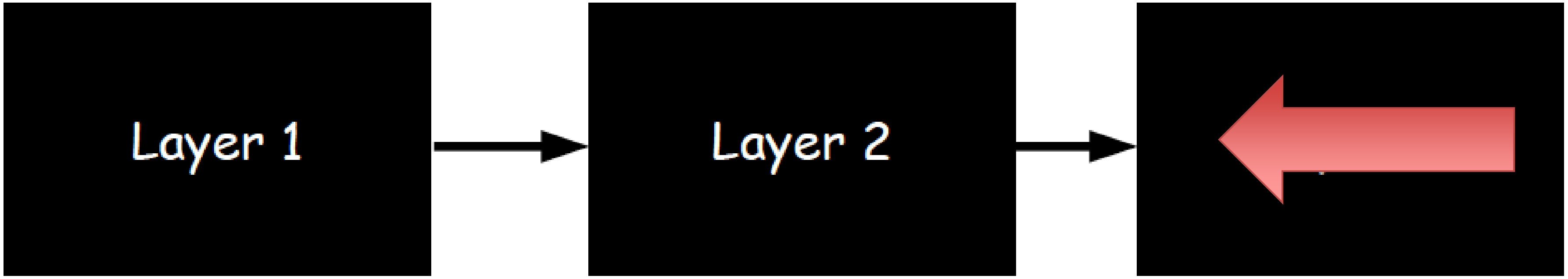


Neural Network Training

- Step 1: Compute Loss on mini-batch [F-Pass]
- Step 2: Compute gradients wrt parameters [B-Pass]



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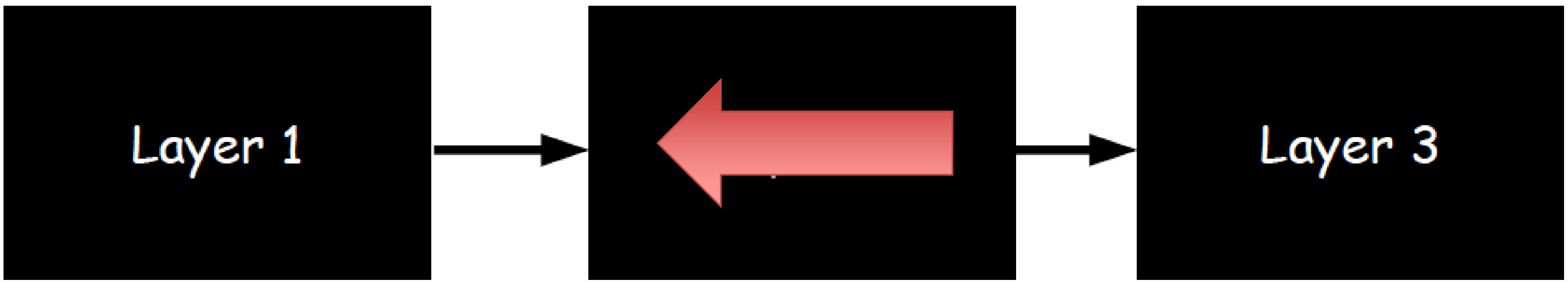

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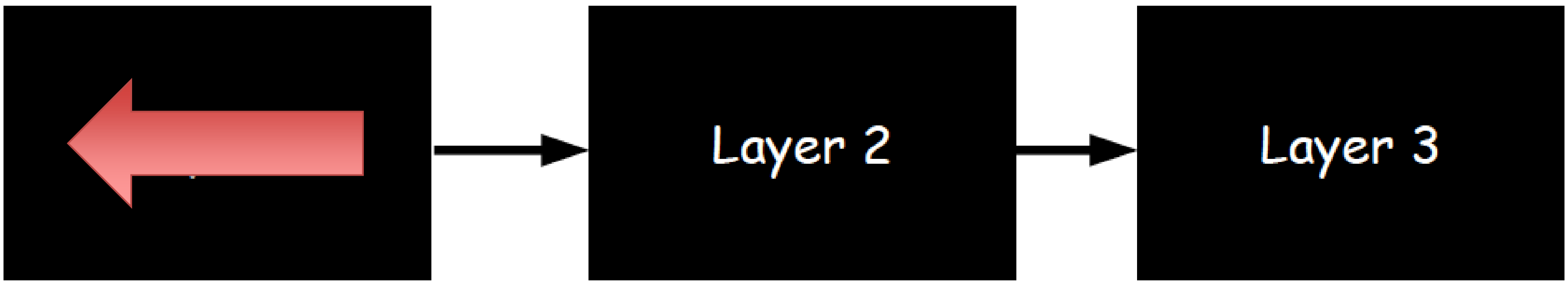
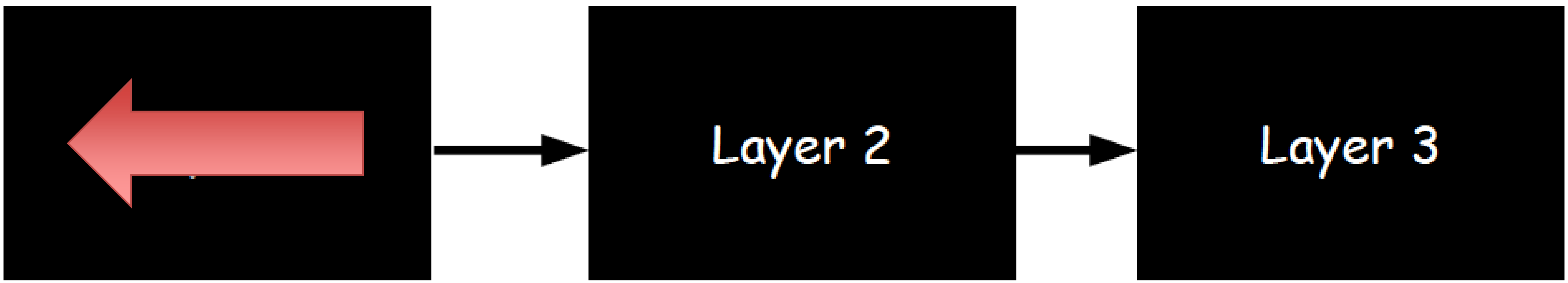


Neural Network Training

- Step 1: Compute Loss on mini-batch [F-Pass]
- Step 2: Compute gradients wrt parameters [B-Pass]
- Step 3: Use gradient to update parameters



$$\theta \leftarrow \theta - \eta \frac{dL}{d\,\theta}$$

Backpropagation: a simple example

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

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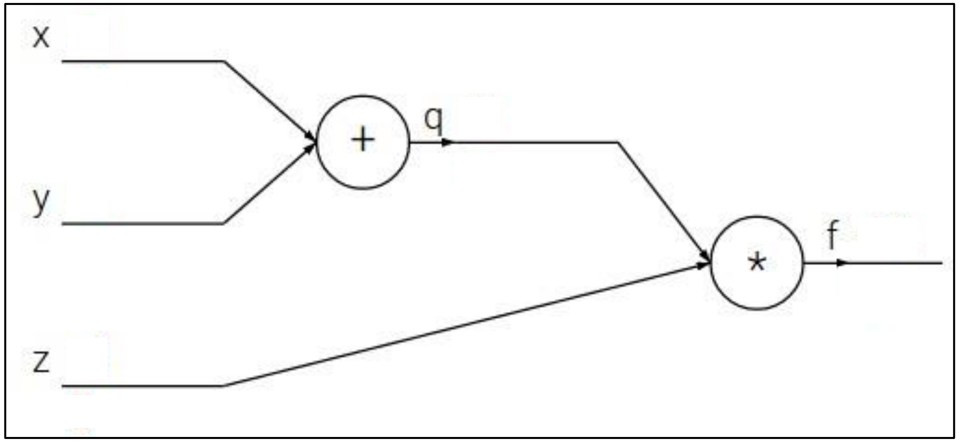
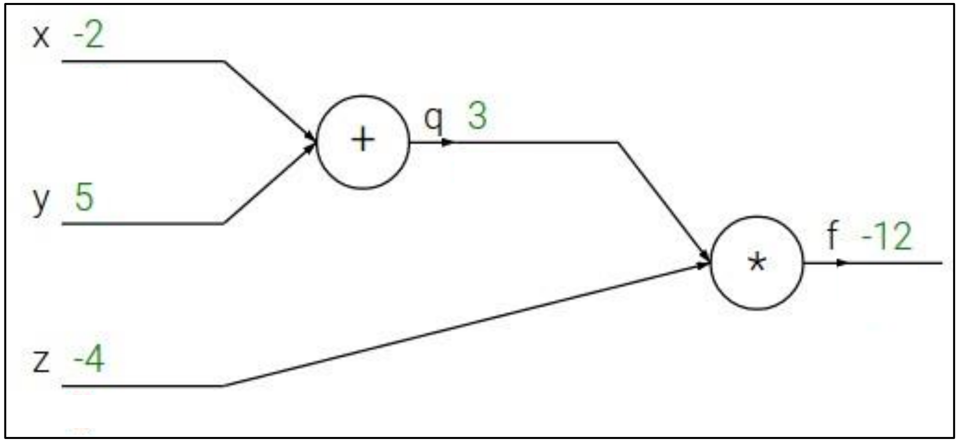
$$f(x, y, z) = (x + y)z$$



Backpropagation: a simple example

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

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



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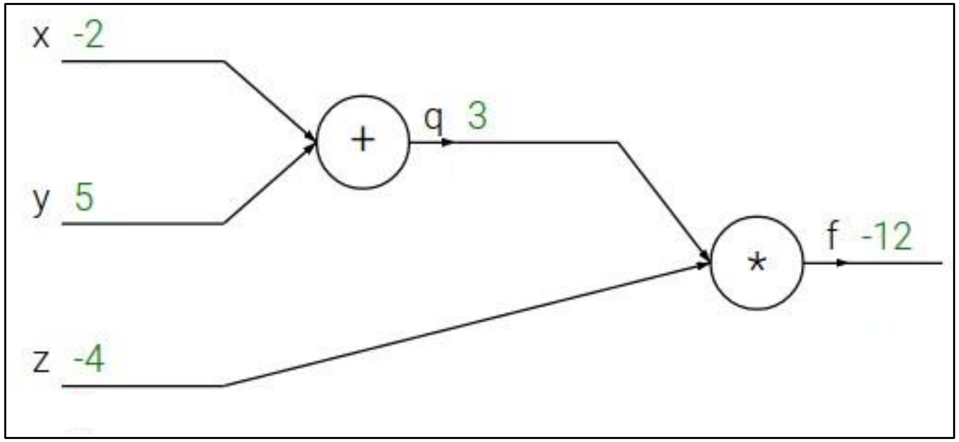

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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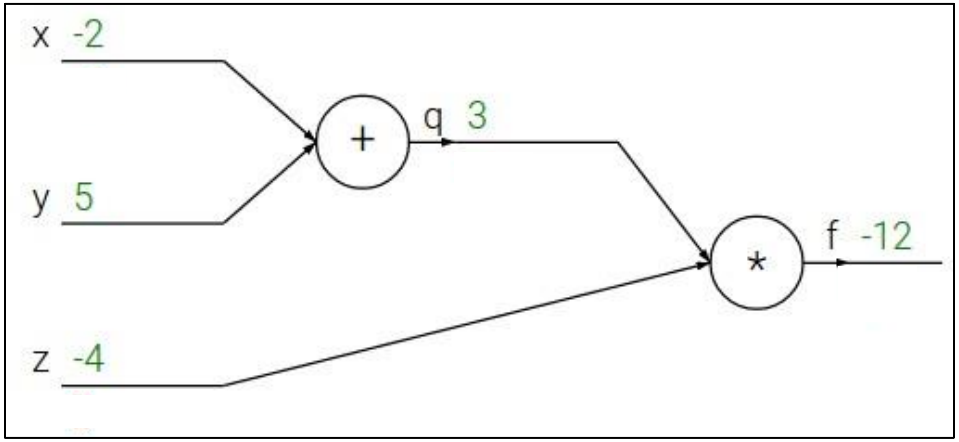

$$\boxed{q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1}$$

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

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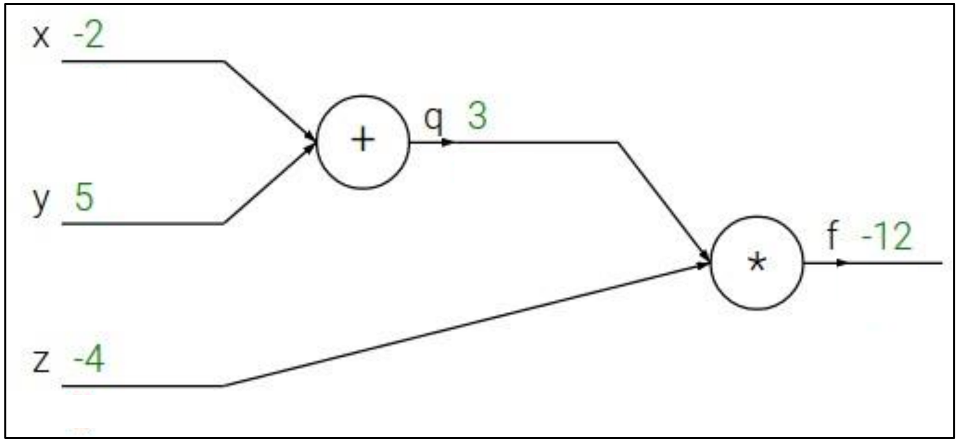

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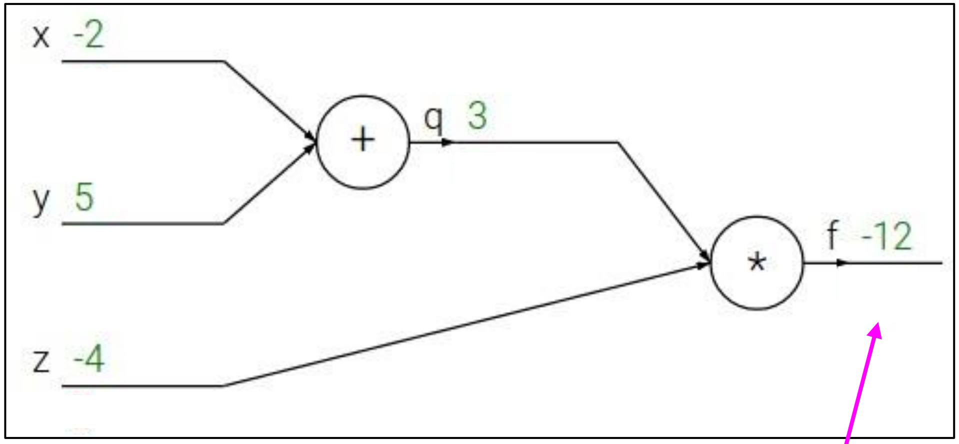
Want: $\dfrac{\partial f}{\partial x}, \dfrac{\partial f}{\partial y}, \dfrac{\partial f}{\partial z}$



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

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

Backpropagation: a simple example

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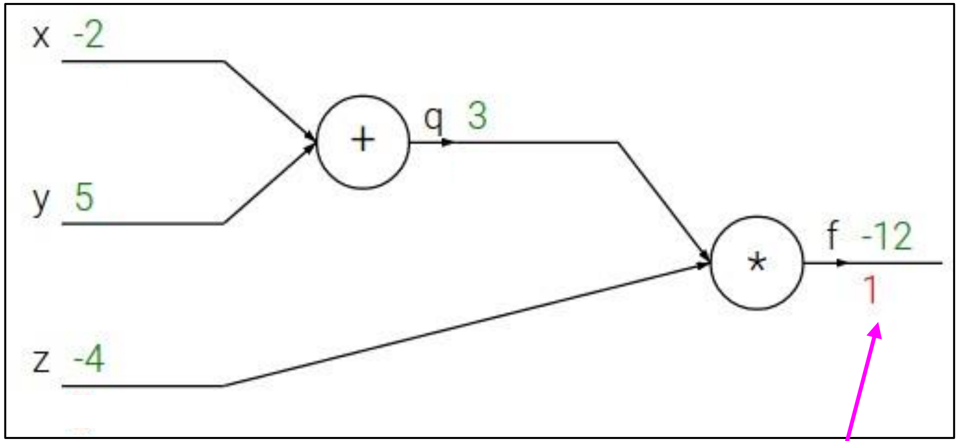

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$$\boxed{\frac{\partial f}{\partial f}}$$

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

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

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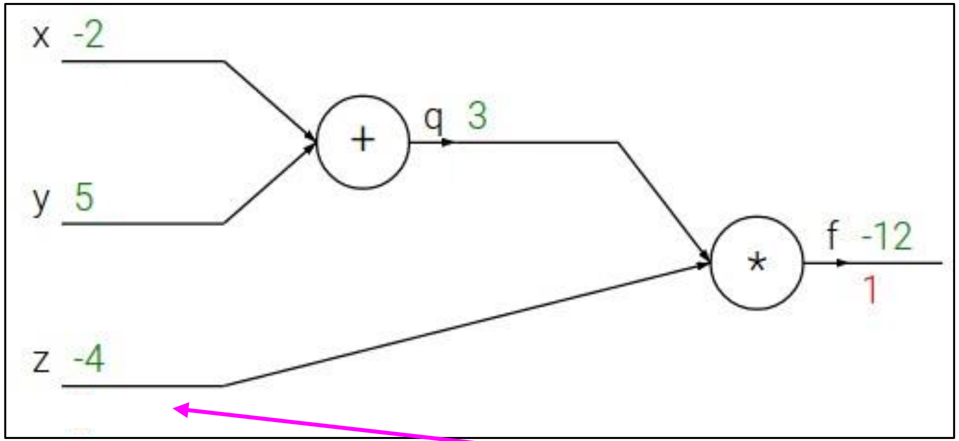

$$\frac{\partial f}{\partial z}$$

Backpropagation: a simple example

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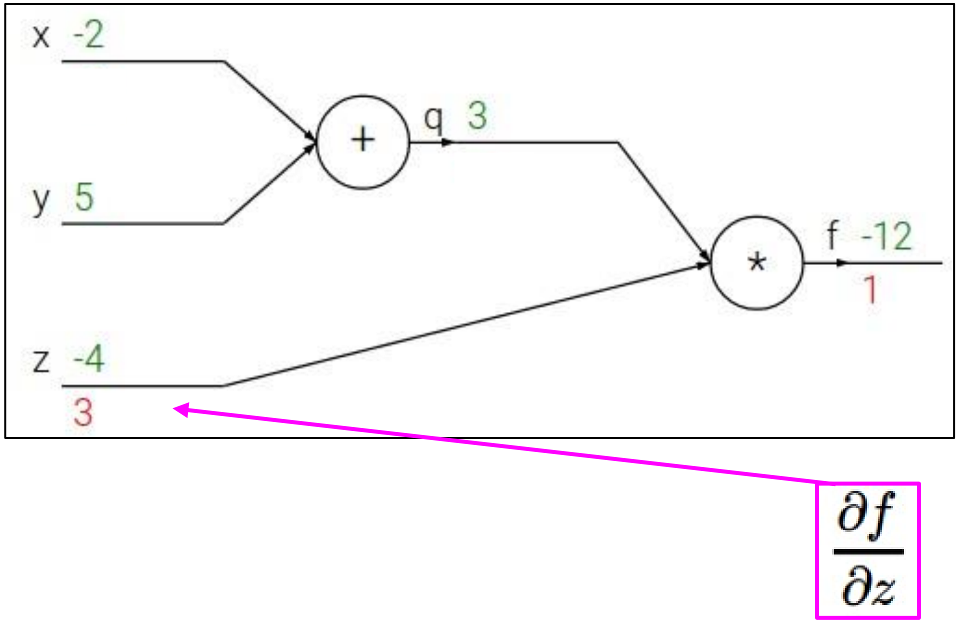

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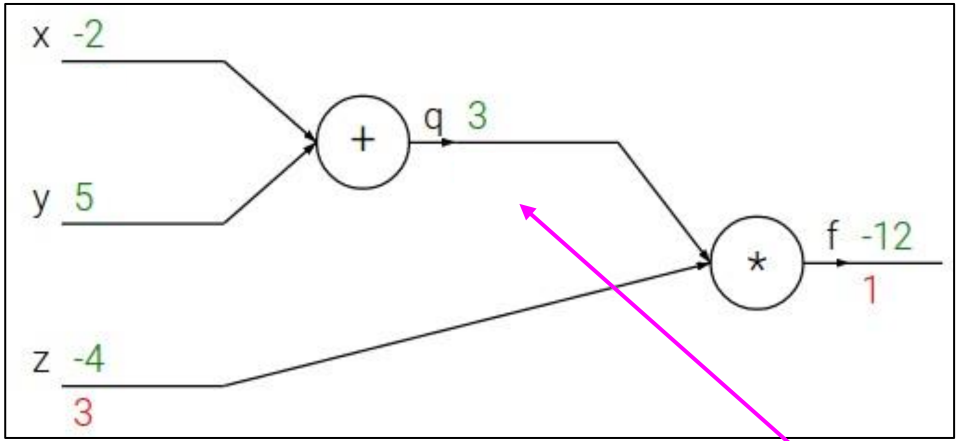

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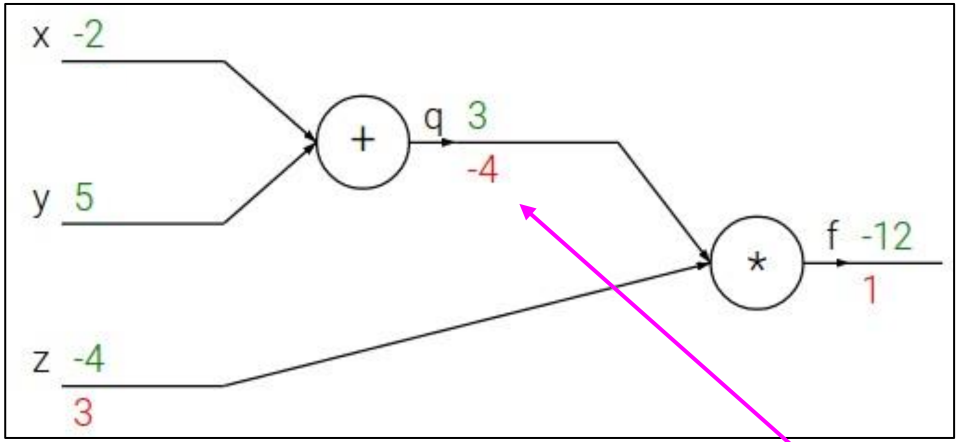

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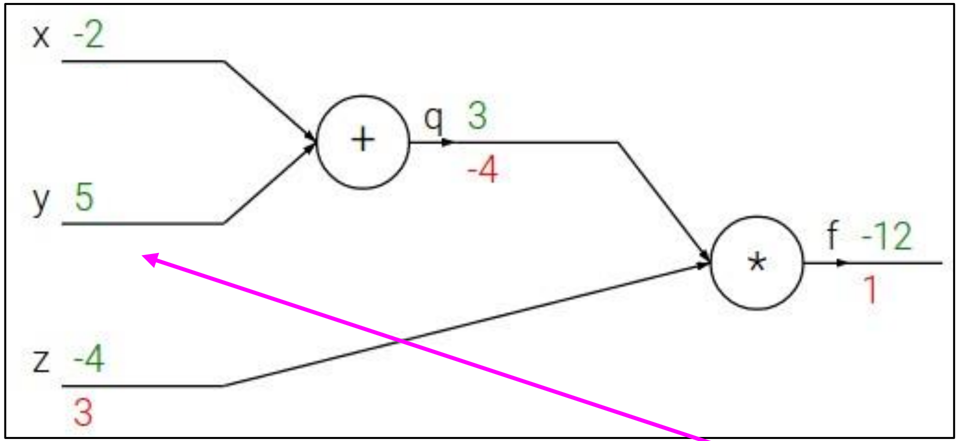

$$\frac{\partial f}{\partial y}$$

Chain rule:

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

Upstream gradient

Local gradient

Backpropagation: a simple example

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

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

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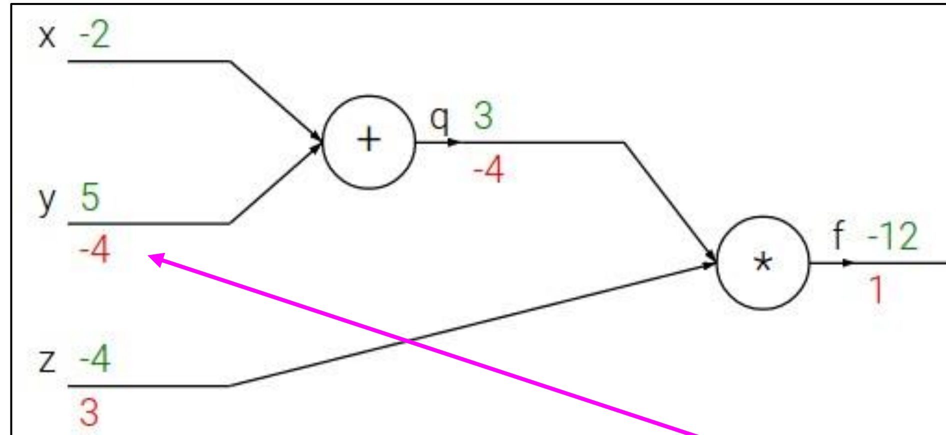

$$\frac{\partial f}{\partial y}$$

Chain rule:

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Upstream gradient

Local gradient

Backpropagation: a simple example

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

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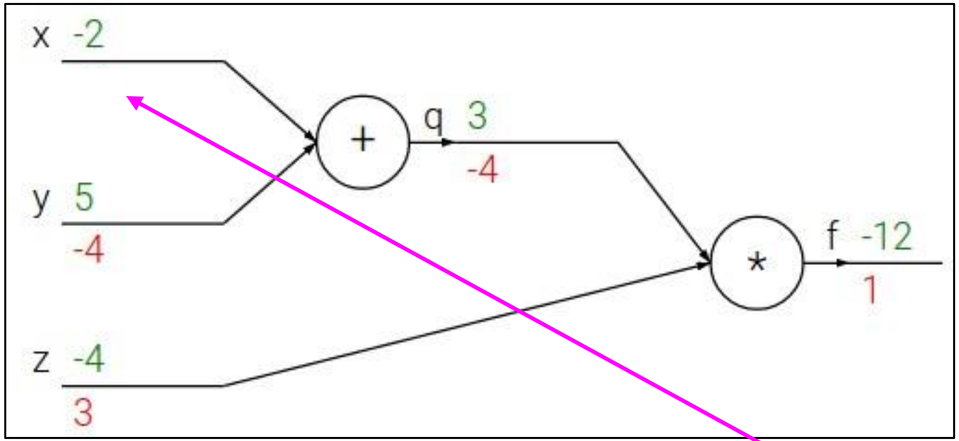

$$\frac{\partial f}{\partial x}$$

Chain rule:

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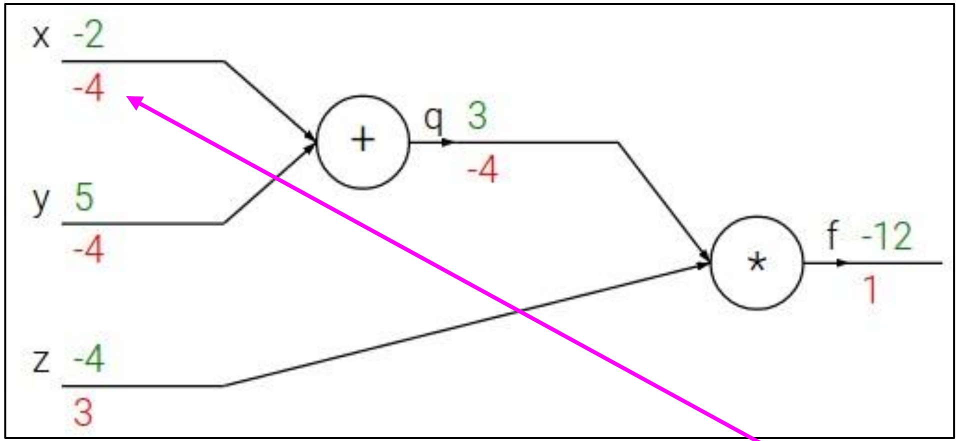

$$\frac{\partial f}{\partial x}$$

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Chain rule:

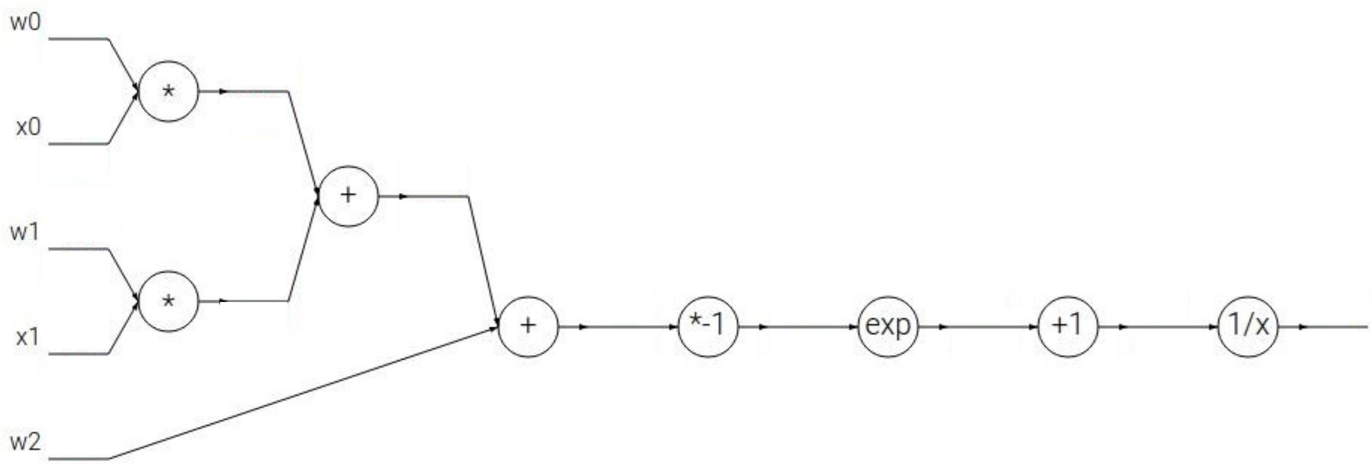
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x}$$

Upstream gradient

Local gradient

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

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



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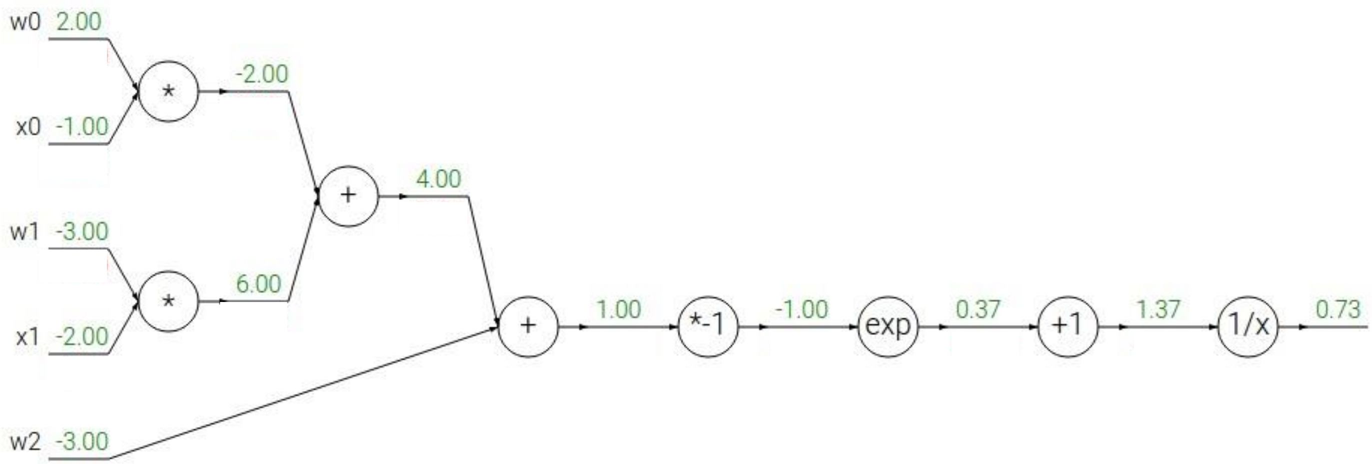

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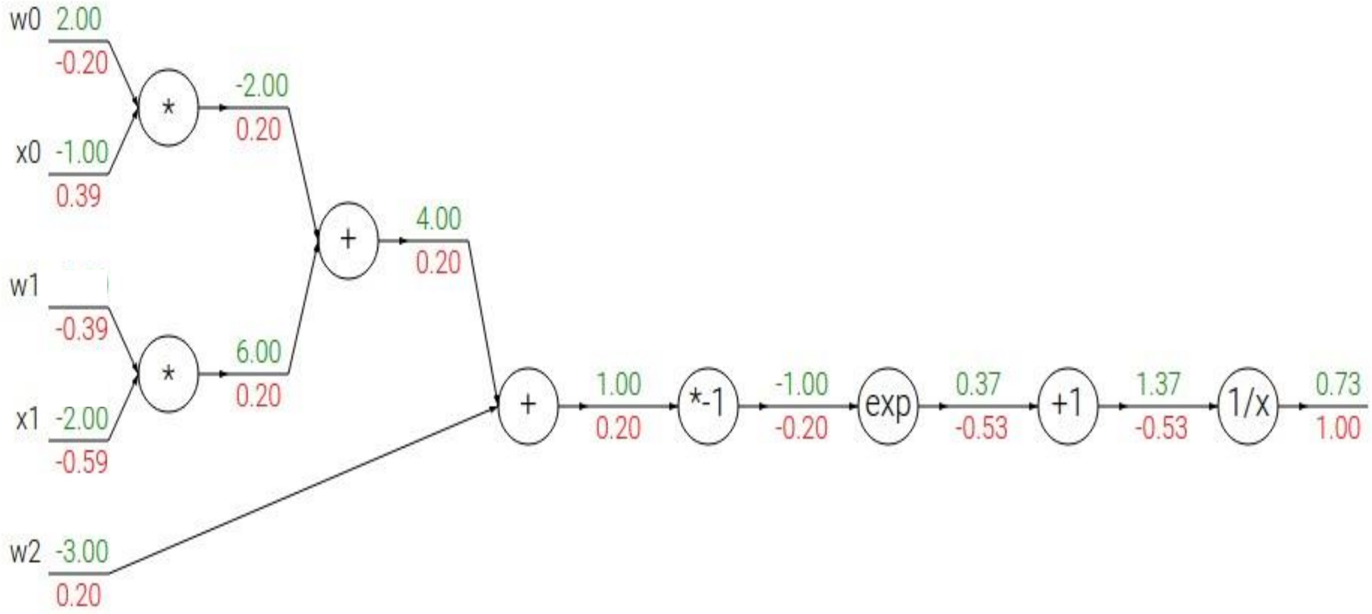
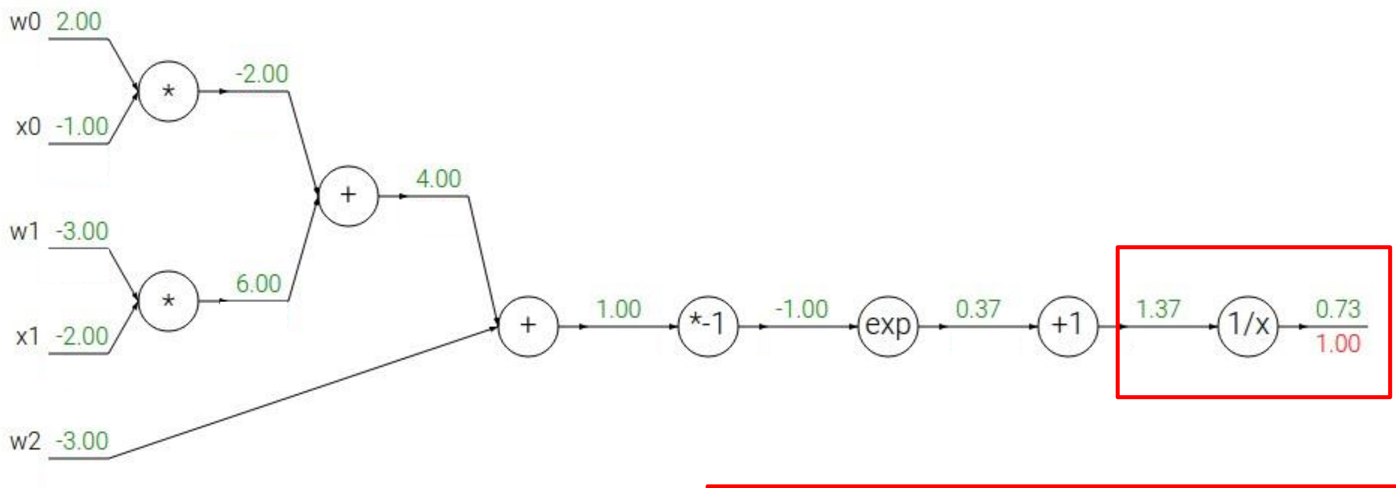


$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$		$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$	
$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$		$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$	

Example:

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



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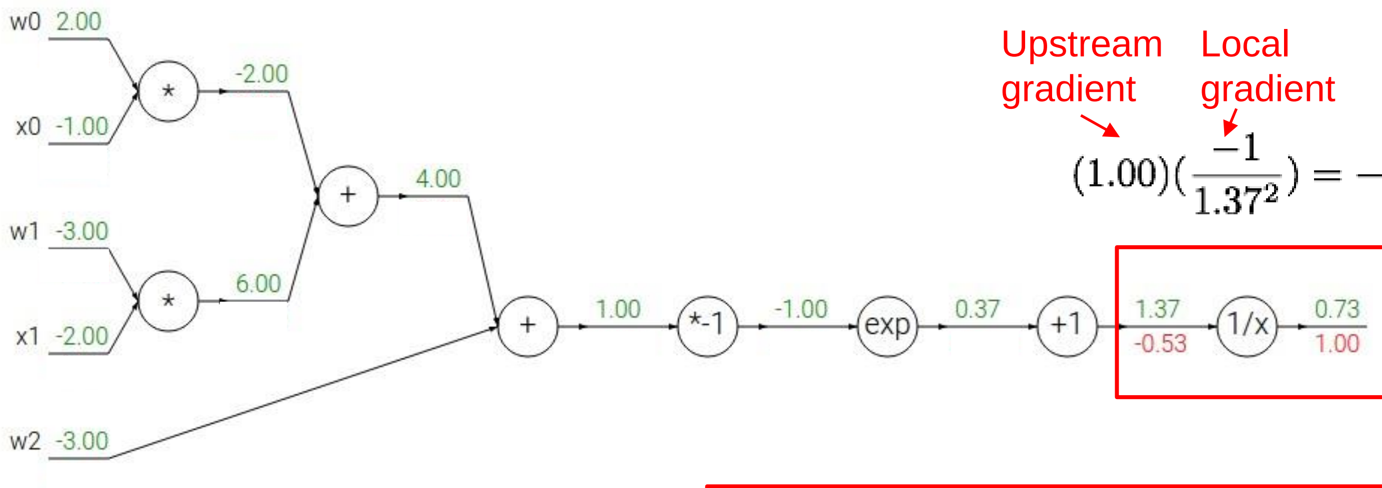
Example:

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

Upstream gradient   Local gradient

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



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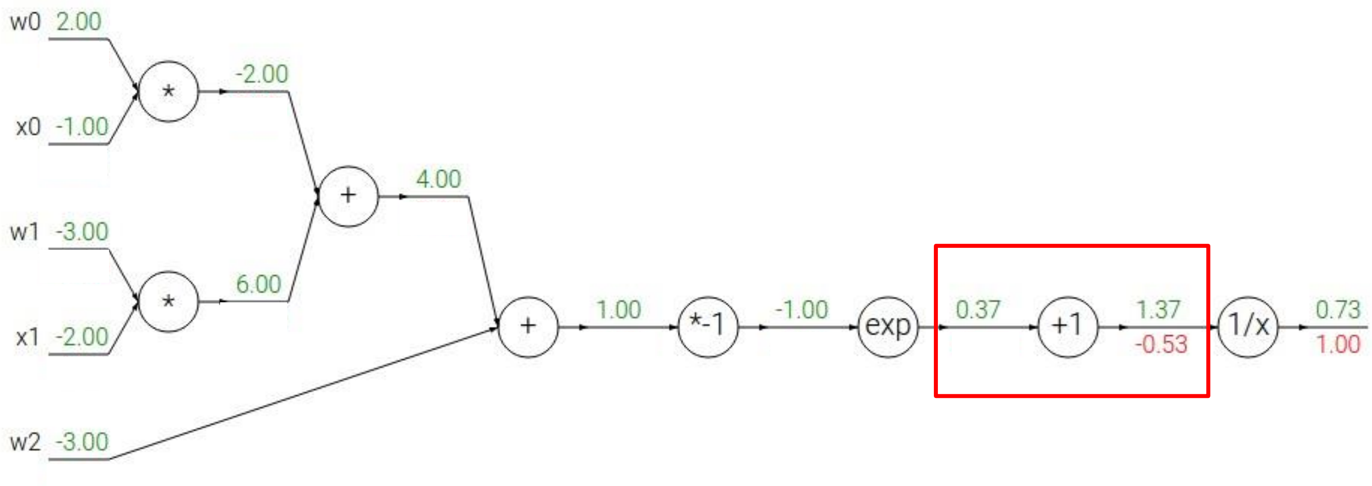

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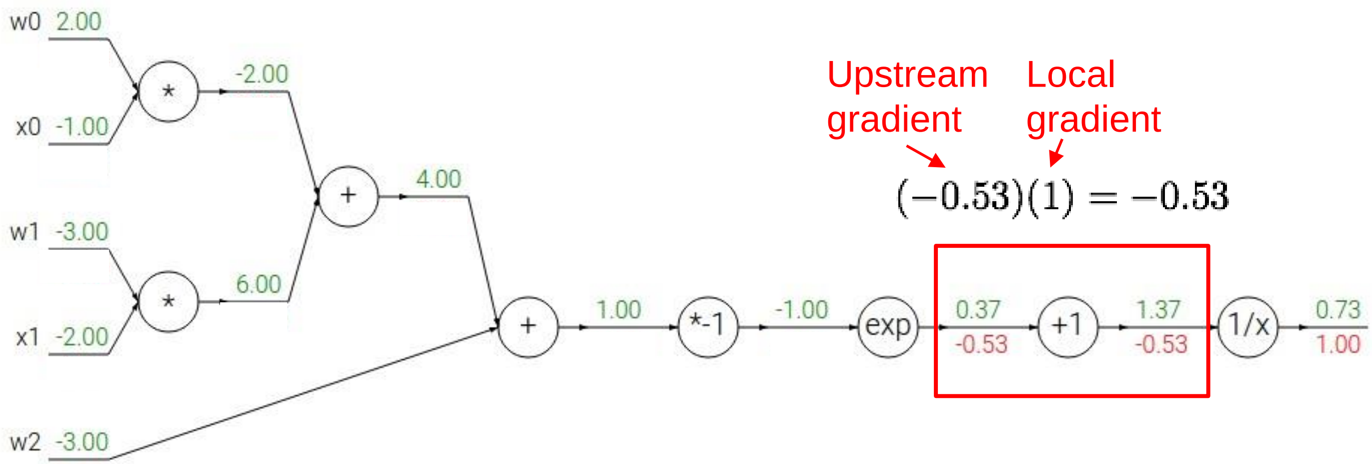

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Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

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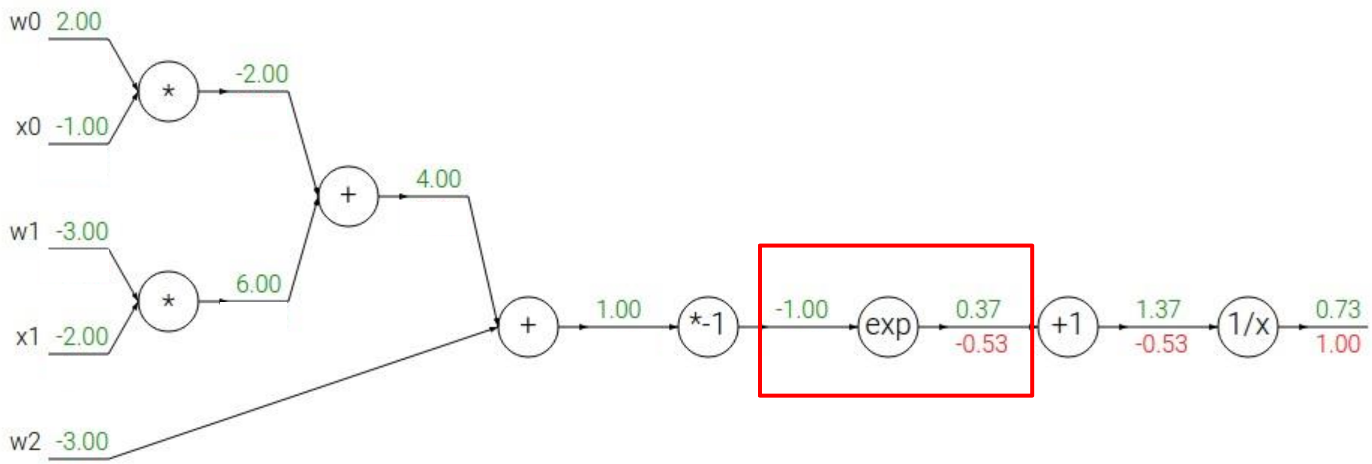

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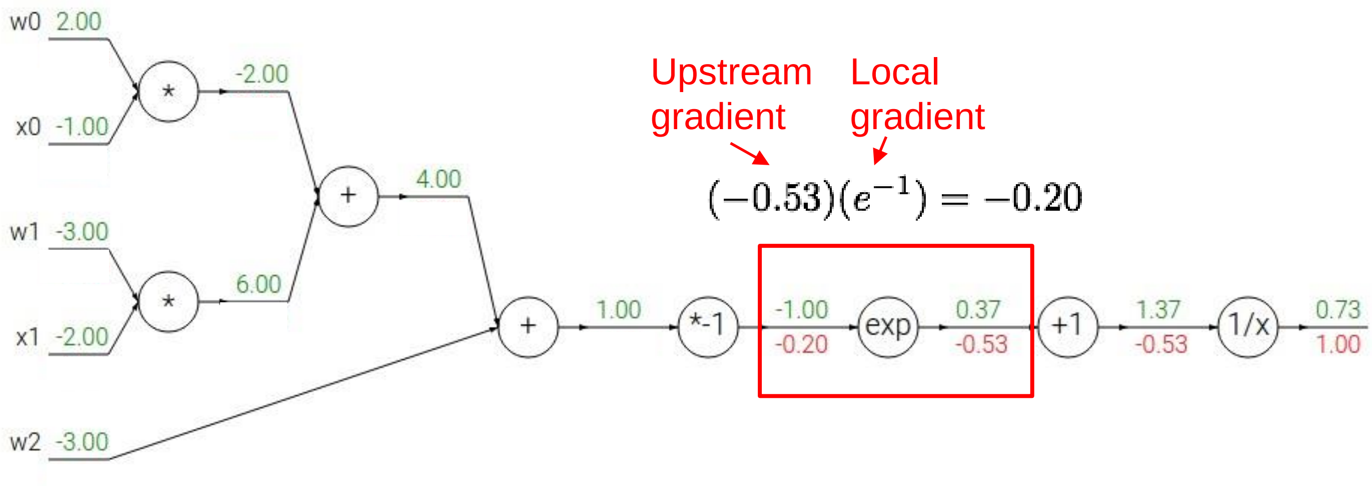

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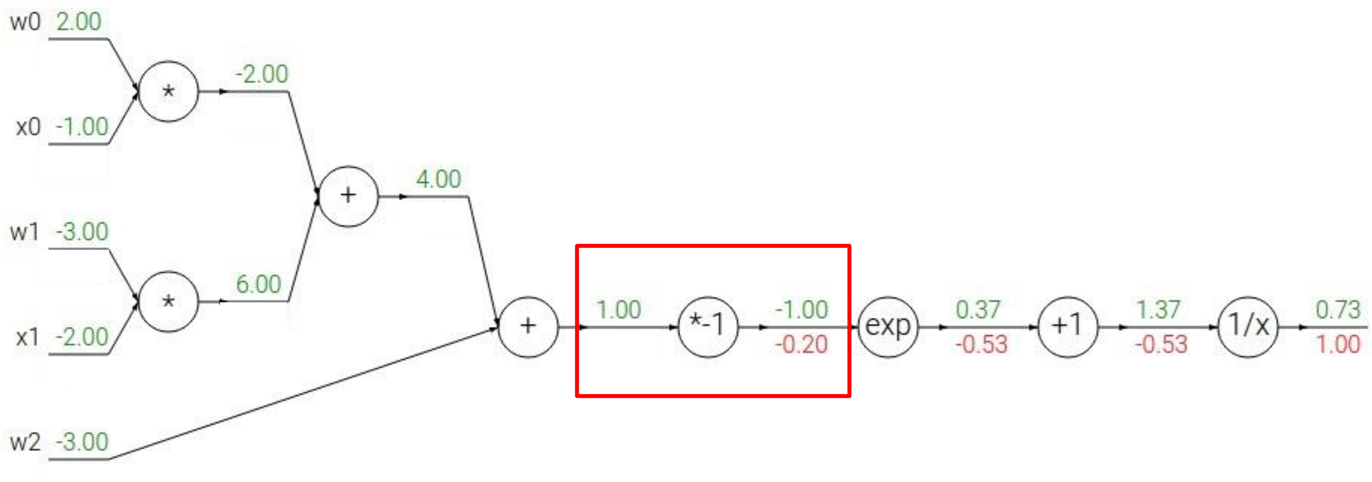

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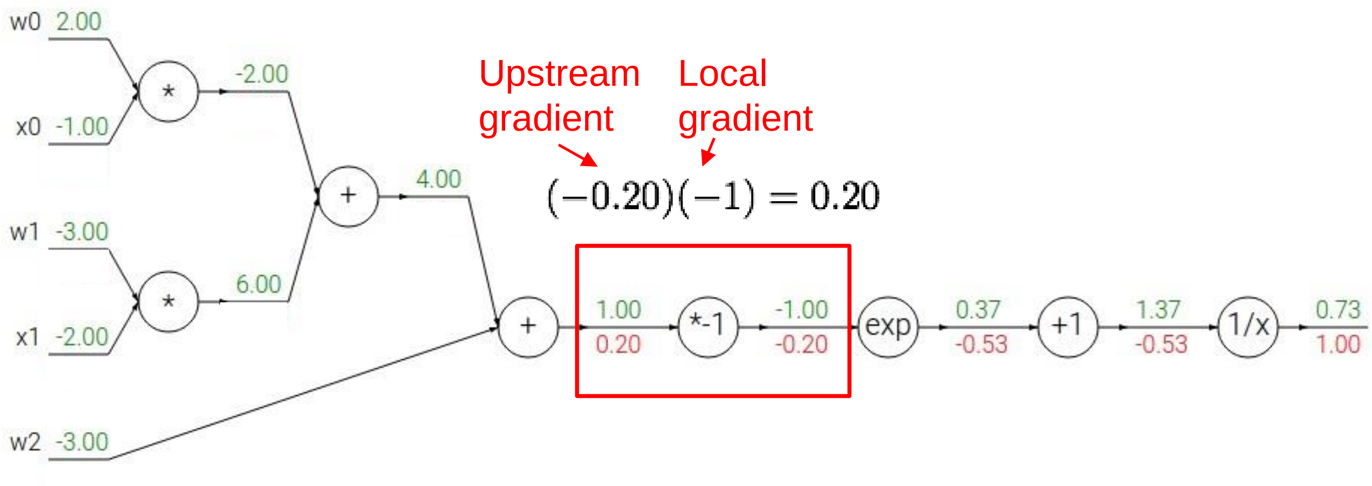

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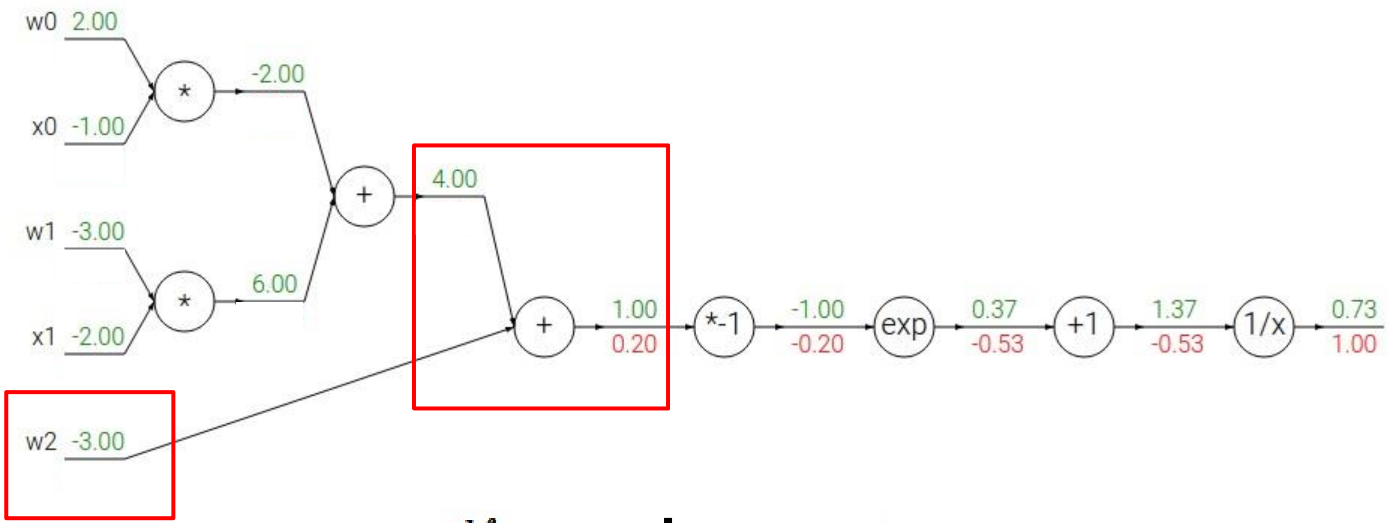

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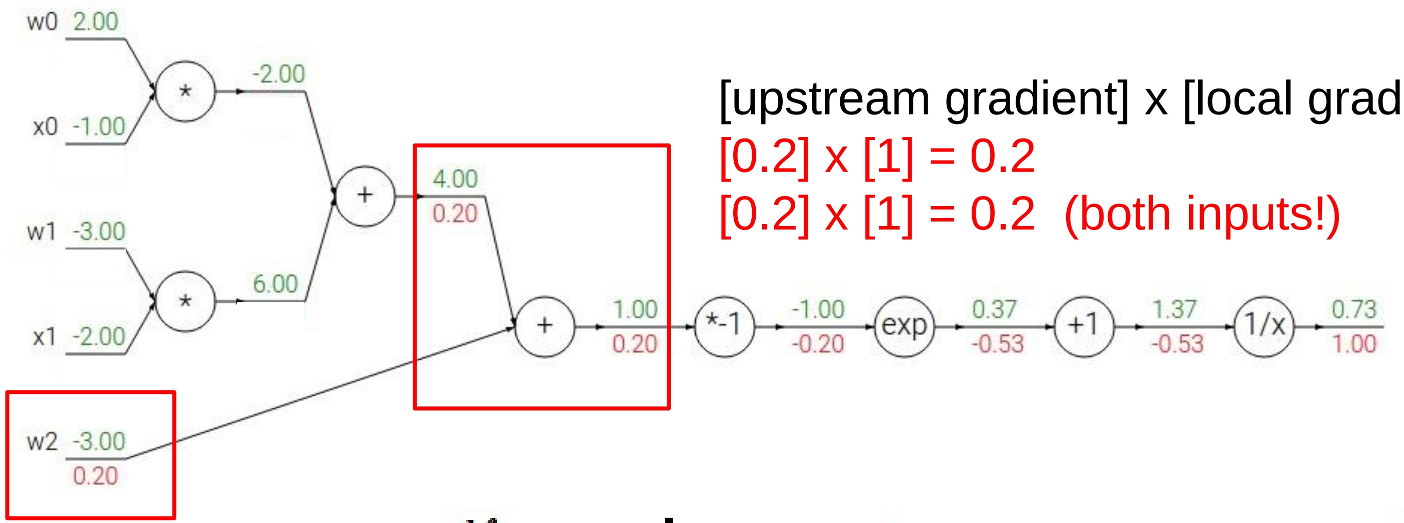

[upstream gradient] x [local gradient]

[0.2] x [1] = 0.2

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

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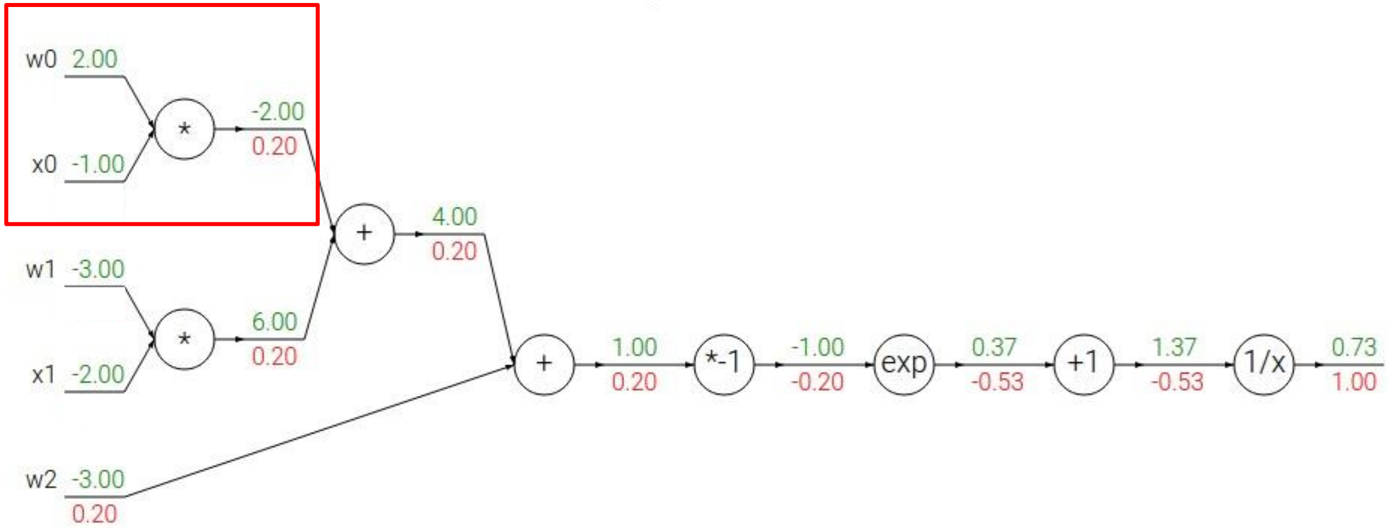

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x \qquad\qquad f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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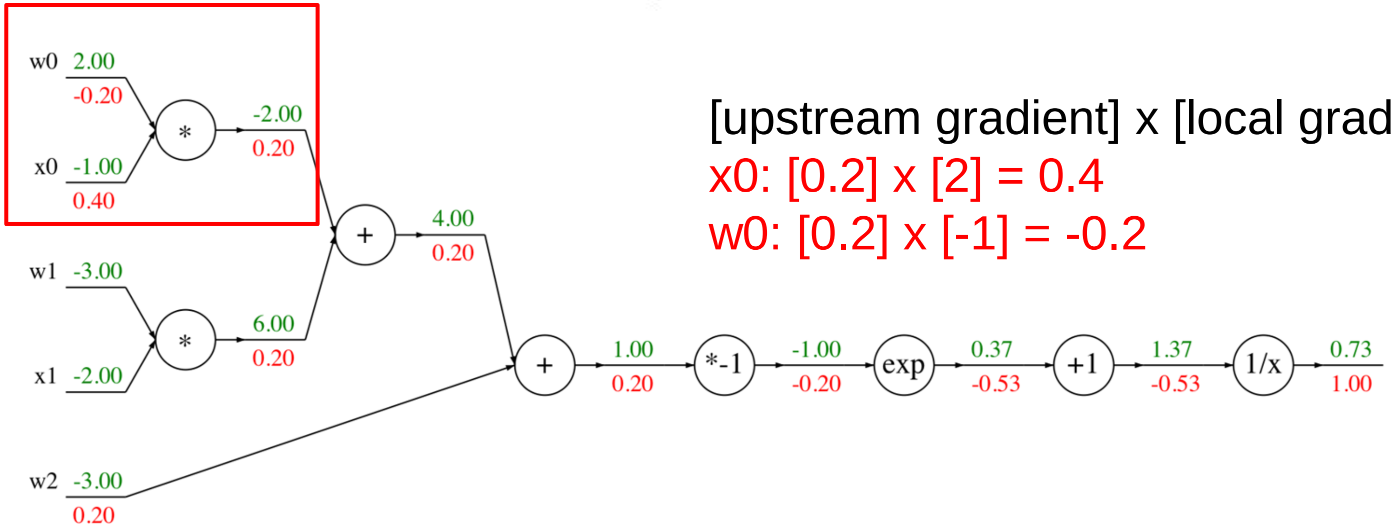


[upstream gradient] x [local gradient]

x0: [0.2] x [2] = 0.4

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

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

Example:

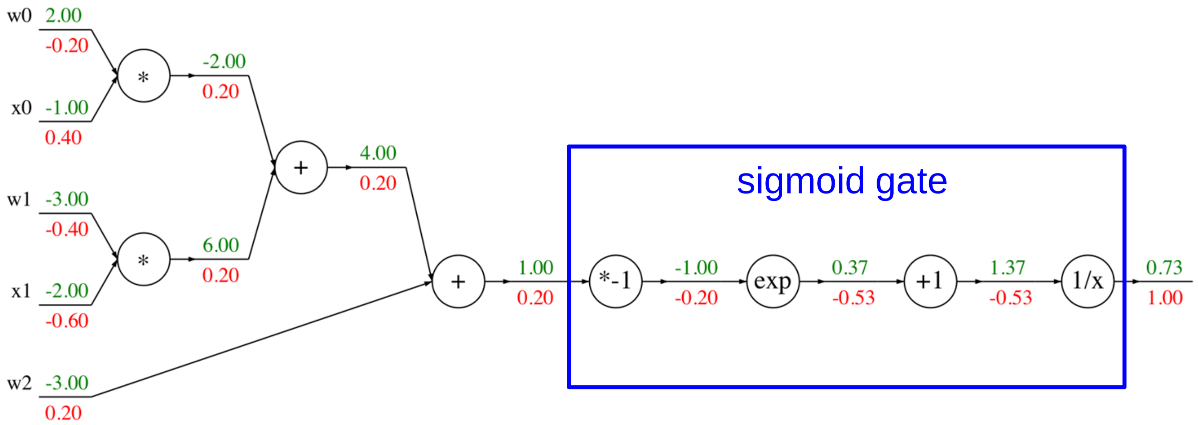
$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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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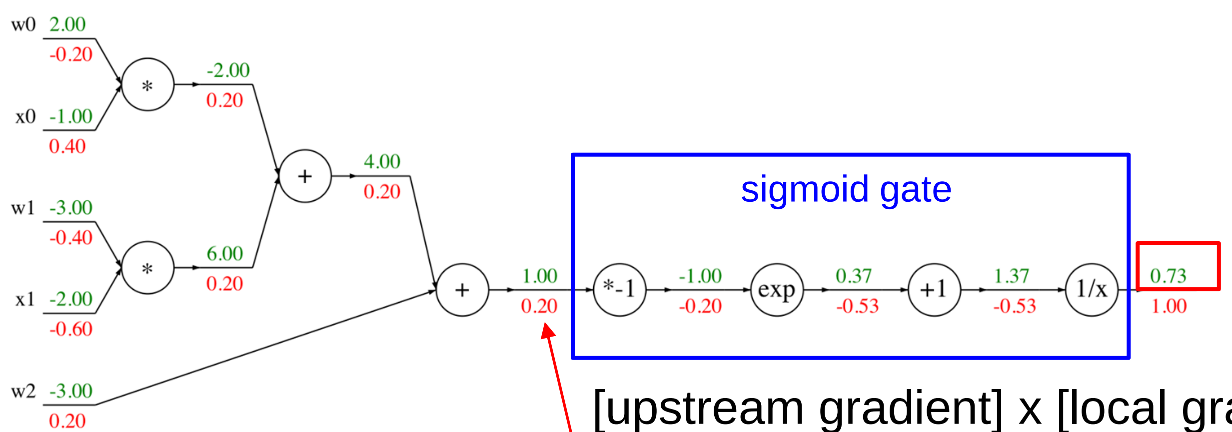
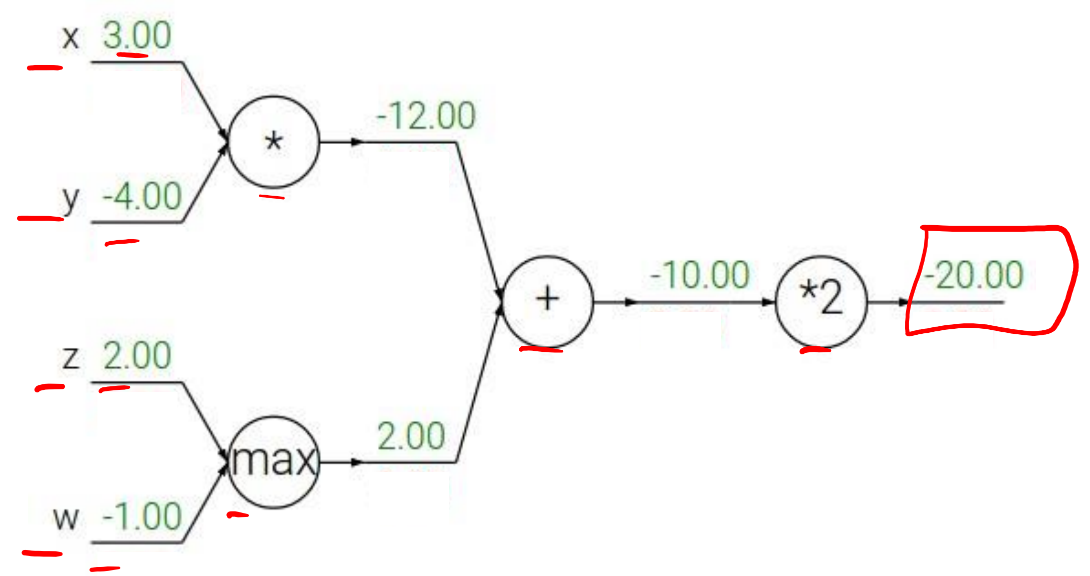


[upstream gradient] x [local gradient]

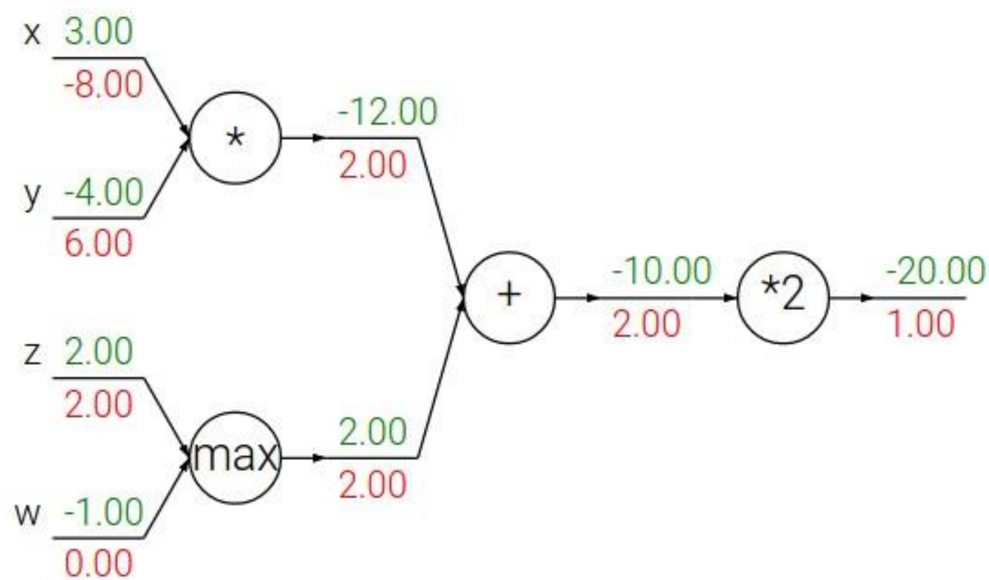
[1.00] x [(1 - 0.73) (0.73)]= 0.2

Patterns in backward flow

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

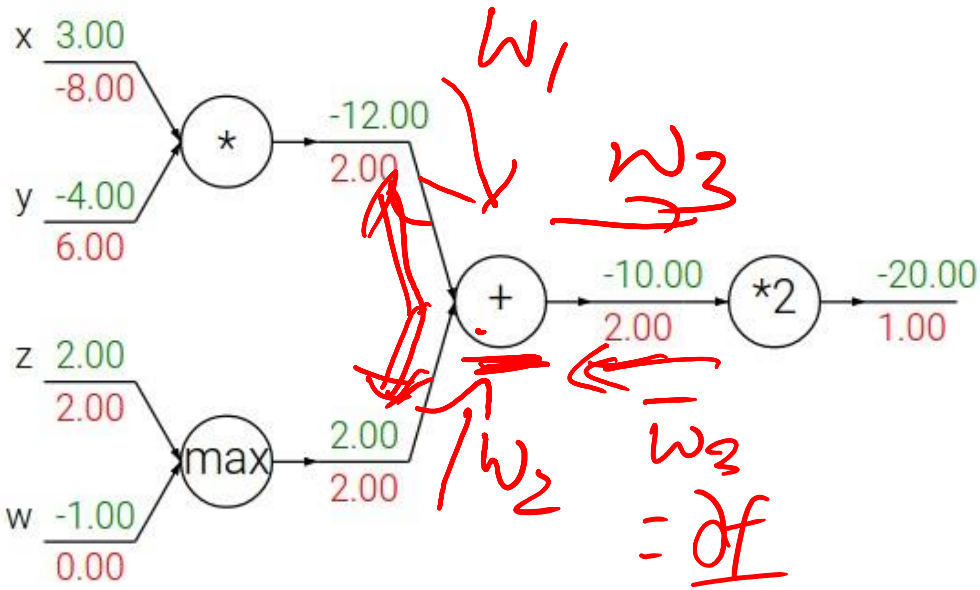


Patterns in backward flow



Patterns in backward flow

add gate: gradient distributor



$$\bar{w}_3 = \frac{\partial f}{\partial w_3}$$

$$w_3 = w_1 + w_2$$

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

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

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

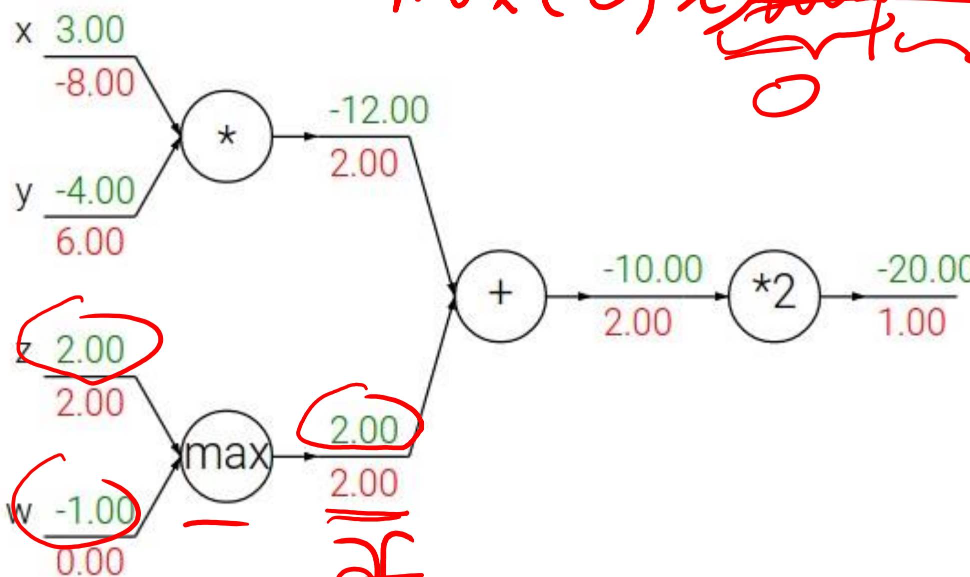
Patterns in backward flow

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

$\max(0, x)$

add gate: gradient distributor

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



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

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

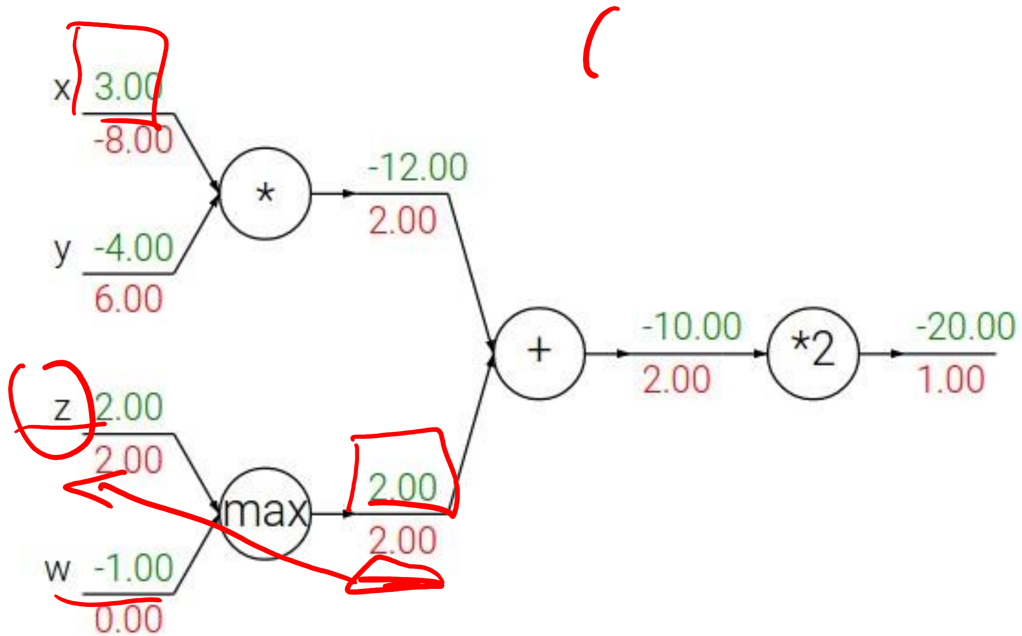
$\frac{\partial f}{\partial w_2}$

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

Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

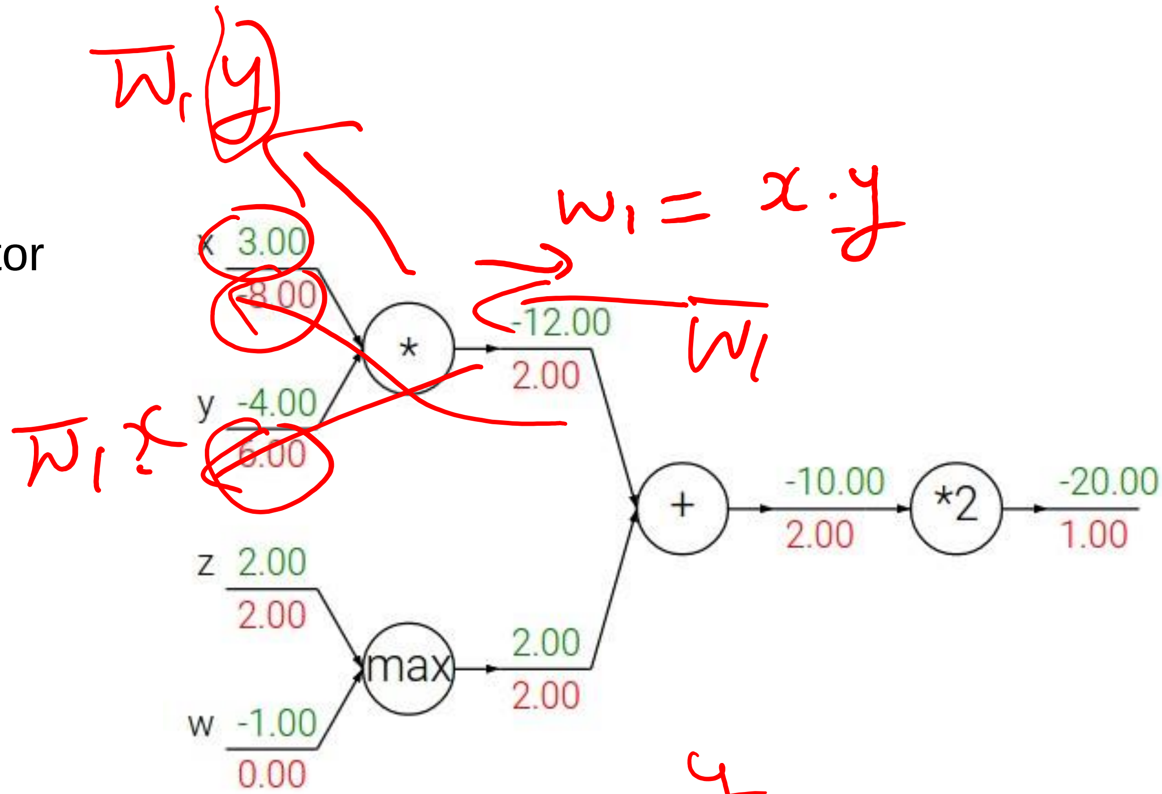


Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

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



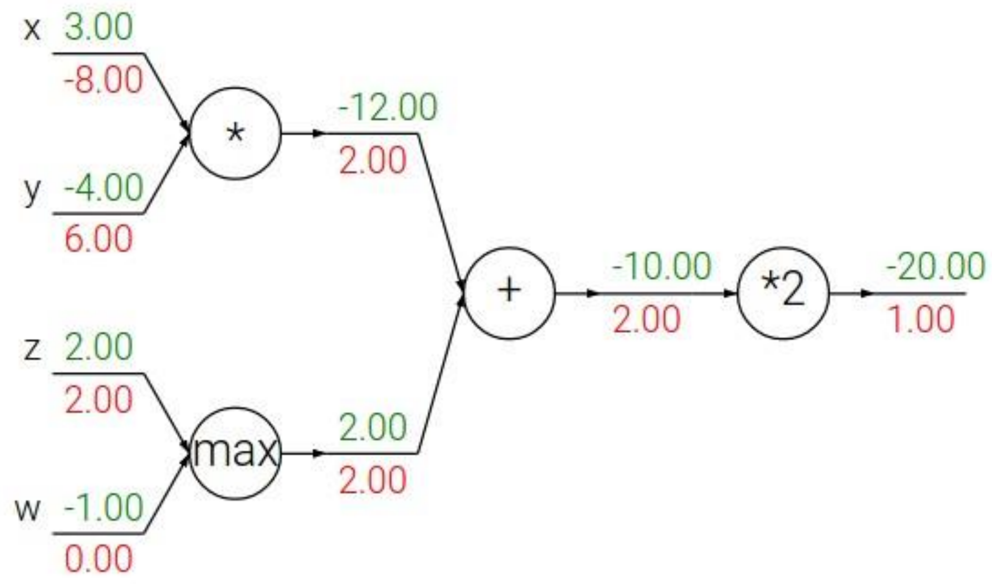
$$\frac{\partial f}{\partial x} = \boxed{\frac{\partial f}{\partial w_1}} \overbrace{\boxed{\frac{\partial w_1}{\partial x}}}^{y}$$

Patterns in backward flow

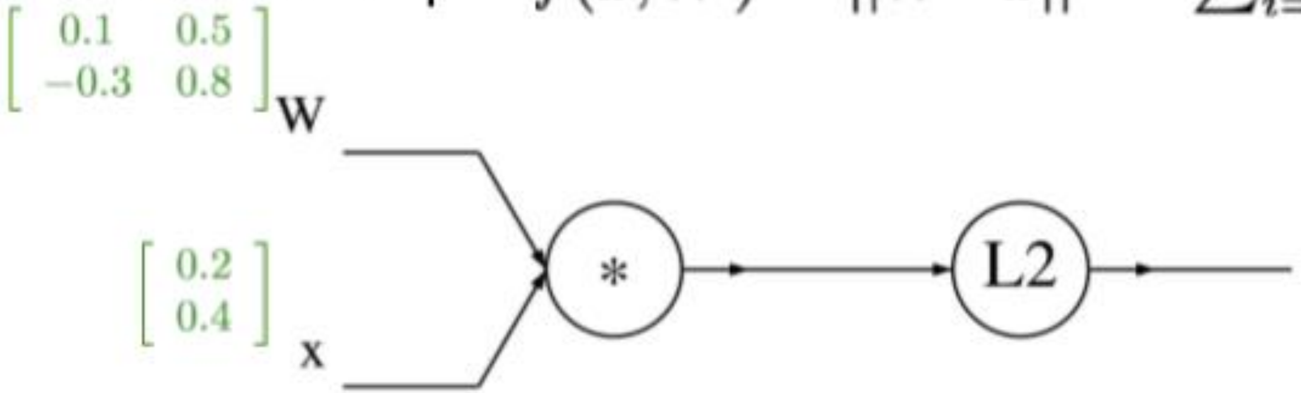
add gate: gradient distributor

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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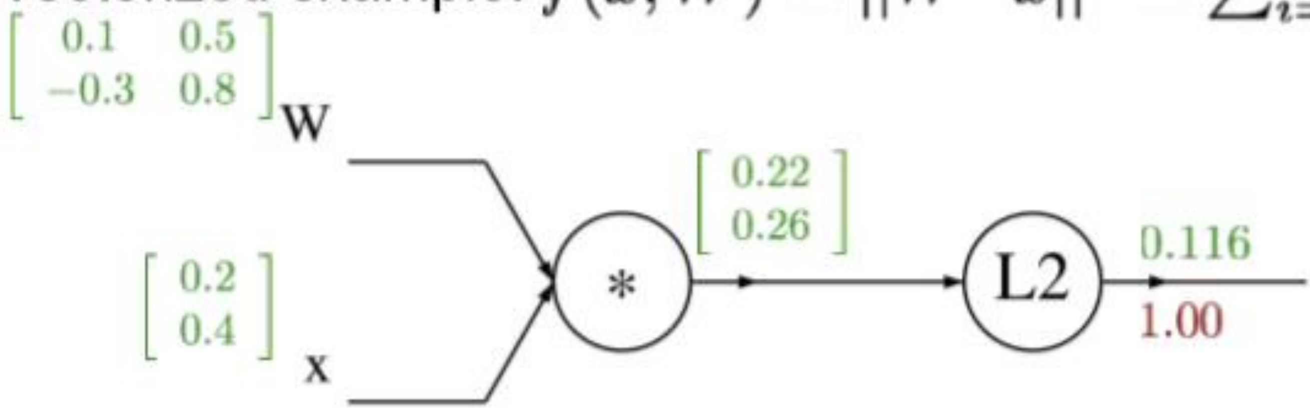

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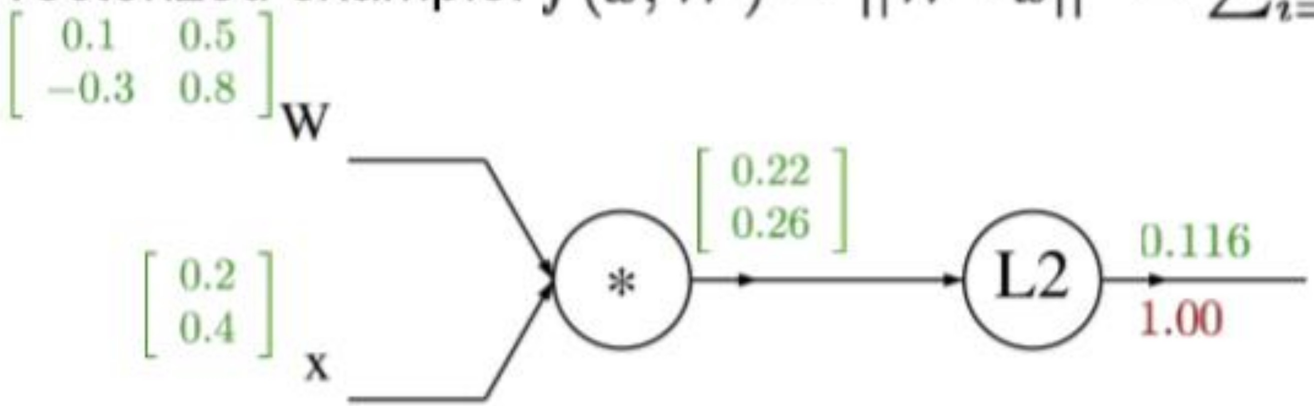

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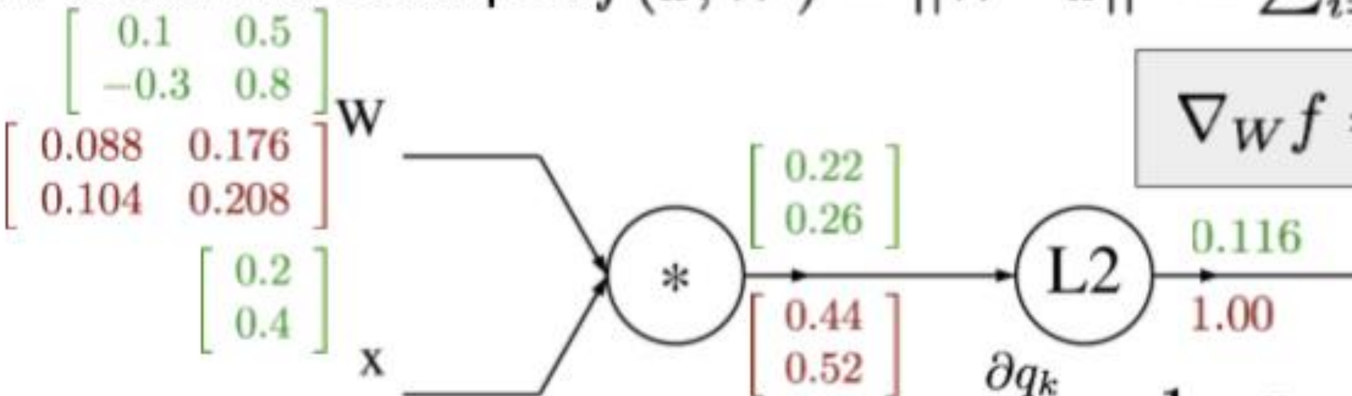
$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

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

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

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



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

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

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

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

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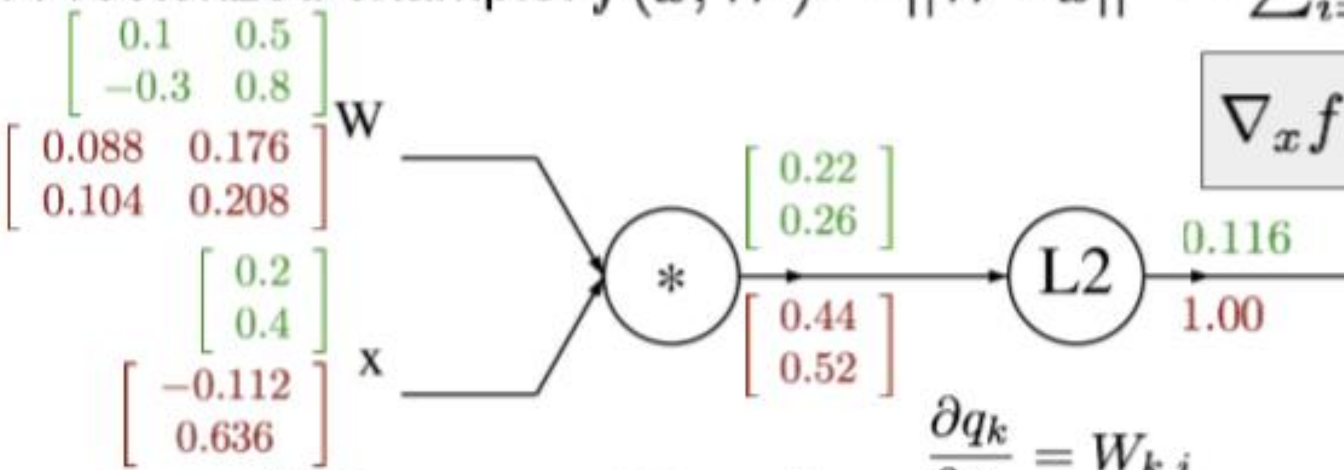

$$\boxed{\nabla_x f = 2W^T \cdot q}$$

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

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

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

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

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

Summary

- We have learned computational graphs and gradient computation methods
- How to apply computational graphs to calculate the gradient during back-propagation
- Notations & examples

- What is next ?
  - Linear classifiers
  - Loss functions : Hinge loss
  - Softmax Classifier (Multinomial Logistic Regression)