Backpropagation

Saurabh Gupta

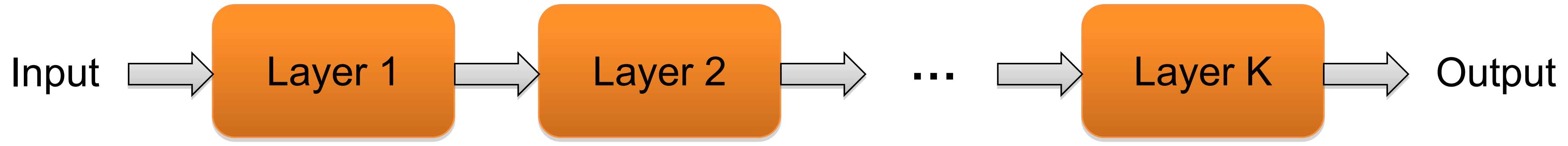
Many slides from Lana Lazebnik

Overview

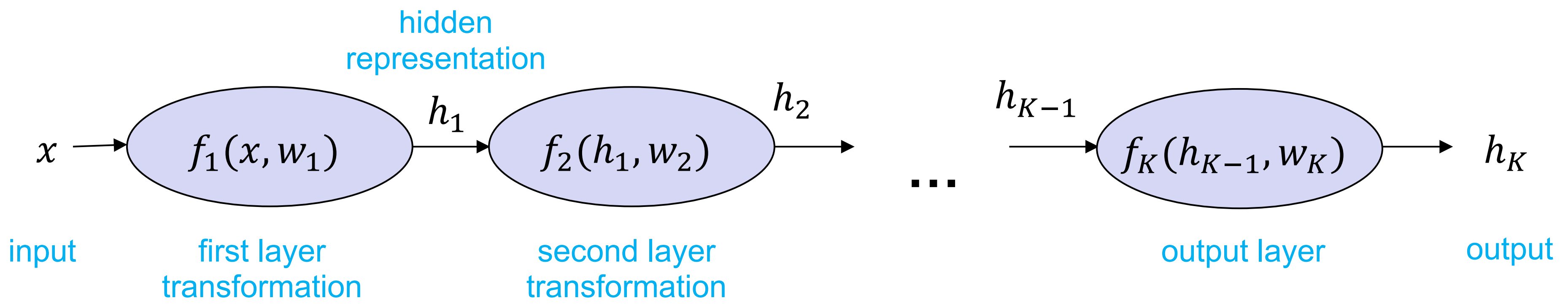
- Computation graphs
- Using the chain rule
- General backpropagation algorithm
- Toy examples of backward pass
- Matrix-vector calculations: ReLU, linear layer

Recall: Multi-layer neural networks

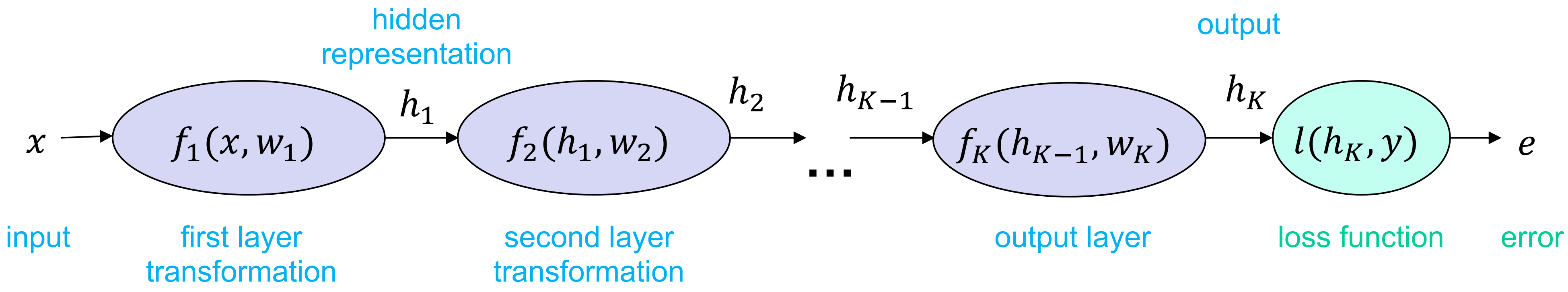
- The function computed by the network is a composition of the functions computed by individual layers (e.g., linear layers and nonlinearities):



- More precisely:



Training a multi-layer network

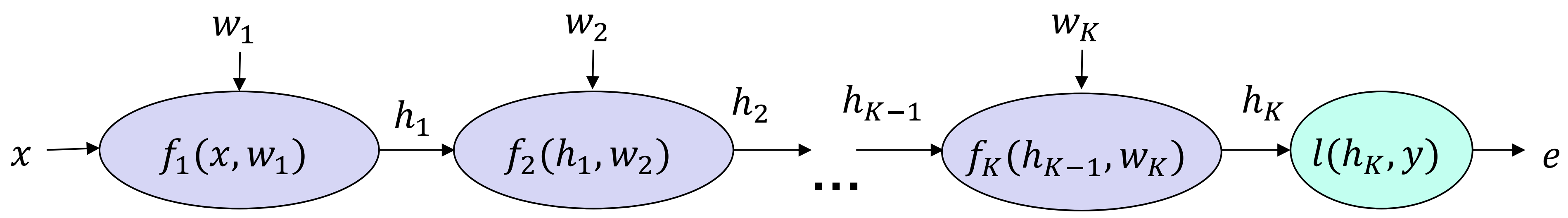


- What is the SGD update for the parameters w_k of the kth layer?

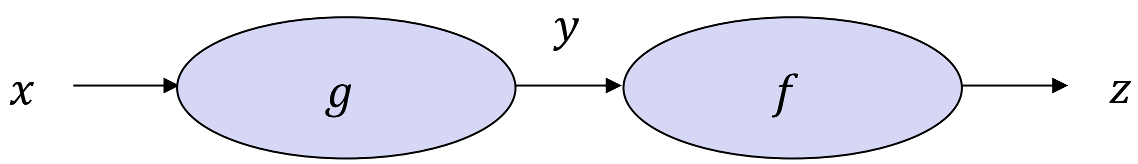
$$w_k \leftarrow w_k - \eta \frac{\partial e}{\partial w_k}$$

- To train the network, we need to find the gradient of the error w.r.t. the parameters of each layer, $\frac{\partial e}{\partial w_k}$

Computation graph



The chain rule



$$\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$$

In calculus, the **chain rule** is a formula that expresses the derivative of the composition of two differentiable functions f and g in terms of the derivatives of f and g. More precisely, if $h = f \circ g$ is the function such that $h(x) = f(g(x))$ for every x, then the chain rule is, in Lagrange's notation,

$$h'(x) = f'(g(x))g'(x).$$

or, equivalently,

$$h' = (f \circ g)' = (f' \circ g) \cdot g'.$$

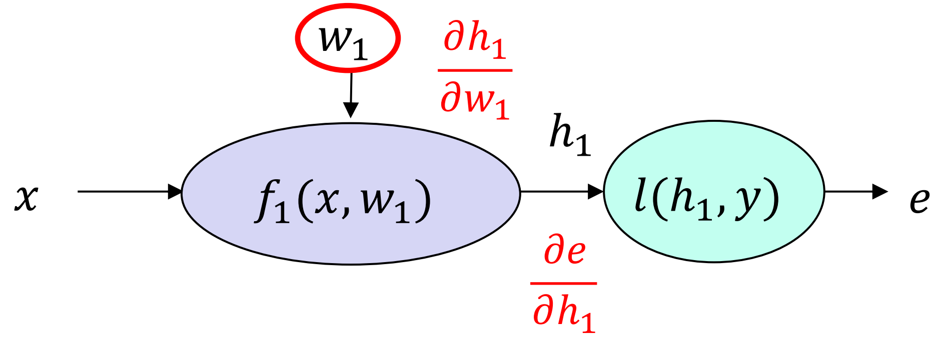
The chain rule may also be expressed in Leibniz's notation. If a variable z depends on the variable y, which itself depends on the variable x (that is, y and z are dependent variables), then z depends on x as well, via the intermediate variable y. In this case, the chain rule is expressed as

$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}$$

https://en.wikipedia.org/wiki/Chain_rule

Applying the chain rule

Let's start with $k = 1$



$e = l(f_1(x, w_1), y)$

Example: $e = (y - w_1^T x)^2$

$h_1 = f_1(x, w_1) = w_1^T x$

$e = l(h_1, y) = (y - h_1)^2$

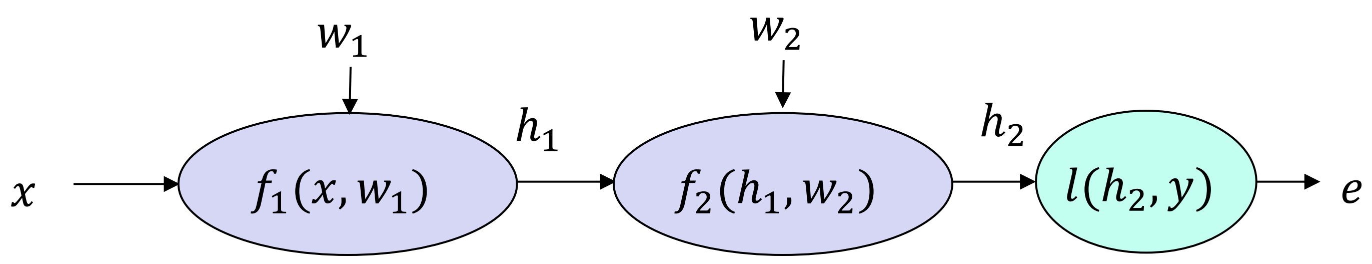
$\frac{\partial h_1}{\partial w_1} =$

$\frac{\partial e}{\partial h_1} =$

$$\frac{\partial e}{\partial w_1} =$$

Applying the chain rule

$k = 2$



$$e = l(f_2(f_1(x, w_1), w_2))$$

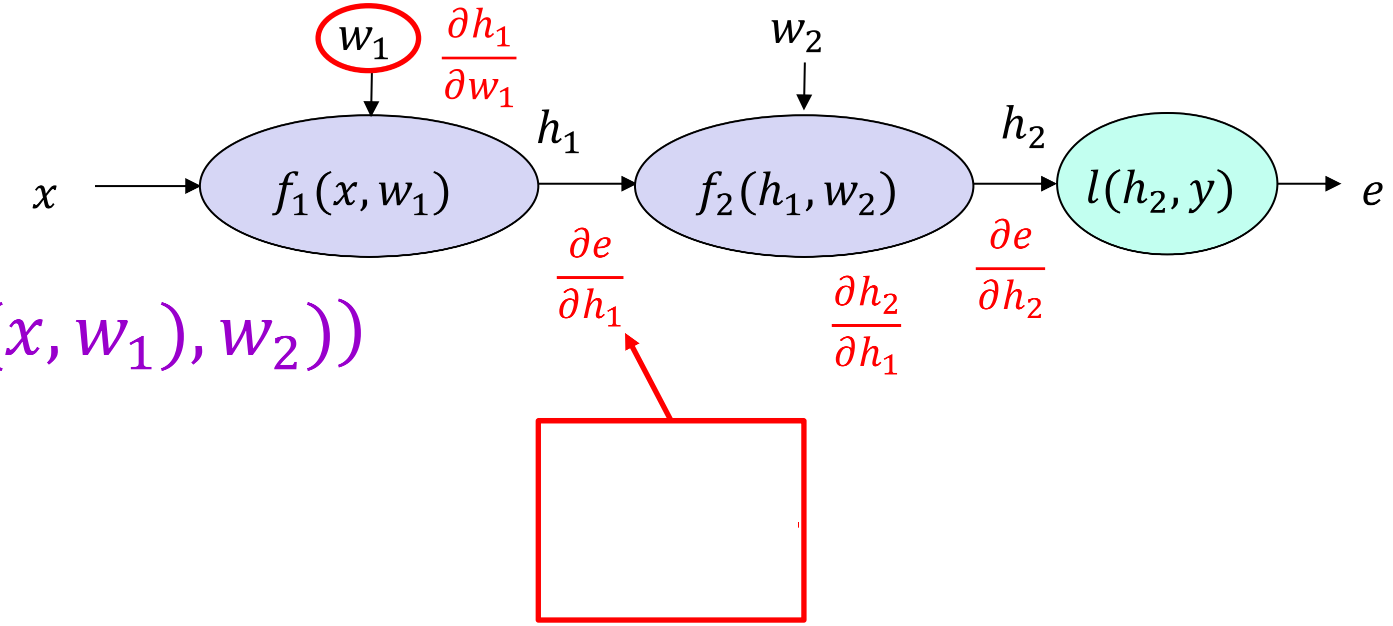
Example: $e = -\log\left(\sigma(w_1^T x)\right)$ (assume $y = 1$)

$$h_1 = f_1(x, w_1) = w_1^T x$$
$$h_2 = f_2(h_1) = \sigma(h_1)$$
$$e = l(h_2, 1) = -\log(h_2)$$

Applying the chain rule

$k = 2$

$e = l(f_2(f_1(x, w_1), w_2))$



Example: $e = -\log\left(\sigma(w_1^T x)\right)$ (assume $y = 1$)

$h_1 = f_1(x, w_1) = w_1^T x$

$h_2 = f_2(h_1) = \sigma(h_1)$

$e = l(h_2, 1) = -\log(h_2)$

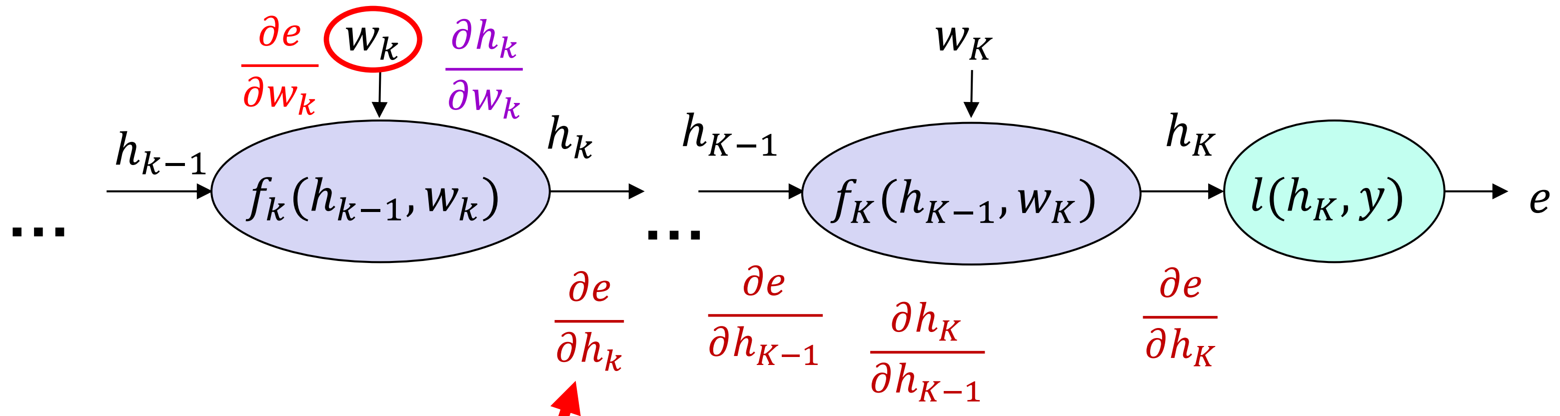
$\frac{\partial h_1}{\partial w_1} =$

$\frac{\partial h_2}{\partial h_1} =$

$\frac{\partial e}{\partial h_2} =$

$\frac{\partial e}{\partial w_1} = \frac{\partial e}{\partial h_2} \frac{\partial h_2}{\partial h_1} \frac{\partial h_1}{\partial w_1} =$

Chain rule: General case

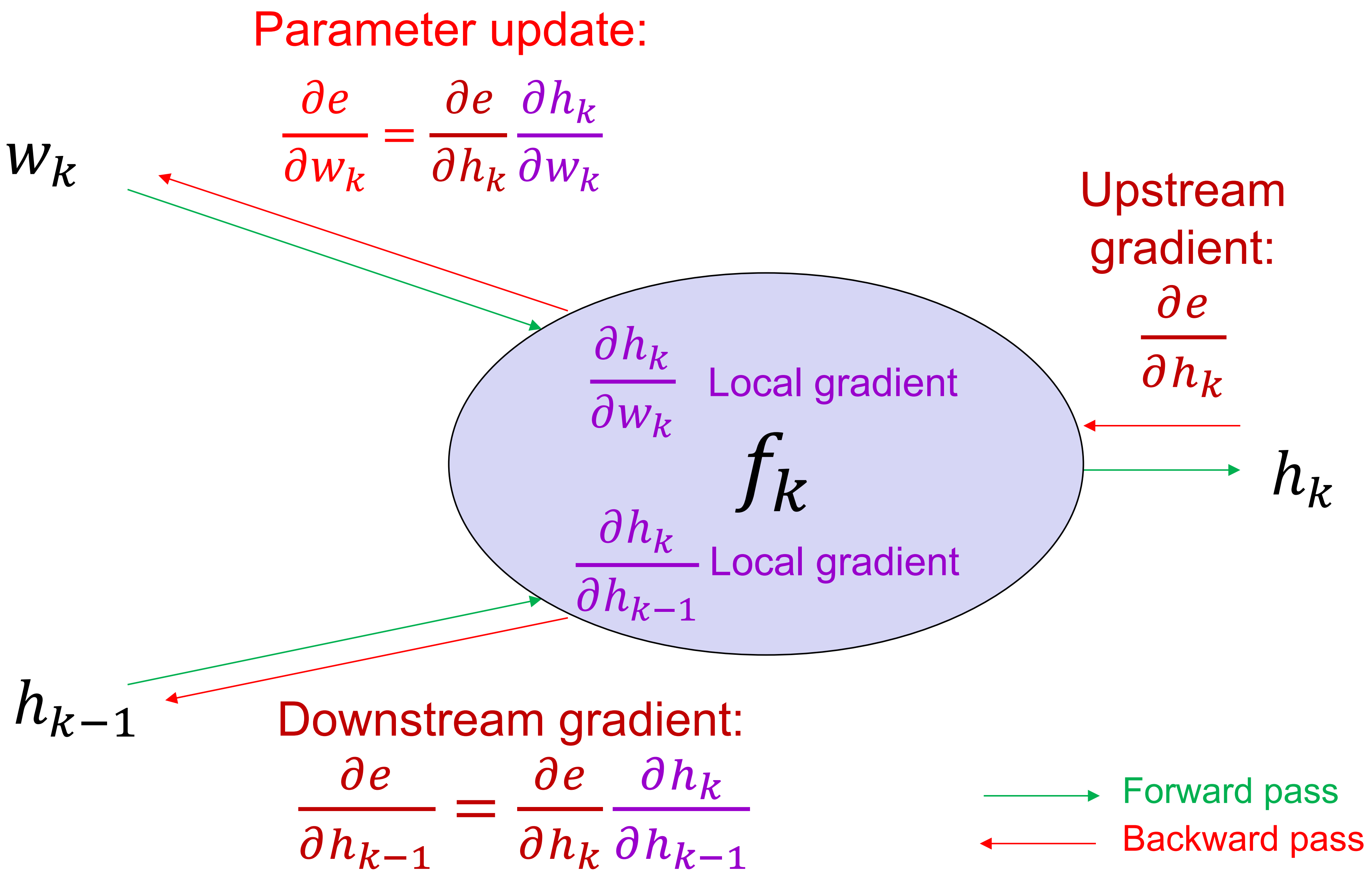


$$\frac{\partial e}{\partial w_k} = \boxed{\frac{\partial e}{\partial h_K} \frac{\partial h_K}{\partial h_{K-1}} \cdots \frac{\partial h_{k+1}}{\partial h_k}} \frac{\partial h_k}{\partial w_k}$$

Upstream gradient $\frac{\partial e}{\partial h_k}$

Local gradient

Backpropagation summary



What about more general computation graphs?

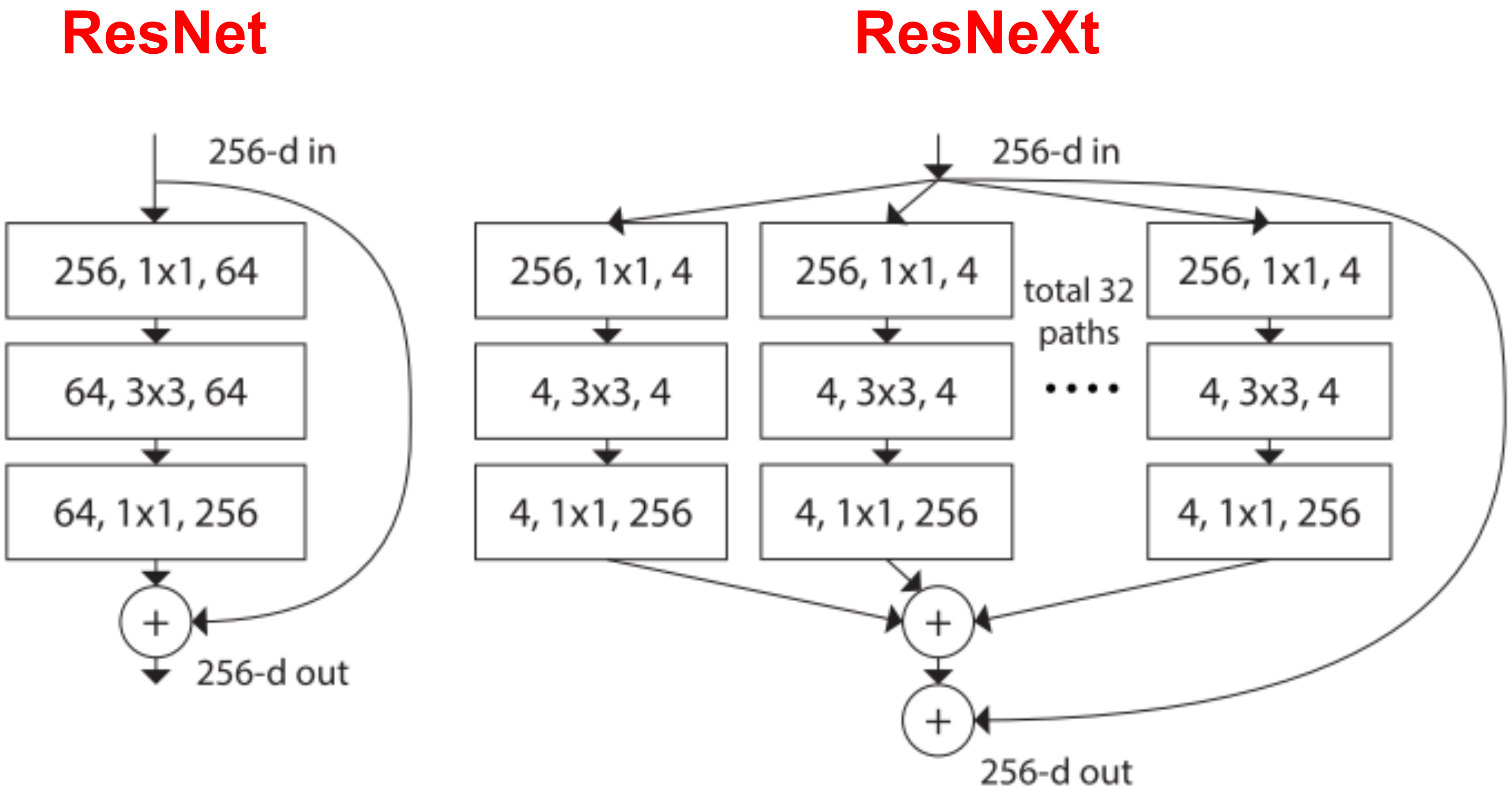
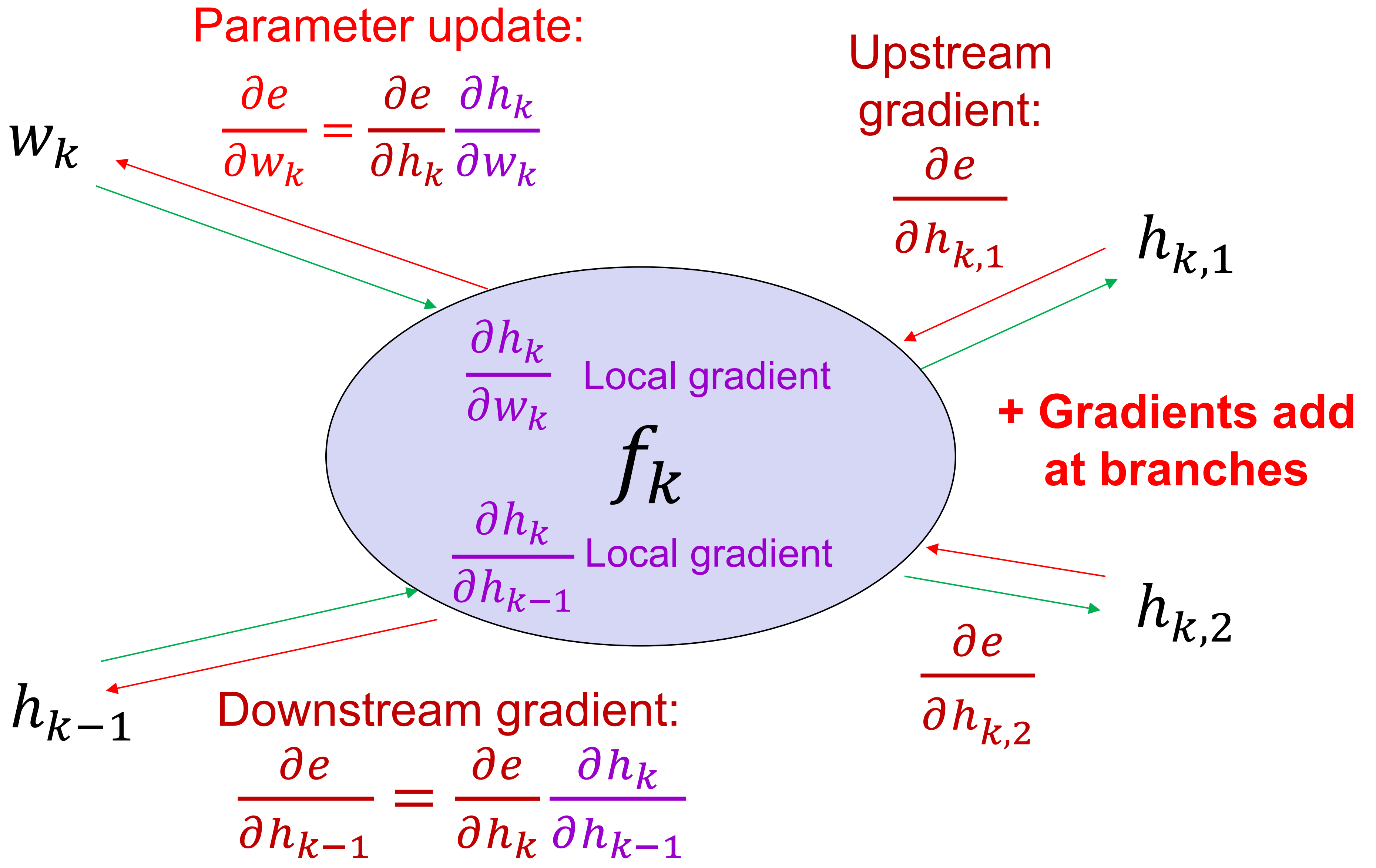


Figure source

What about more general computation graphs?

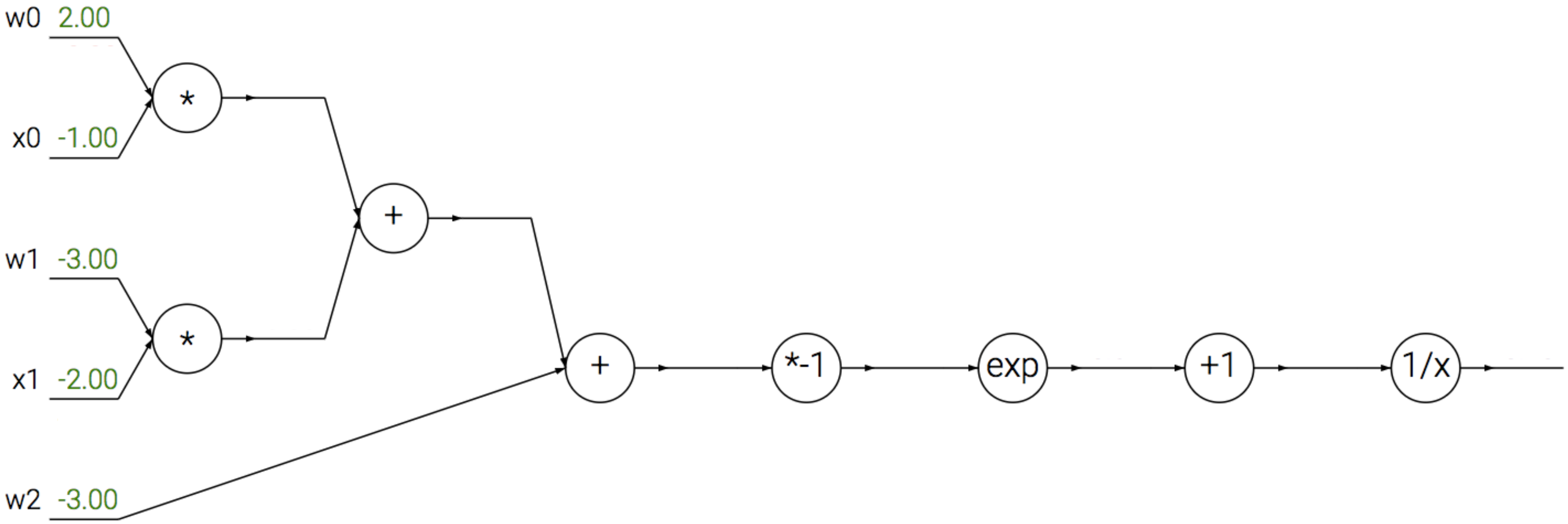


Overview

- Computation graphs
- Using the chain rule
- General backprop algorithm
- Toy examples of backward pass

A detailed example

$$f(x, w) = \frac{1}{1 + \exp[-(w^{(0)}x^{(0)} + w^{(1)}x^{(1)} + w^{(2)})]}$$



Source: [Stanford 231n]()

A detailed example

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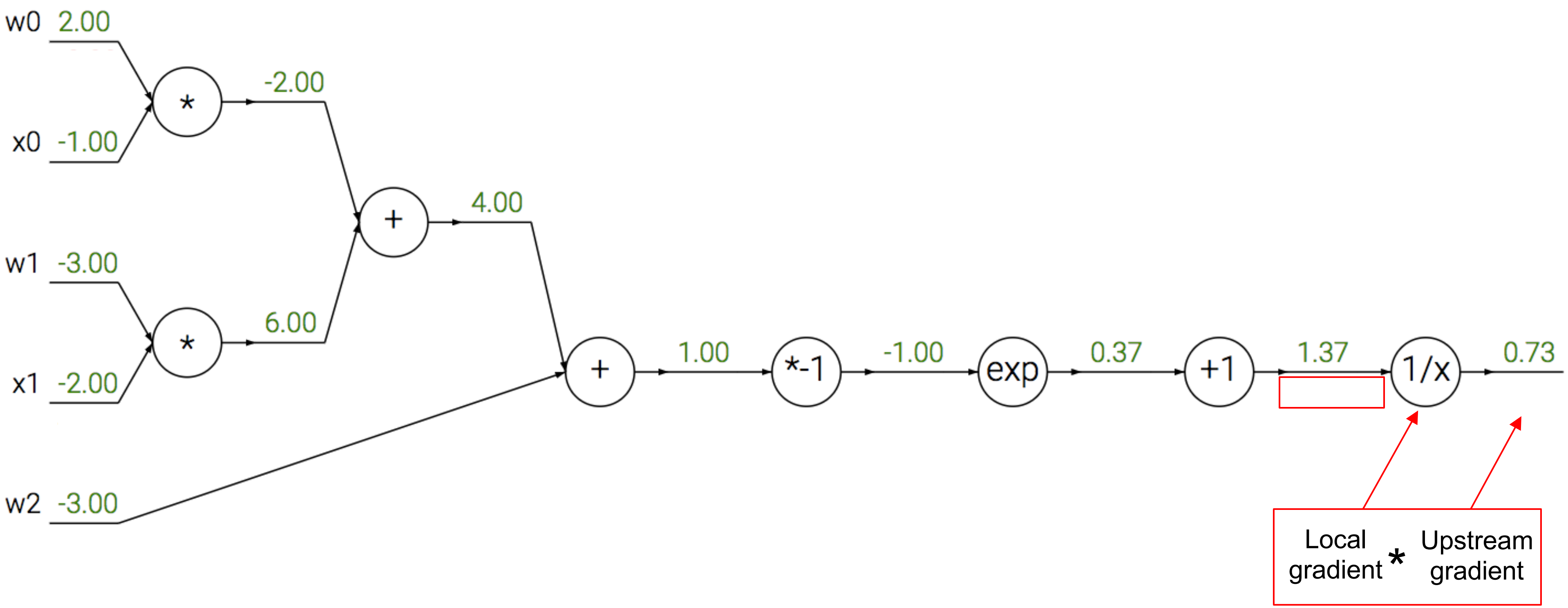


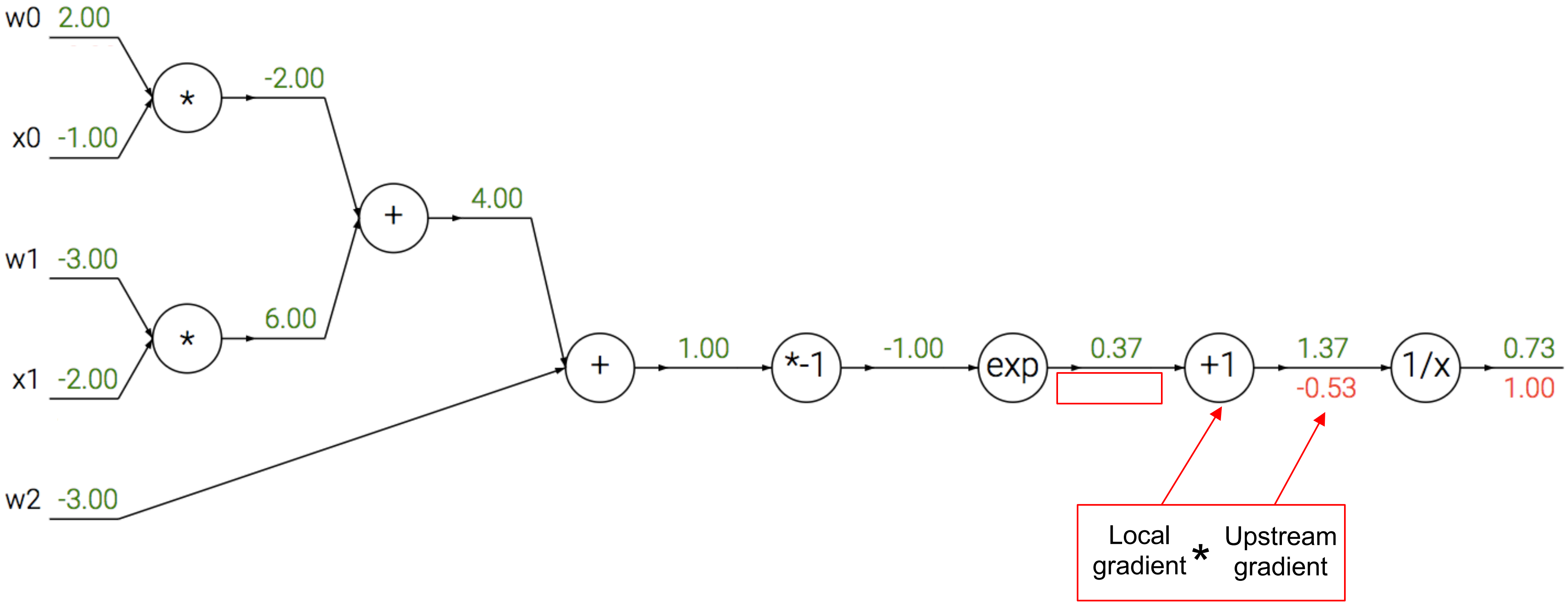
$$(1/x)' = -1/x^2$$

$$-\frac{1}{1.37^2} * 1 = -0.53$$

Source: [Stanford 231n]

A detailed example

$$f(x,w) = \frac{1}{1 + \exp[-(w^{(0)}x^{(0)} + w^{(1)}x^{(1)} + w^{(2)})]}$$



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A detailed example

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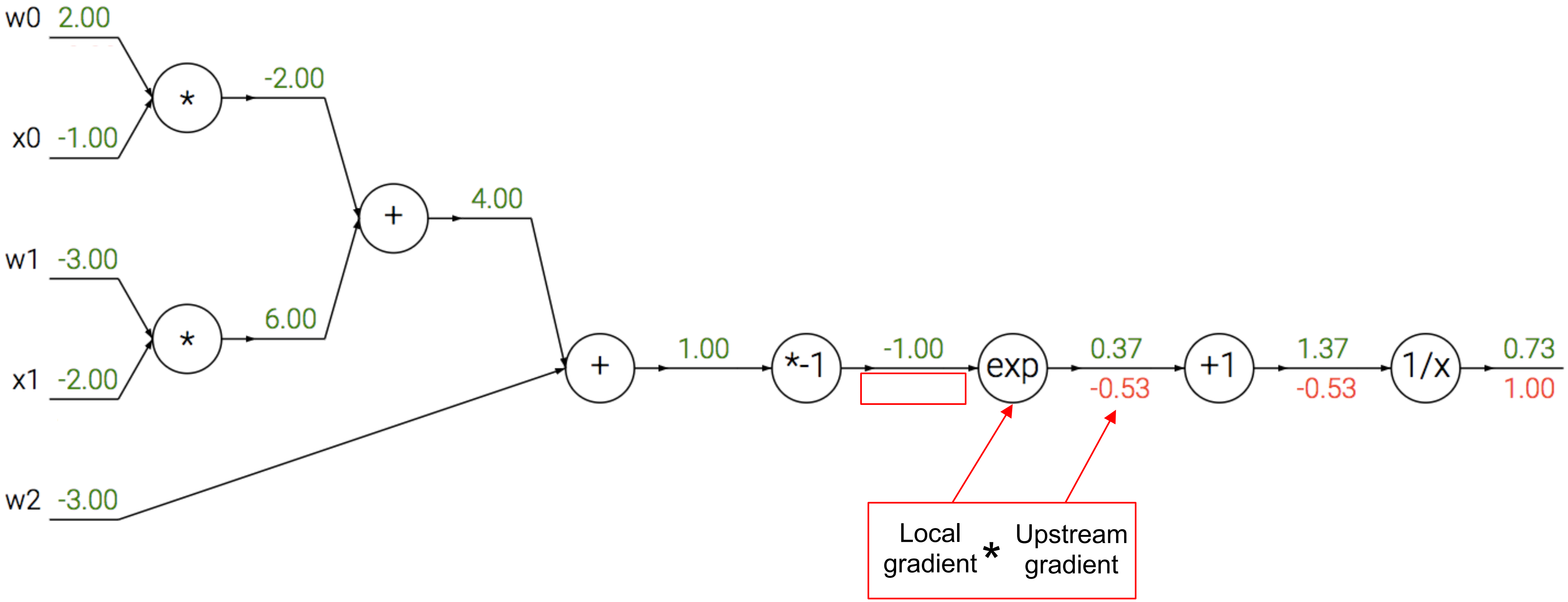

$$\exp(-1) * (-0.53) = -0.20$$

Source: [Stanford 231n]()

A detailed example

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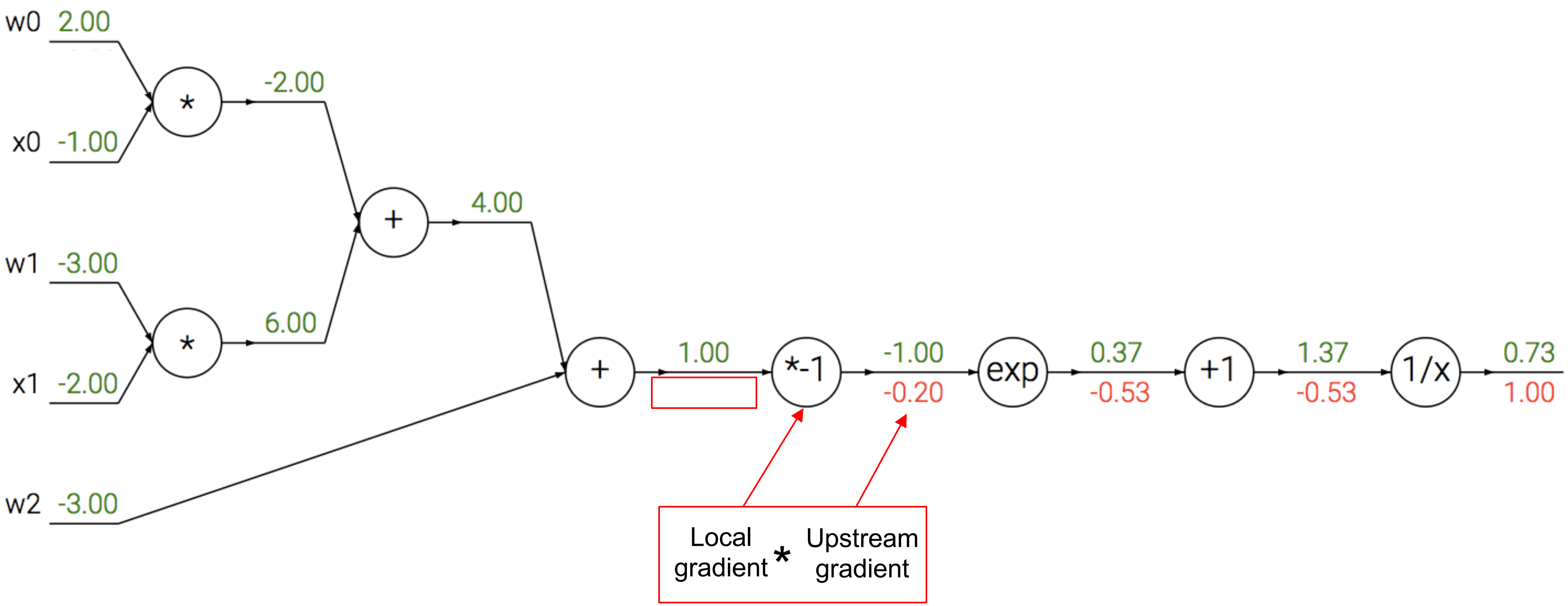

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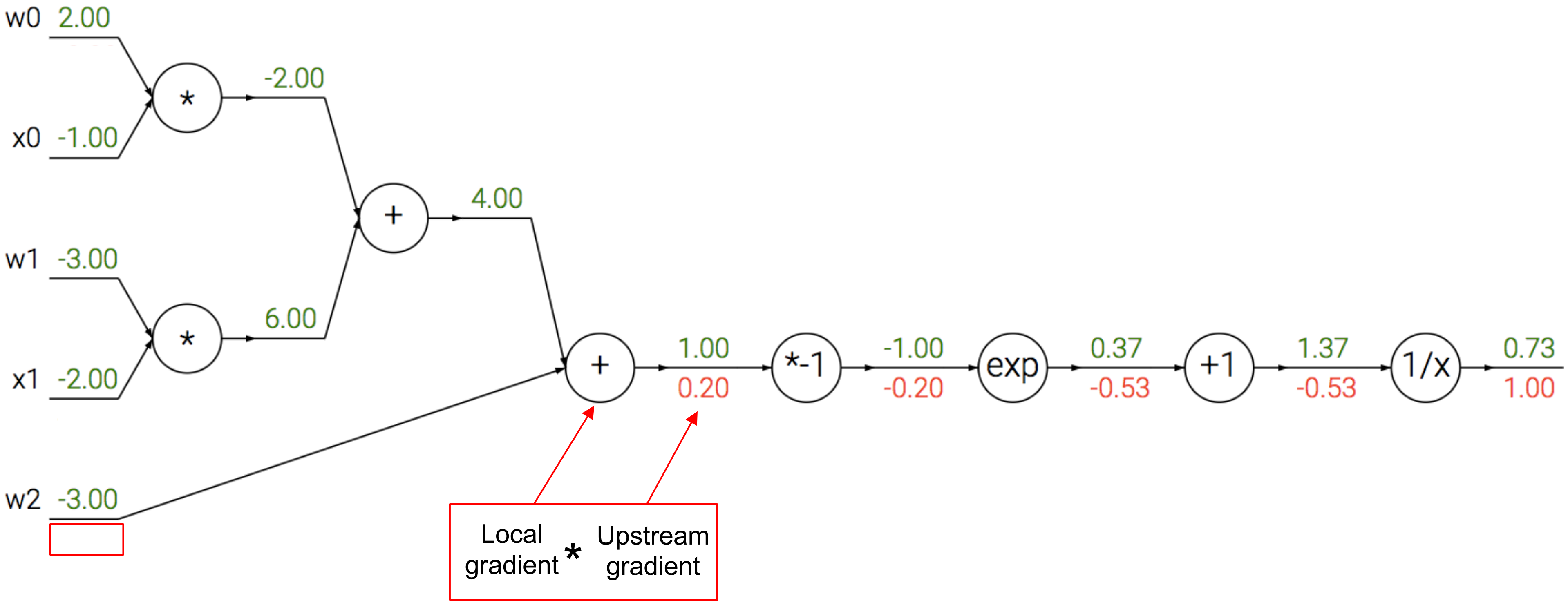

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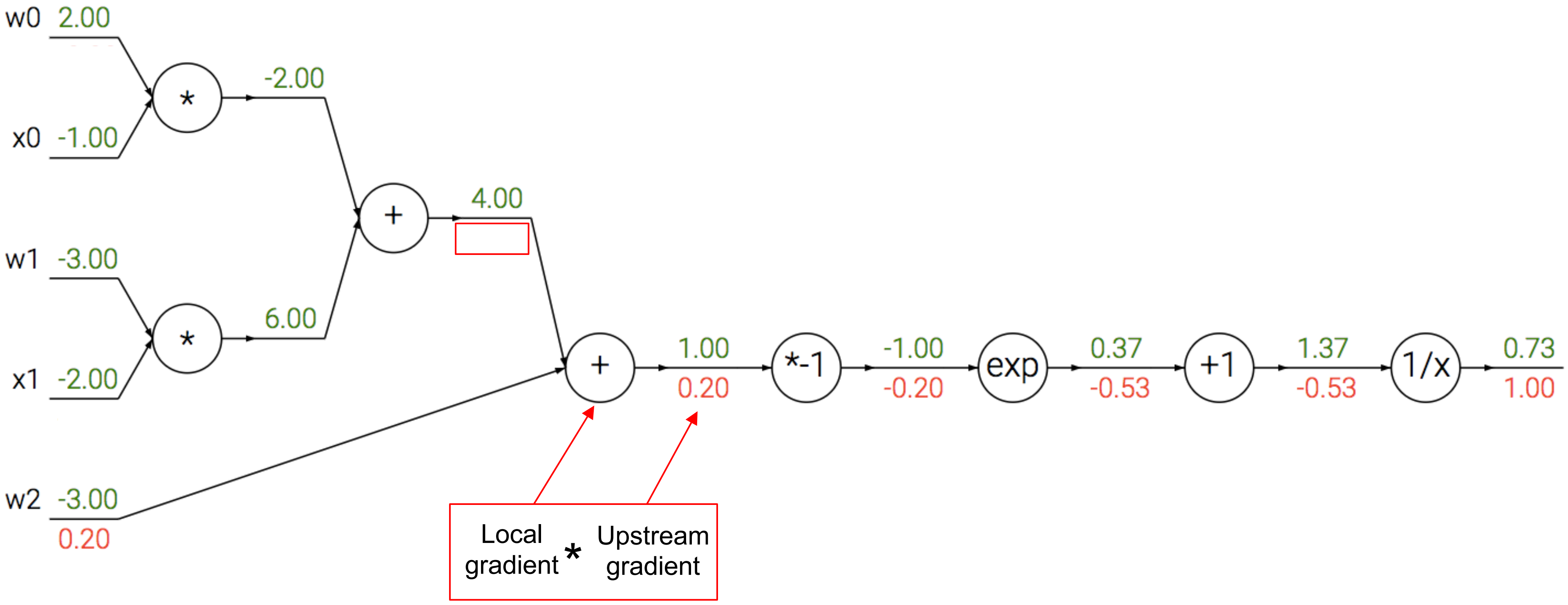

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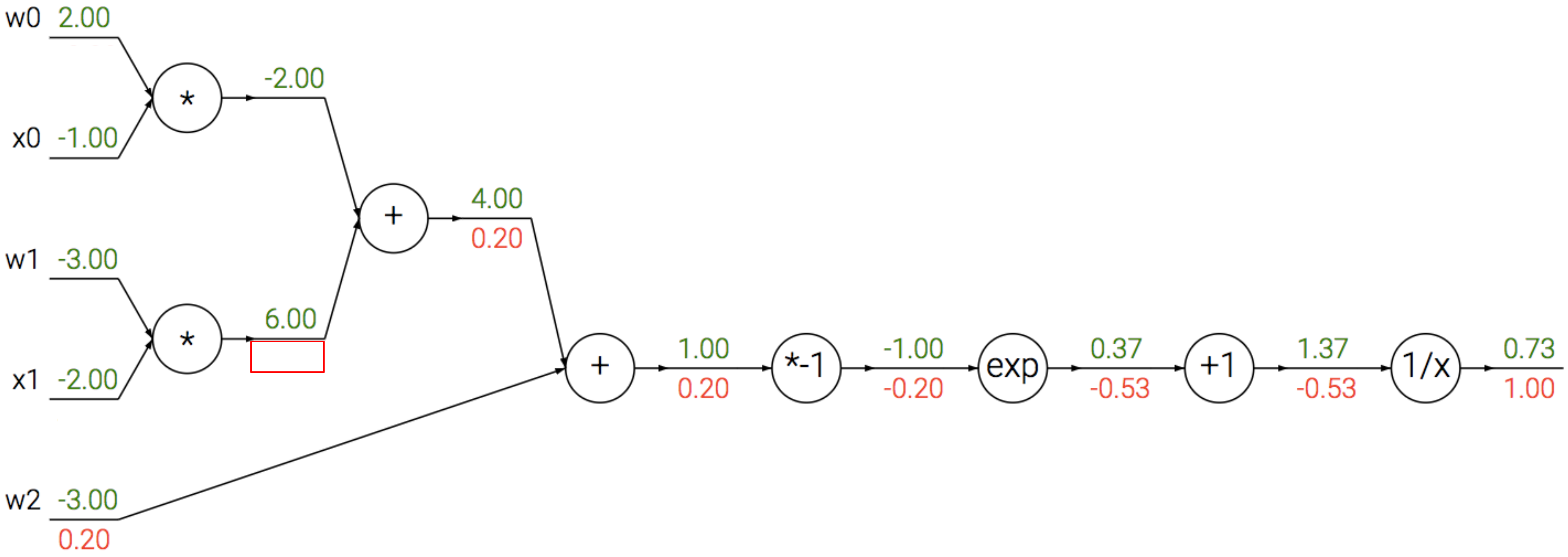

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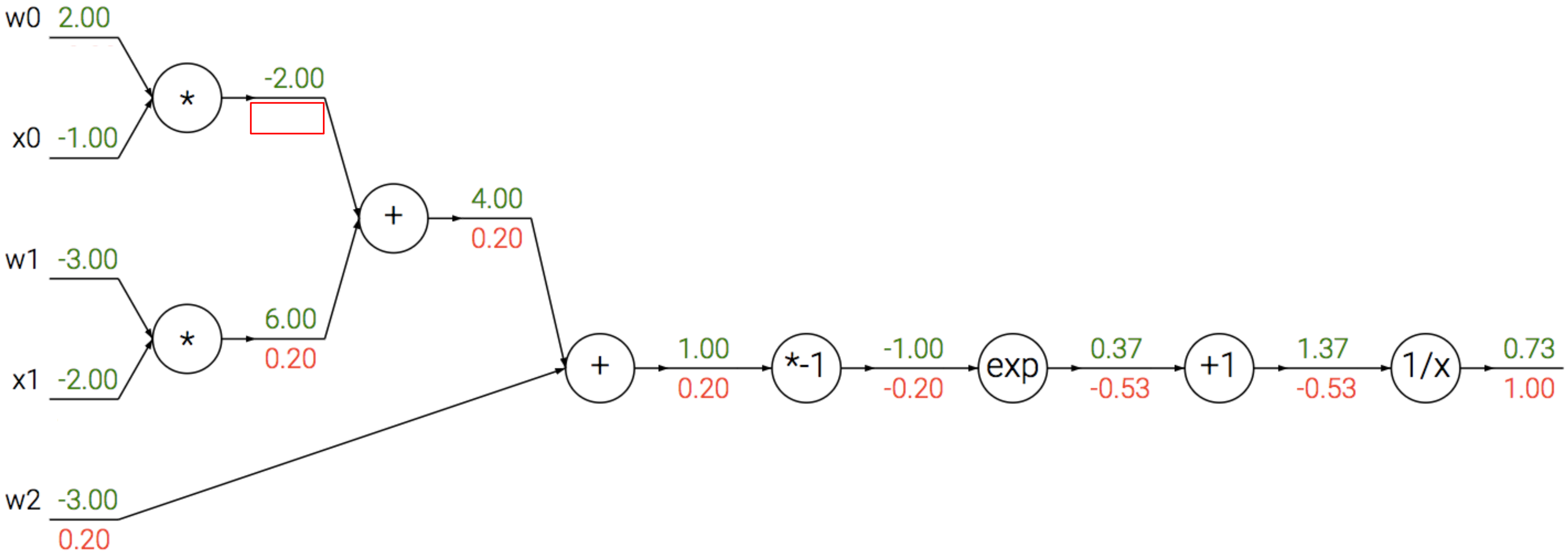

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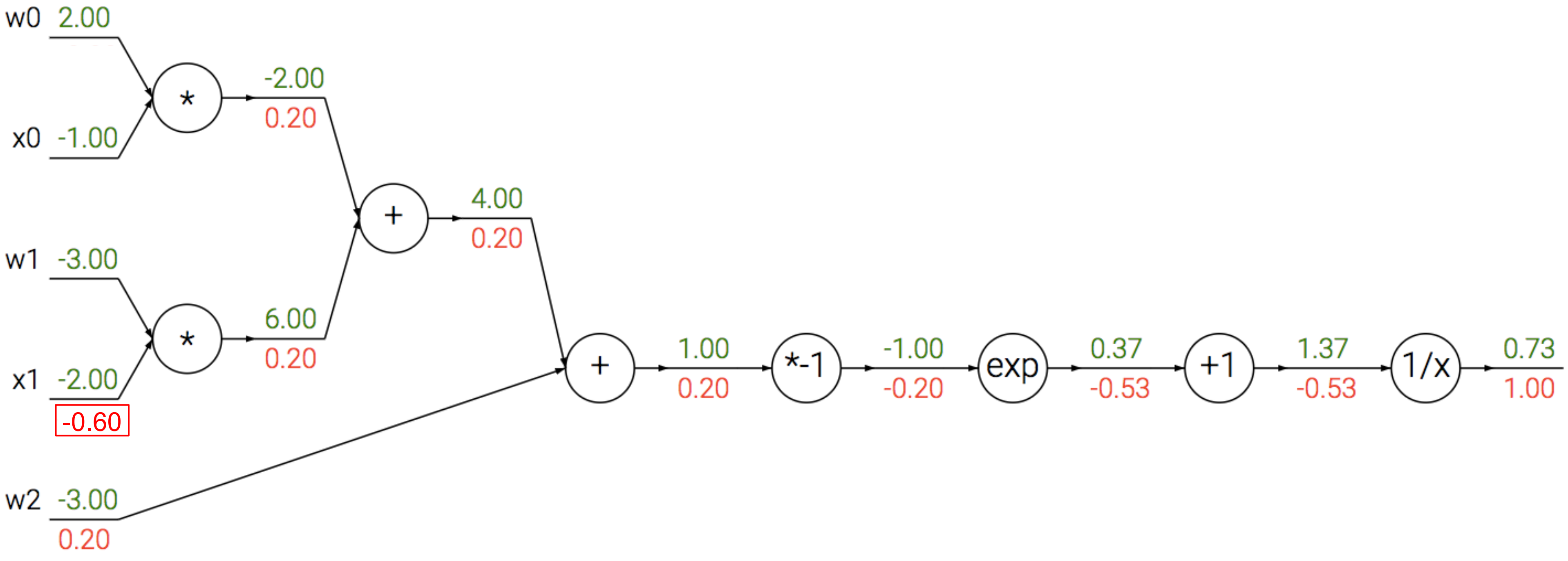

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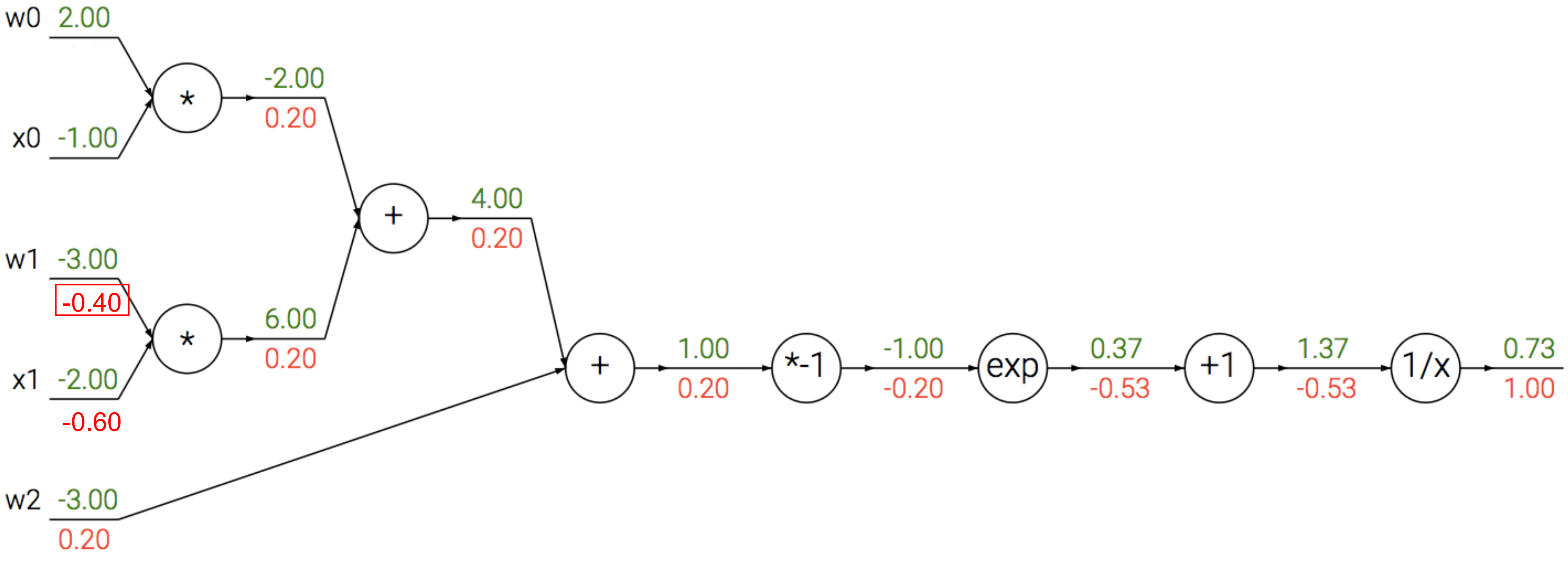

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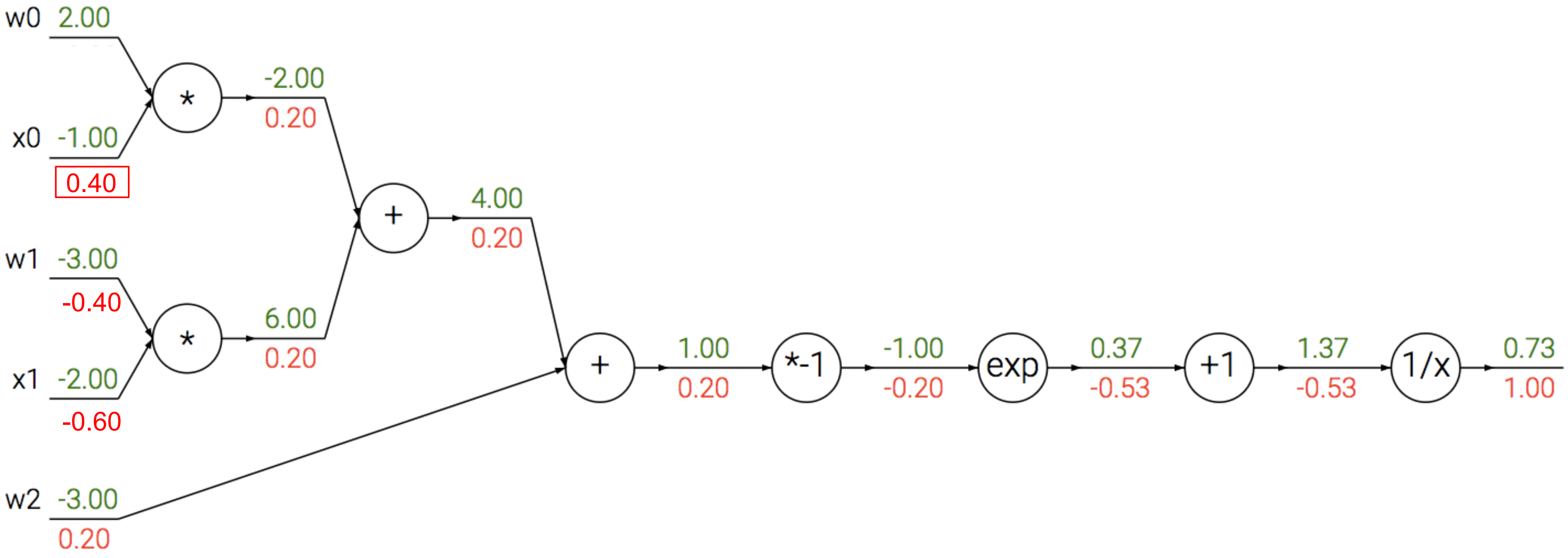

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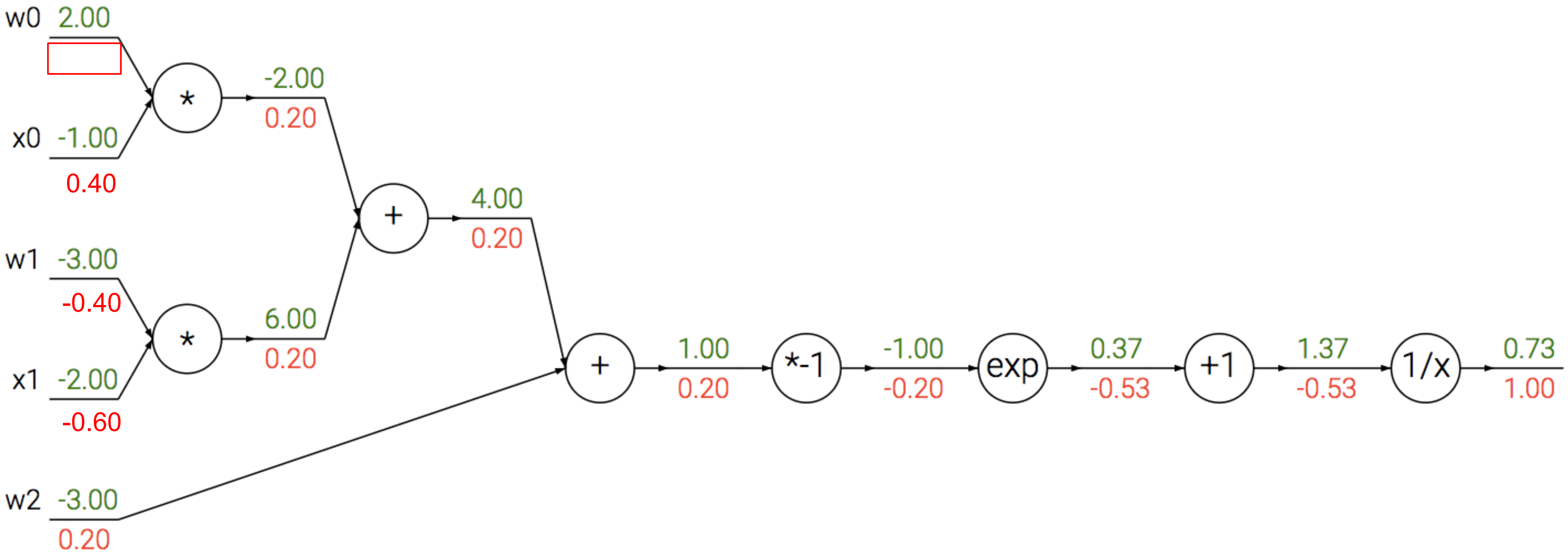

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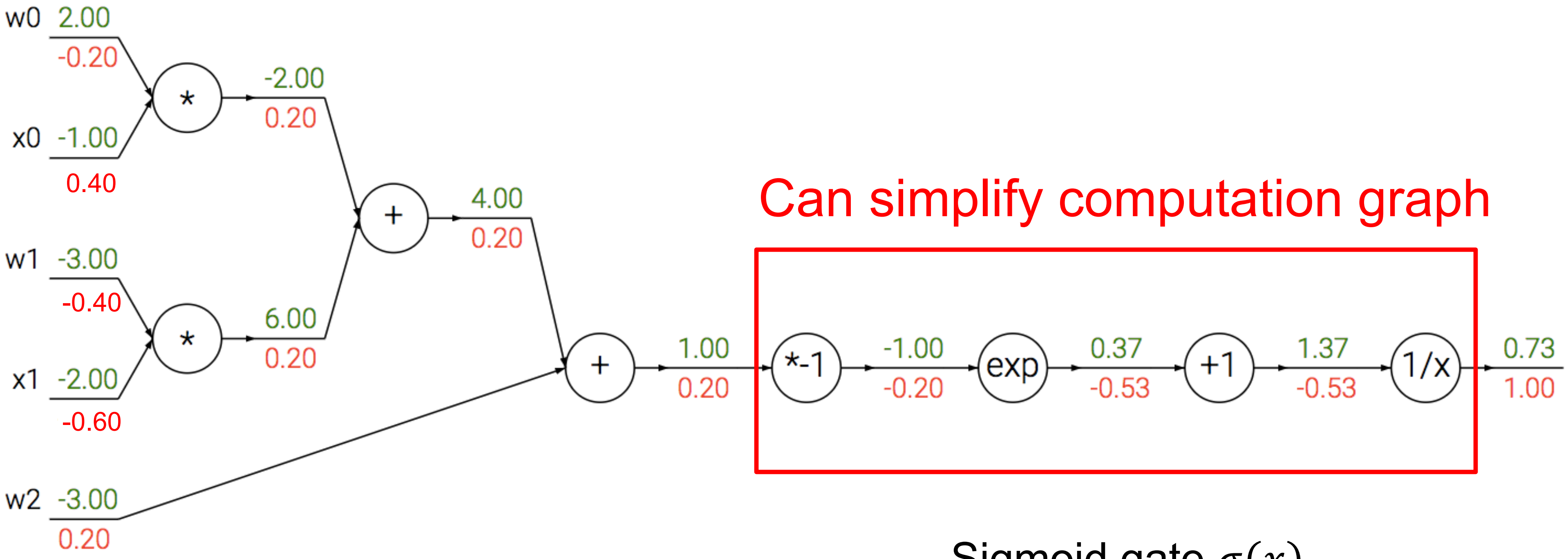


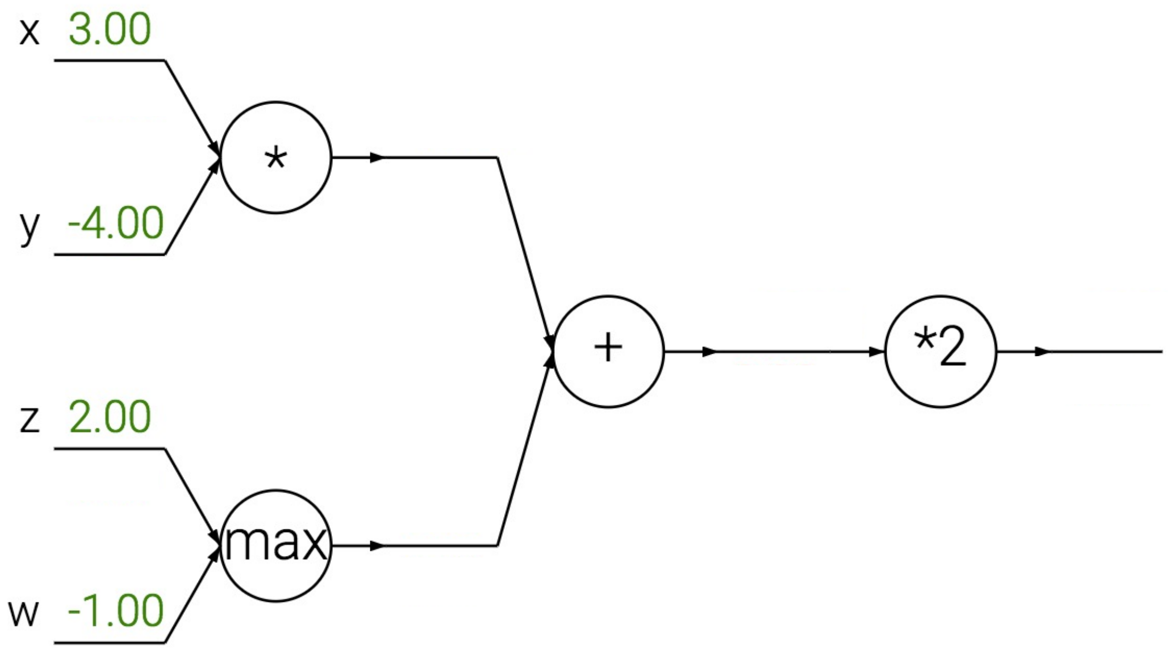
Sigmoid gate $\sigma(x)$

$$\sigma'(x) = \sigma(x)\big(1 - \sigma(x)\big)$$

$$\sigma(1)\big(1 - \sigma(1)\big) = 0.73 * (1 - 0.73) = 0.20$$

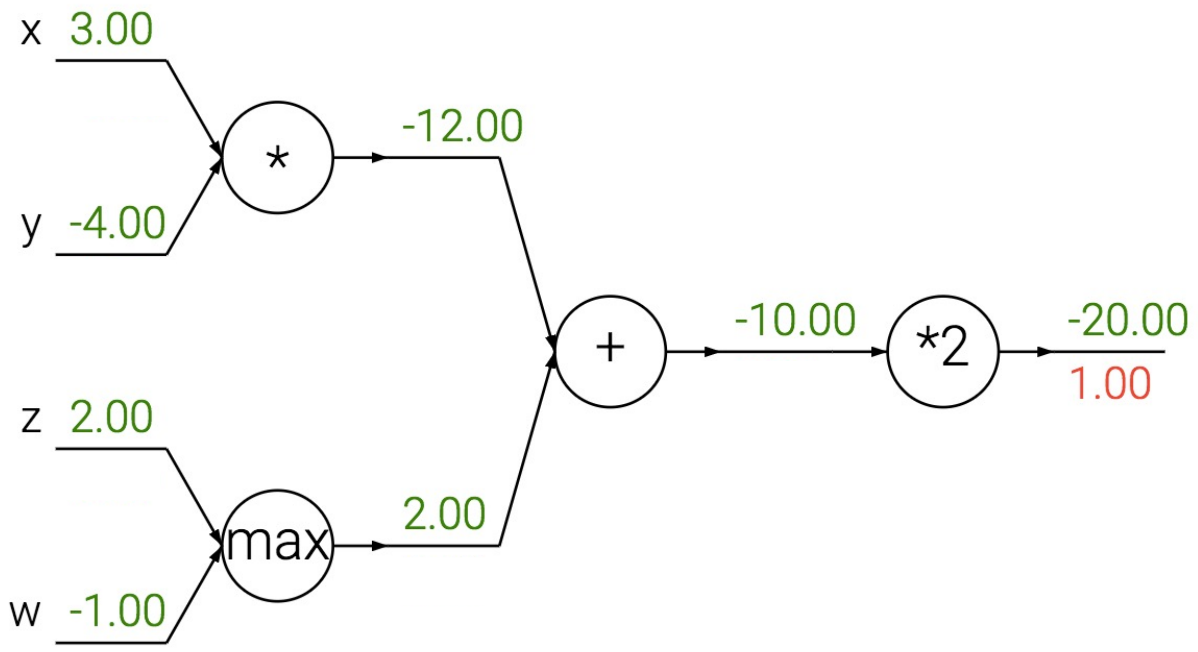
Source: [Stanford 231n]

Another example



Source: [Stanford 231n]

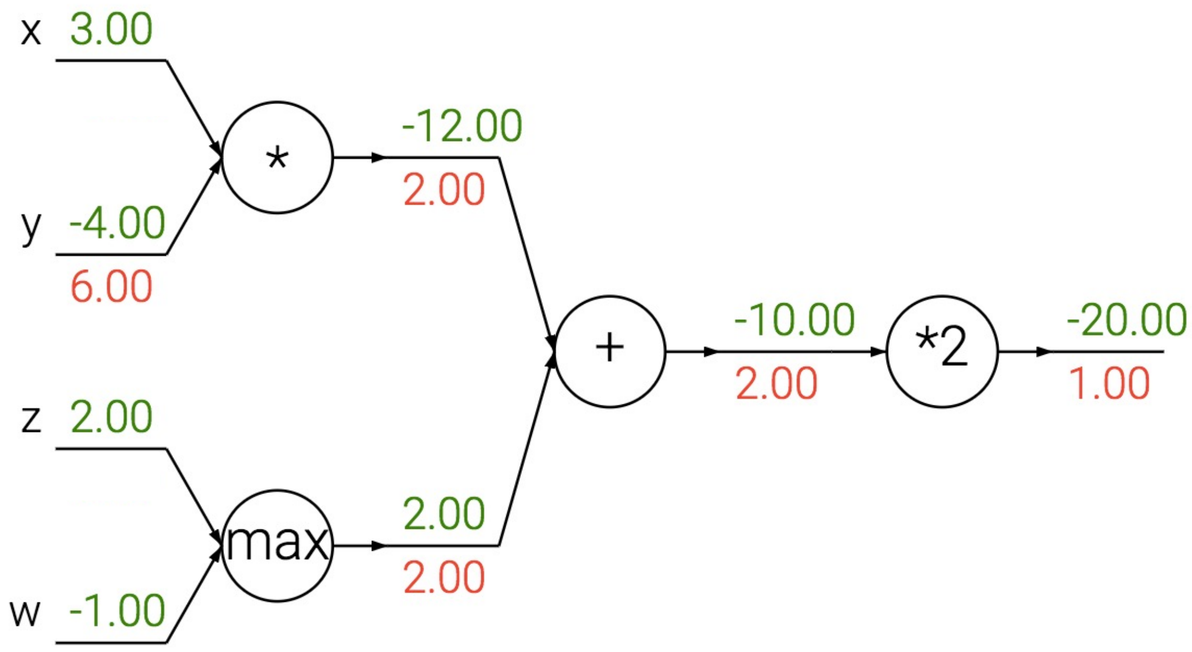
Another example



Add gate: “gradient distributor”

Source: [Stanford 231n]

Another example

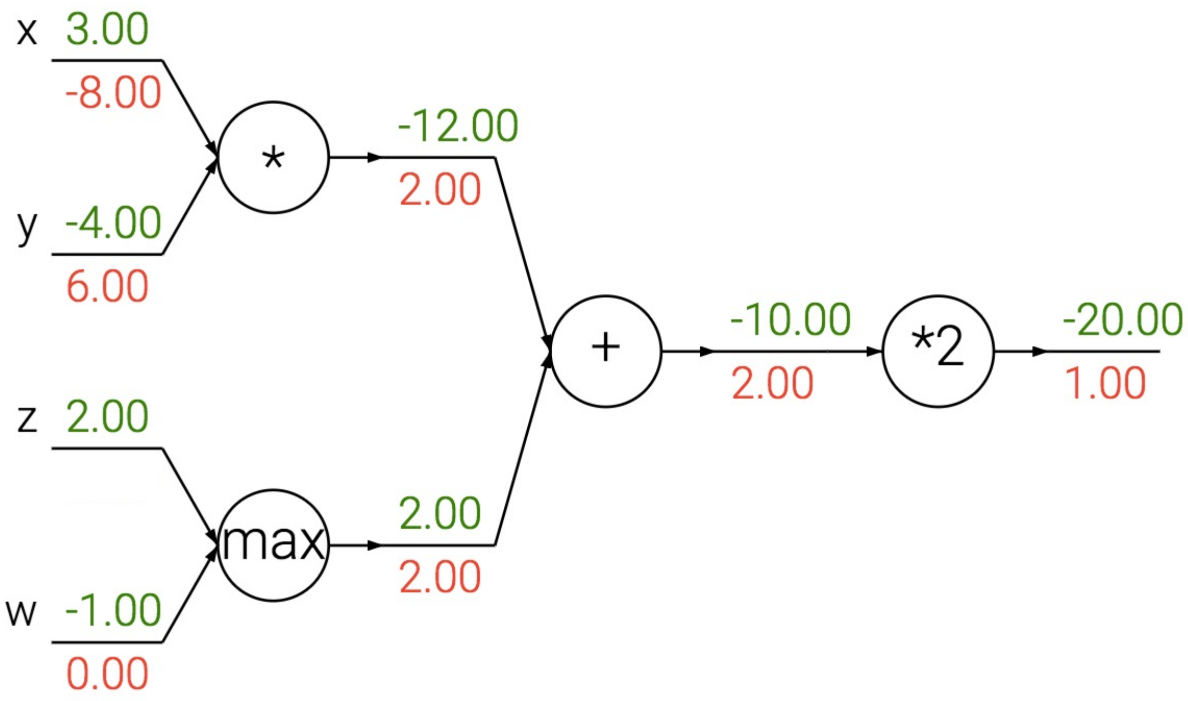


Add gate: “gradient distributor”

Multiply gate: “gradient switcher”

Source: [Stanford 231n]()

Another example



Add gate: “gradient distributor”

Multiply gate: “gradient switcher”

Max gate: “gradient router”

Source: [Stanford 231n]

Overview: Backpropagation

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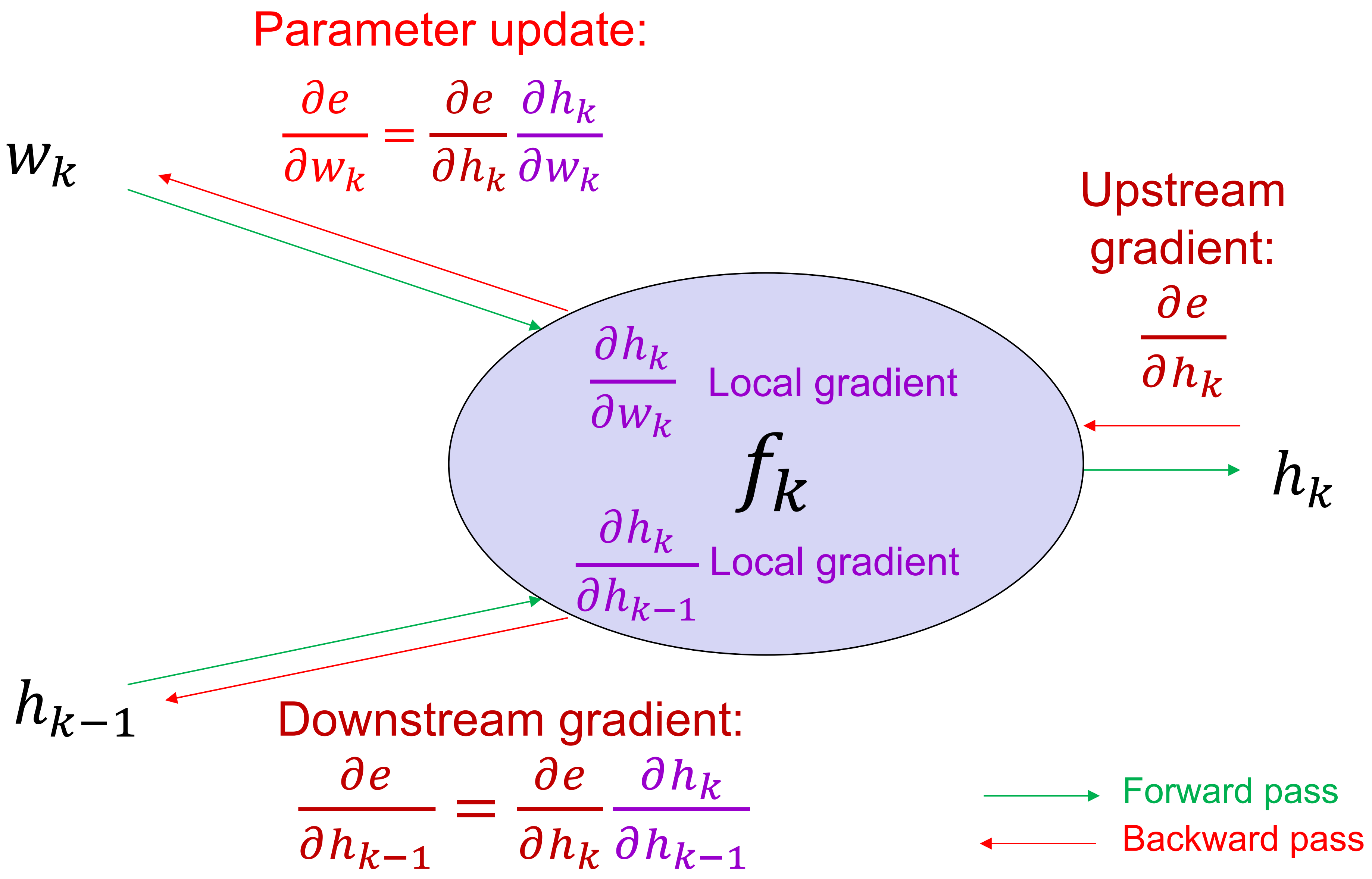
- Matrix-vector calculations: ReLU, linear layer

Backpropagation summary

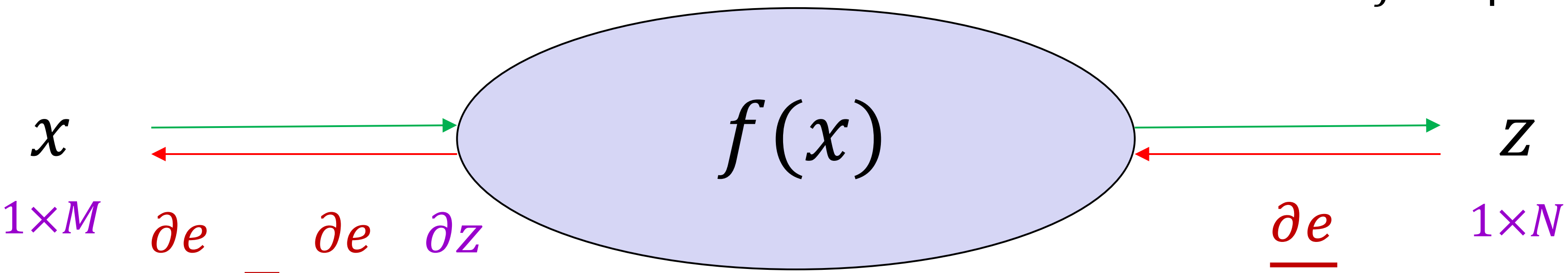


Dealing with vectors

$$\frac{\partial z}{\partial x} = \begin{pmatrix} \frac{\partial z^{(1)}}{\partial x^{(1)}} & \cdots & \frac{\partial z^{(1)}}{\partial x^{(M)}} \\ \vdots & \ddots & \vdots \\ \frac{\partial z^{(N)}}{\partial x^{(1)}} & \cdots & \frac{\partial z^{(N)}}{\partial x^{(M)}} \end{pmatrix}$$

$N \times M$ Jacobian

Jacobian: row indices correspond to outputs, column indices correspond to inputs. The i, jth element of the Jacobian is the partial derivative of the ith output w.r.t. jth input



x: $1 \times M$

z: $1 \times N$

$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z}\frac{\partial z}{\partial x}$$

$1 \times M$ $1 \times N$ $N \times M$

$$\frac{\partial e}{\partial z}$$

$1 \times N$

Simple case: Elementwise operation

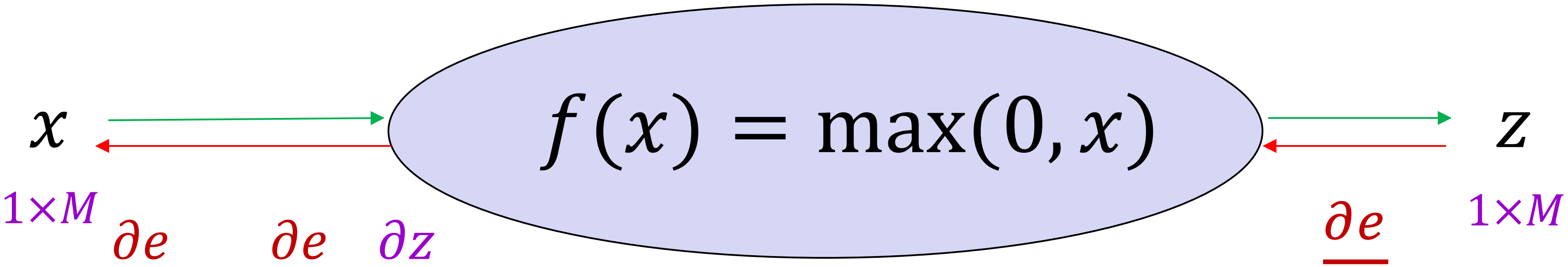
Simple case: Elementwise operation (ReLU layer)

$$\frac{\partial z}{\partial x} = \begin{pmatrix} \frac{\partial z^{(1)}}{\partial x^{(1)}} & \cdots & \frac{\partial z^{(1)}}{\partial x^{(M)}} \\ \vdots & \ddots & \vdots \\ \frac{\partial z^{(M)}}{\partial x^{(1)}} & \cdots & \frac{\partial z^{(M)}}{\partial x^{(M)}} \end{pmatrix}$$

$M \times M$

Jacobian

What does the Jacobian for an elementwise function look like?



$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z} \frac{\partial z}{\partial x}$$

$1 \times M \quad 1 \times M \quad M \times M$

$$\frac{\partial e}{\partial z}$$

$1 \times M$

Simple case: Elementwise operation (ReLU layer)

$$\frac{\partial z}{\partial x} = \begin{pmatrix} \frac{\partial z^{(1)}}{\partial x^{(1)}} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{\partial z^{(M)}}{\partial x^{(M)}} \end{pmatrix}$$

$M \times M$

Jacobian

What does the Jacobian for an elementwise function look like?

x → $f(x) = \max(0, x)$ → z

x: $1 \times M$

z: $1 \times M$

$$\frac{\partial e}{\partial z}$$

$1 \times M$

$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z} \frac{\partial z}{\partial x}$$

$1 \times M \quad 1 \times M \quad M \times M$

Simple case: Elementwise operation (ReLU layer)

$$\underbrace{\frac{\partial z}{\partial x}}_{M\times M} = \begin{pmatrix} \mathbb{I}[x^{(1)} > 0] & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \mathbb{I}[x^{(M)} > 0] \end{pmatrix}$$

Jacobian

x ($1\times M$) → $f(x) = \max(0, x)$ → z ($1\times M$)

$\frac{\partial e}{\partial z}$ ($1\times M$)

$$\underset{1\times M}{\frac{\partial e}{\partial x}} = \underset{1\times M}{\frac{\partial e}{\partial z}} \; \underset{M\times M}{\frac{\partial z}{\partial x}}$$

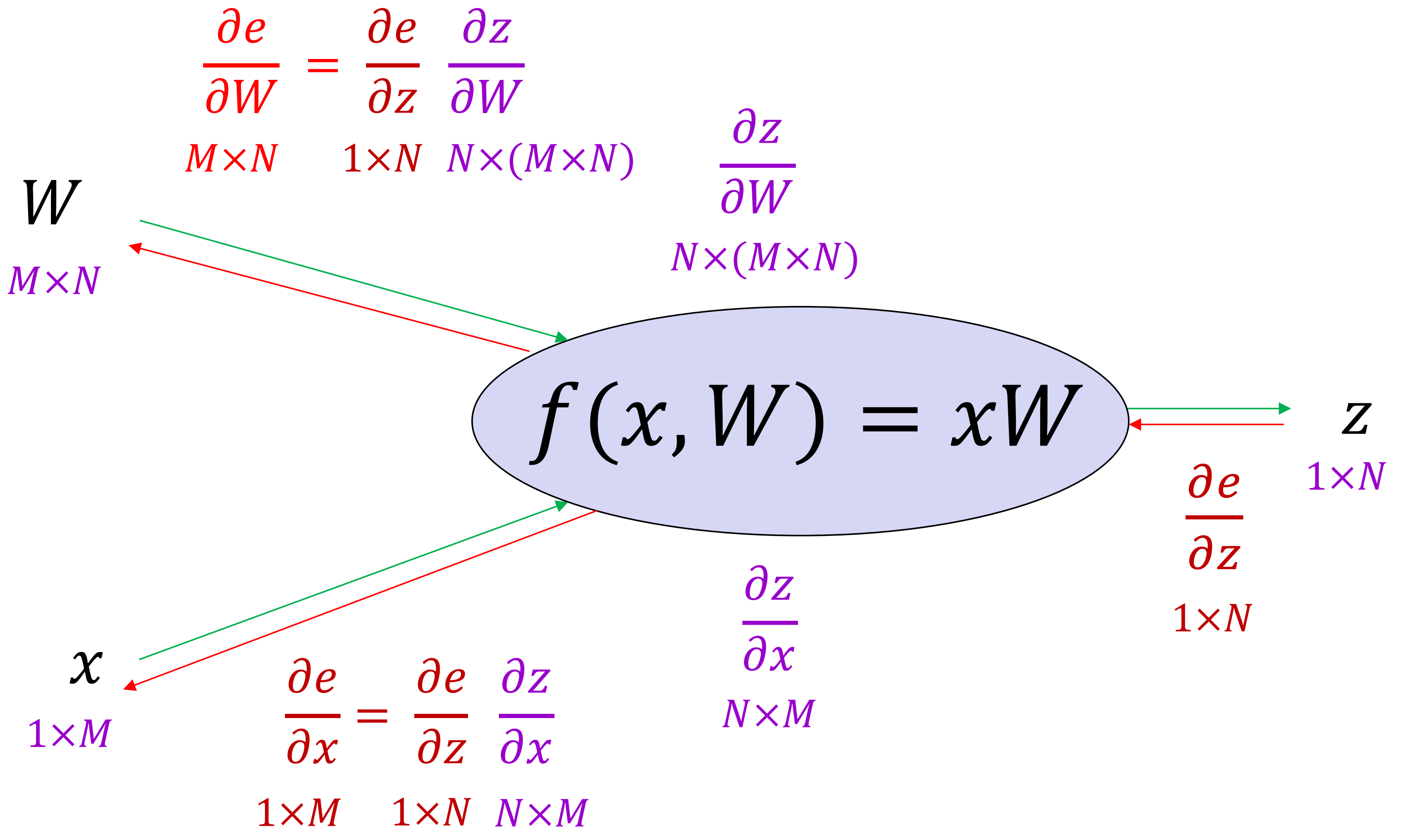
$$\frac{\partial e}{\partial x^{(i)}} = \frac{\partial e}{\partial z^{(i)}} \mathbb{I}[x^{(i)} > 0]$$

$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z} \odot \mathbb{I}[x > 0]$$

What happens if some $x^{(i)}$ is always negative?

This is known as the “dead ReLU” problem

Matrix-vector multiplication (linear layer)



Matrix-vector multiplication (linear layer)

$$\begin{pmatrix} z^{(1)} & \dots & z^{(N)} \end{pmatrix} = \begin{pmatrix} x^{(1)} & \dots & x^{(M)} \end{pmatrix} \begin{pmatrix} W^{(11)} & \cdots & W^{(1N)} \\ \vdots & \ddots & \vdots \\ W^{(M1)} & \cdots & W^{(MN)} \end{pmatrix}$$

$$z^{(j)} = \sum_{i=1}^{M} x^{(i)} W^{(ij)}$$

Want: $\dfrac{\partial e}{\partial x} = \dfrac{\partial e}{\partial z} \boxed{\dfrac{\partial z}{\partial x}}$

$1 \times M \qquad 1 \times N \qquad N \times M$

$$\frac{\partial z^{(j)}}{\partial x^{(i)}} =$$

jth row, ith column of Jacobian

$$\frac{\partial z}{\partial x} = W^T$$

Matrix-vector multiplication (linear layer)

$$\begin{pmatrix} z^{(1)} & \dots & z^{(N)} \end{pmatrix} = \begin{pmatrix} x^{(1)} & \dots & x^{(M)} \end{pmatrix} \begin{pmatrix} W^{(11)} & \dots & W^{(1N)} \\ \vdots & \ddots & \vdots \\ W^{(M1)} & \dots & W^{(MN)} \end{pmatrix}$$

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Want: $\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z} \boxed{\frac{\partial z}{\partial x}}$

$1 \times M \quad 1 \times N \quad N \times M$

$$\frac{\partial z^{(j)}}{\partial x^{(i)}} = W^{(ij)}$$

jth row, ith column of Jacobian

$$\frac{\partial z}{\partial x} = W^T$$

$$\boxed{\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z} \frac{\partial z}{\partial x} = \frac{\partial e}{\partial z} W^T}$$

Matrix-vector multiplication (linear layer)

$$\begin{pmatrix} z^{(1)} & \dots & z^{(N)} \end{pmatrix} = \begin{pmatrix} x^{(1)} & \dots & x^{(M)} \end{pmatrix} \begin{pmatrix} W^{(11)} & \dots & W^{(1N)} \\ \vdots & \ddots & \vdots \\ W^{(M1)} & \dots & W^{(MN)} \end{pmatrix}$$

$$z^{(j)} = \sum_{i=1}^{M} x^{(i)} W^{(ij)}$$

Want: $$\underset{M \times N}{\frac{\partial e}{\partial W}} = \underset{1 \times N}{\frac{\partial e}{\partial z}} \underset{N \times (M \times N)}{\boxed{\frac{\partial z}{\partial W}}}$$

$$\frac{\partial z^{(k)}}{\partial W^{(ij)}}$$

$z^{(k)}$ depends only on kth column of W

Matrix-vector multiplication (linear layer)

$$\begin{pmatrix} z^{(1)} & \dots & z^{(N)} \end{pmatrix} = \begin{pmatrix} x^{(1)} & \dots & x^{(M)} \end{pmatrix} \begin{pmatrix} W^{(11)} & \dots & W^{(1N)} \\ \vdots & \ddots & \vdots \\ W^{(M1)} & \dots & W^{(MN)} \end{pmatrix}$$

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Want: $$\underset{M \times N}{\frac{\partial e}{\partial W}} = \underset{1 \times N}{\frac{\partial e}{\partial z}} \underset{N \times (M \times N)}{\boxed{\frac{\partial z}{\partial W}}}$$

$$\frac{\partial z^{(k)}}{\partial W^{(ij)}} = \mathbb{I}[k = j] x^{(i)}$$

$z^{(k)}$ depends only on kth column of W

$$\frac{\partial e}{\partial W^{(ij)}} = \frac{\partial e}{\partial z} \frac{\partial z}{\partial W^{(ij)}}$$

Matrix-vector multiplication (linear layer)

$$\left(z^{(1)} \quad \dots \quad z^{(N)}\right) = \left(x^{(1)} \quad \dots \quad x^{(M)}\right) \begin{pmatrix} W^{(11)} & \dots & W^{(1N)} \\ \vdots & \ddots & \vdots \\ W^{(M1)} & \dots & W^{(MN)} \end{pmatrix}$$

$$z^{(j)} = \sum_{i=1}^{M} x^{(i)} W^{(ij)}$$

Want: $\boxed{\frac{\partial e}{\partial W}} = \frac{\partial e}{\partial z} \frac{\partial z}{\partial W}$

$M \times N \qquad 1 \times N \qquad N \times (M \times N)$

$$\frac{\partial e}{\partial W^{(ij)}} = \frac{\partial e}{\partial z^{(j)}} x^{(i)}$$

$$\frac{\partial e}{\partial W} = \begin{pmatrix} \frac{\partial e}{\partial z^{(1)}} x^{(1)} & \dots & \frac{\partial e}{\partial z^{(N)}} x^{(1)} \\ \vdots & \ddots & \vdots \\ \frac{\partial e}{\partial z^{(1)}} x^{(M)} & \dots & \frac{\partial e}{\partial z^{(N)}} x^{(M)} \end{pmatrix}$$

Matrix-vector multiplication (linear layer)

$$\begin{pmatrix} z^{(1)} & \dots & z^{(N)} \end{pmatrix} = \begin{pmatrix} x^{(1)} & \dots & x^{(M)} \end{pmatrix} \begin{pmatrix} W^{(11)} & \dots & W^{(1N)} \\ \vdots & \ddots & \vdots \\ W^{(M1)} & \dots & W^{(MN)} \end{pmatrix}$$

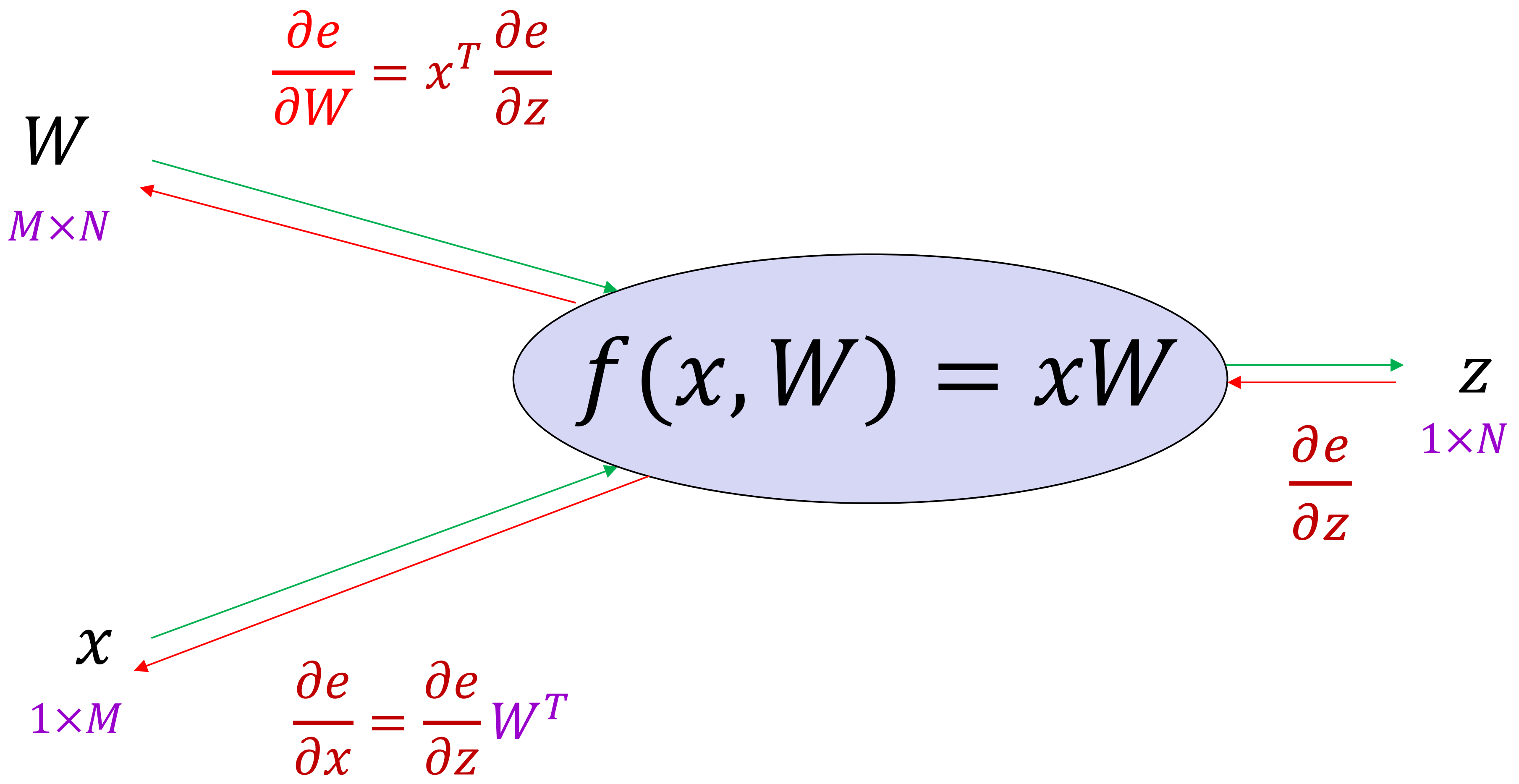
$$z^{(j)} = \sum_{i=1}^{M} x^{(i)} W^{(ij)}$$

Want: $\underset{M \times N}{\boxed{\frac{\partial e}{\partial W}}} = \underset{1 \times N}{\frac{\partial e}{\partial z}} \; \underset{N \times (M \times N)}{\frac{\partial z}{\partial W}}$

$$\boxed{\frac{\partial e}{\partial W} = x^T \frac{\partial e}{\partial z}}$$

Matrix-vector multiplication (linear layer)

- Summary of backward pass:



General tips

- Derive error signal (upstream gradient) directly, avoid explicit computation of huge local derivatives
- Write out expression for a single element of the Jacobian, then deduce the overall formula
- Keep consistent indexing conventions, order of operations
- Use dimension analysis
- Compare analytical gradients to numerical gradient

- **For further reading:**
  - Lecture 4 of Stanford 231n and associated links in the syllabus
  - Yes you should understand backprop by Andrej Karpathy