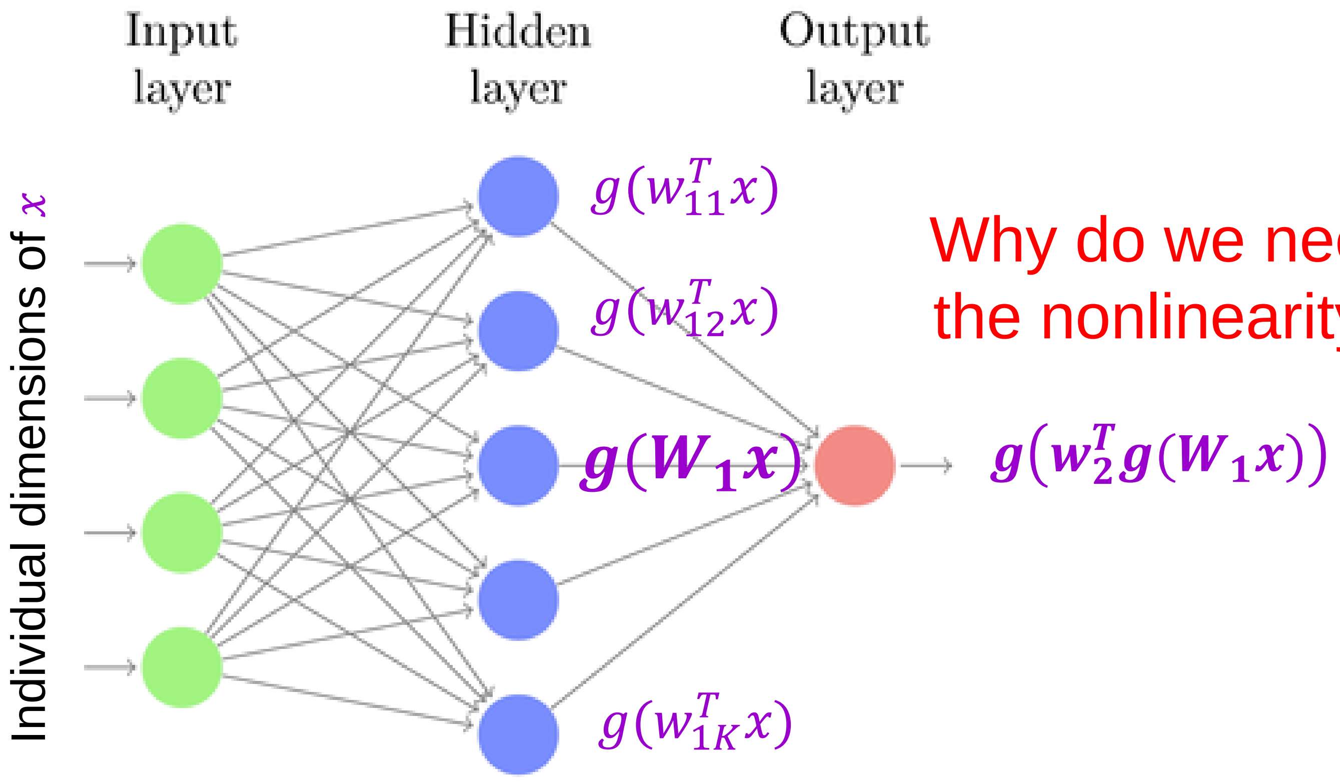
Multi-layer neural networks and backpropagation

Jianguo Zhang

Two-layer neural network

- Introduce a *hidden layer* of perceptrons computing linear combinations of inputs followed by a *nonlinearity*



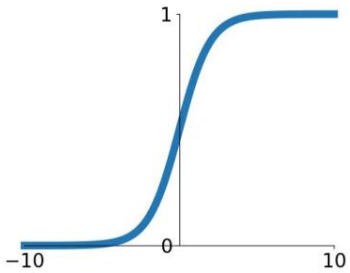
Why do we need the nonlinearity?

$\boldsymbol{W_1}$ – matrix with rows w_{1j}^T

Common nonlinearities

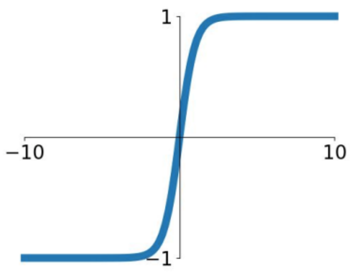
Sigmoid

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



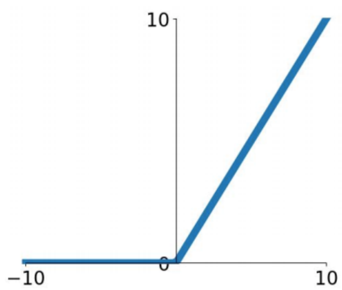
tanh

$\tanh(x)$



ReLU

$\max(0, x)$



Source: [Stanford 231n]

Two-layer neural network

- Introduce a *hidden layer* of perceptrons computing linear combinations of inputs followed by a *nonlinearity*
- This gives a *universal function approximator*
  - But the hidden layer may need to be huge

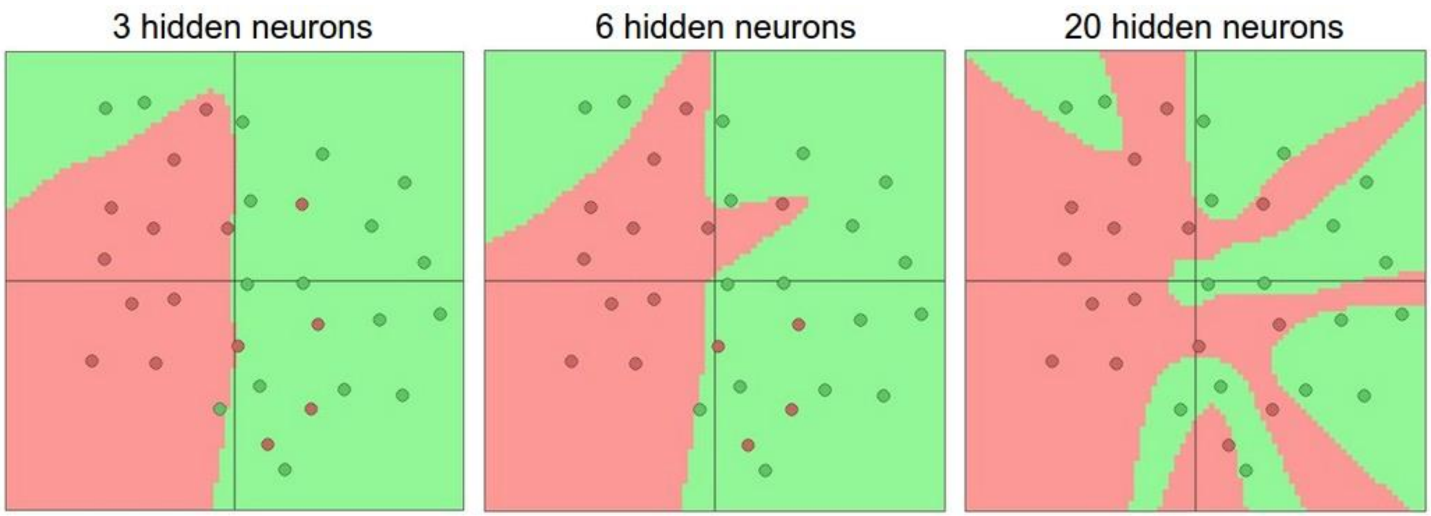
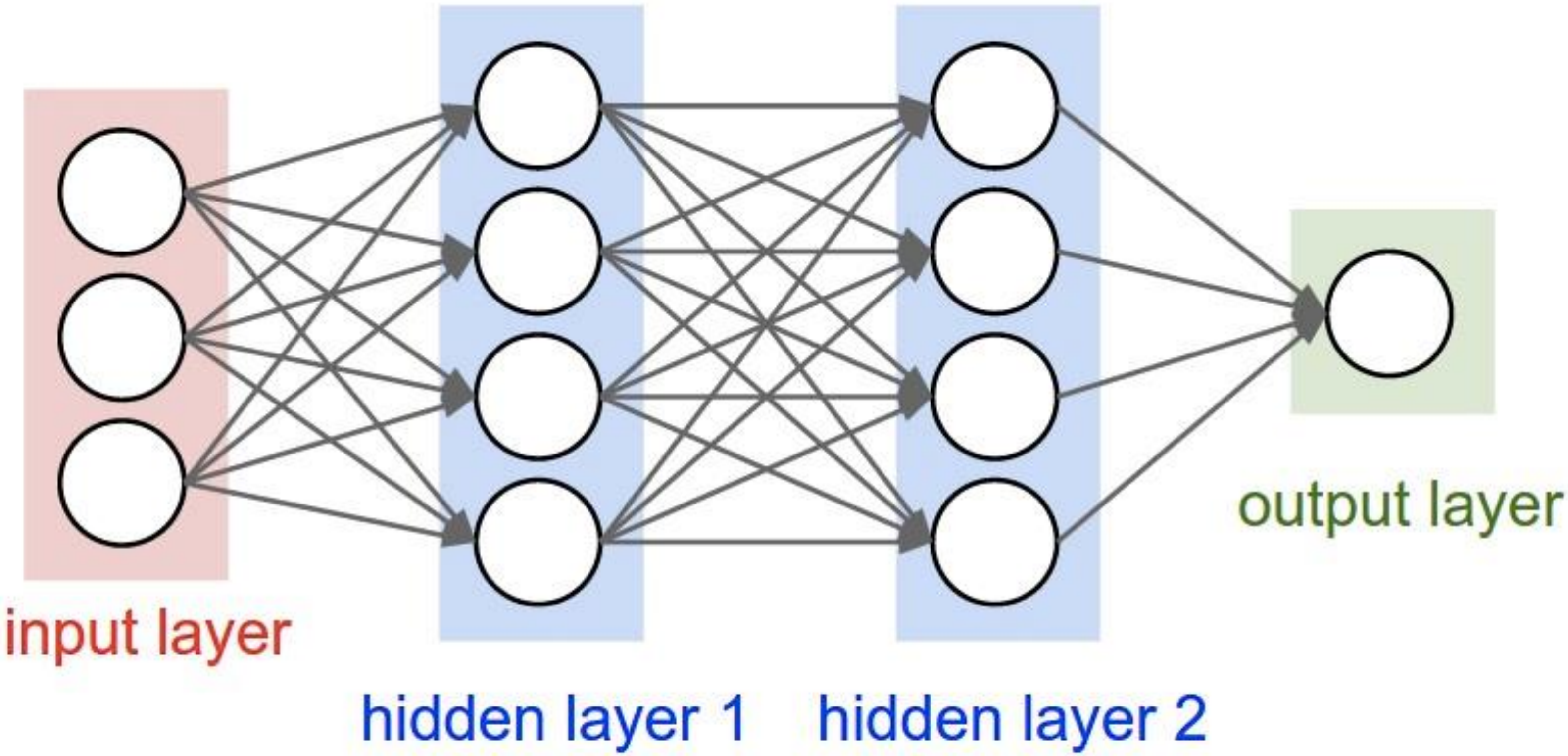
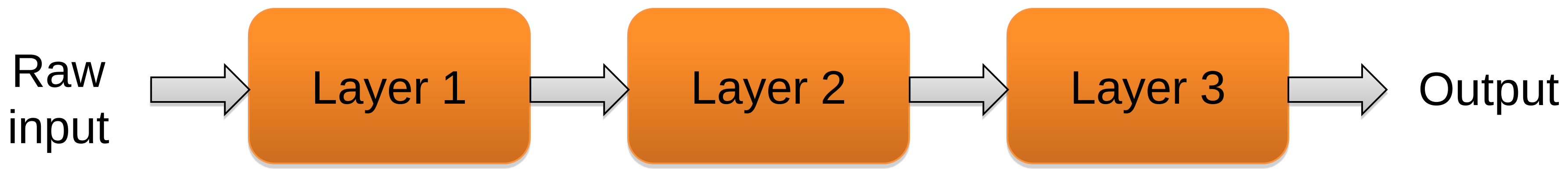


Figure source

Beyond two layers

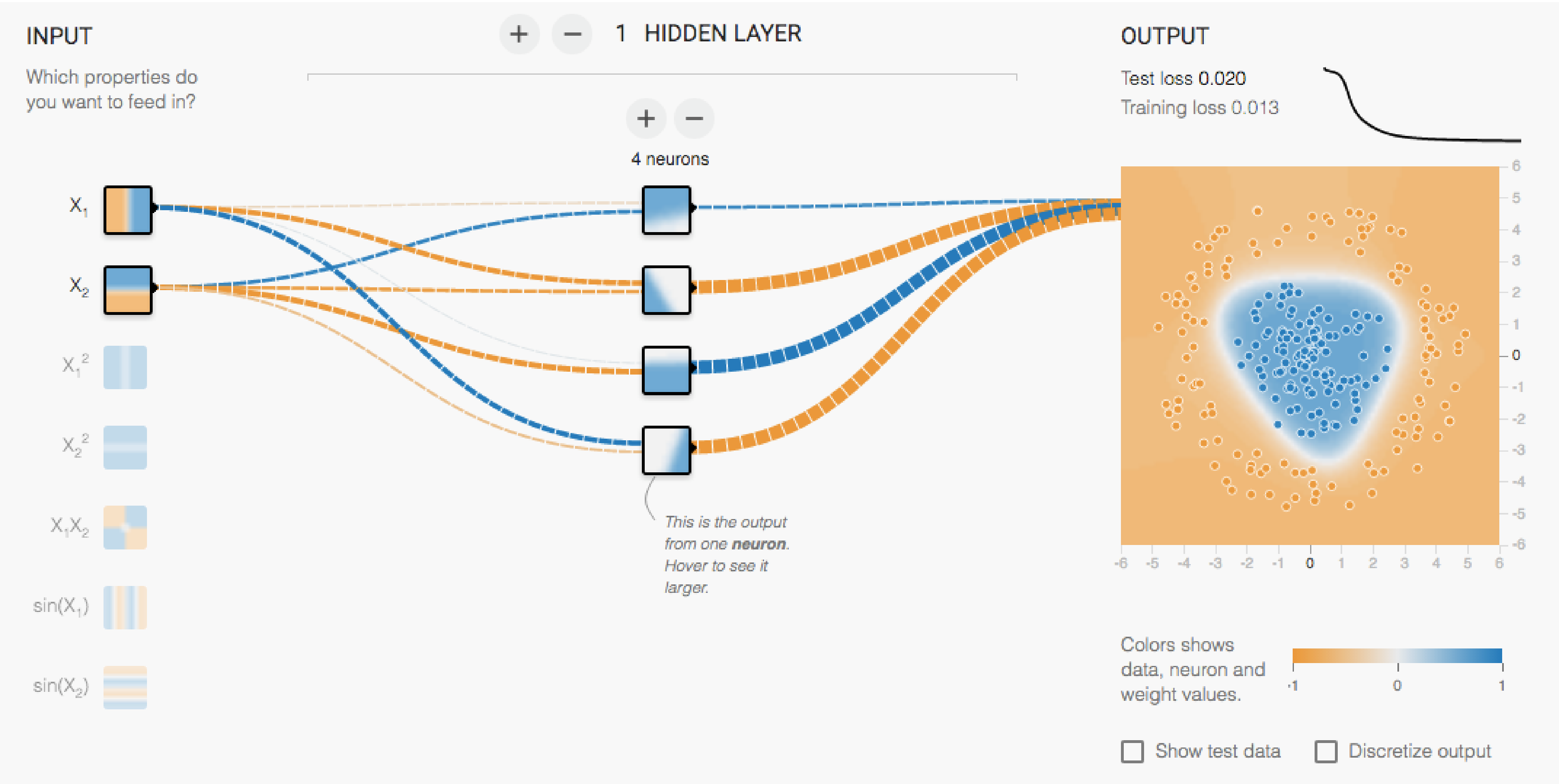


“Deep” pipeline



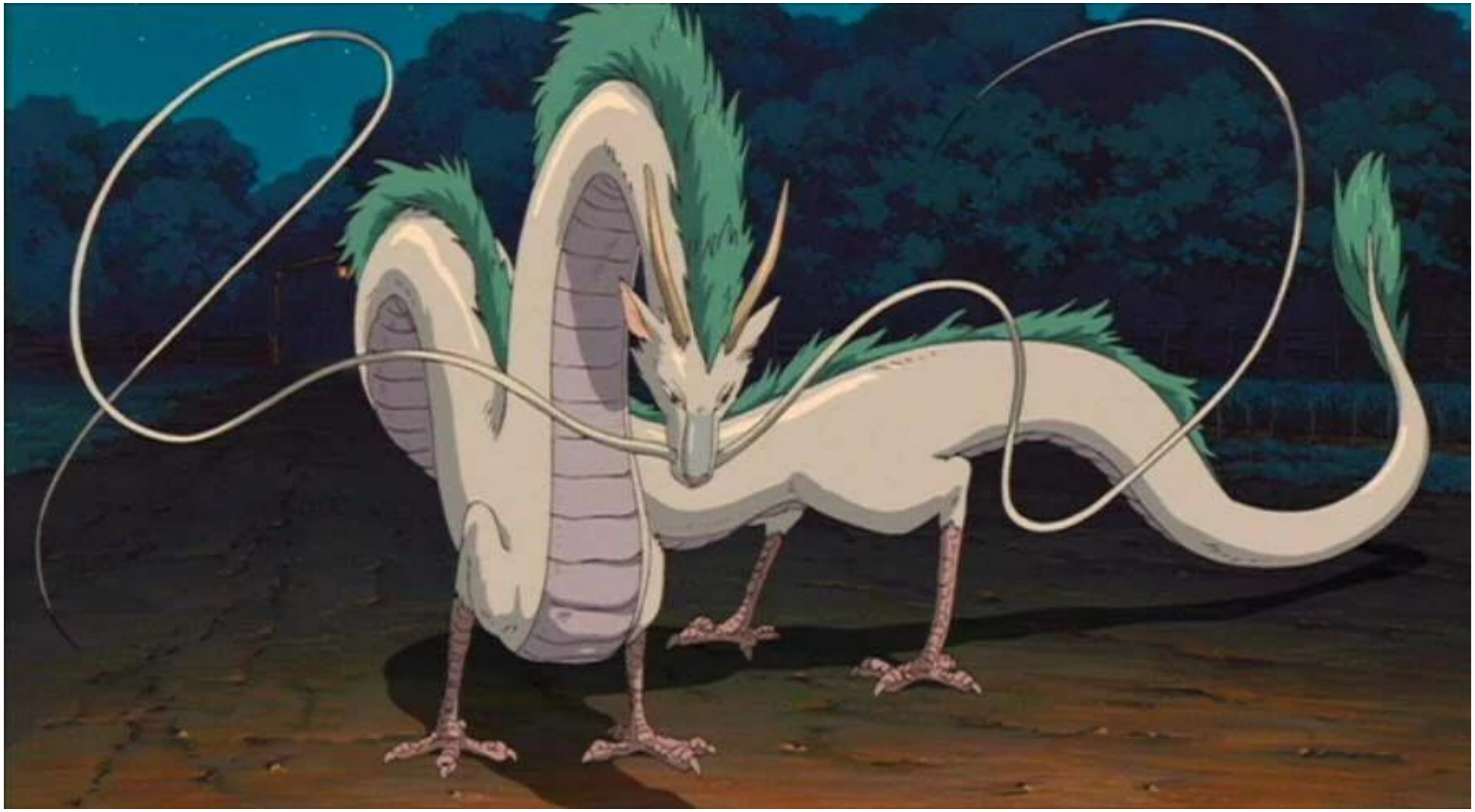
- Learn a *feature hierarchy*
- Each layer extracts features from the output of previous layer
- All layers are trained jointly

Multi-Layer network demo

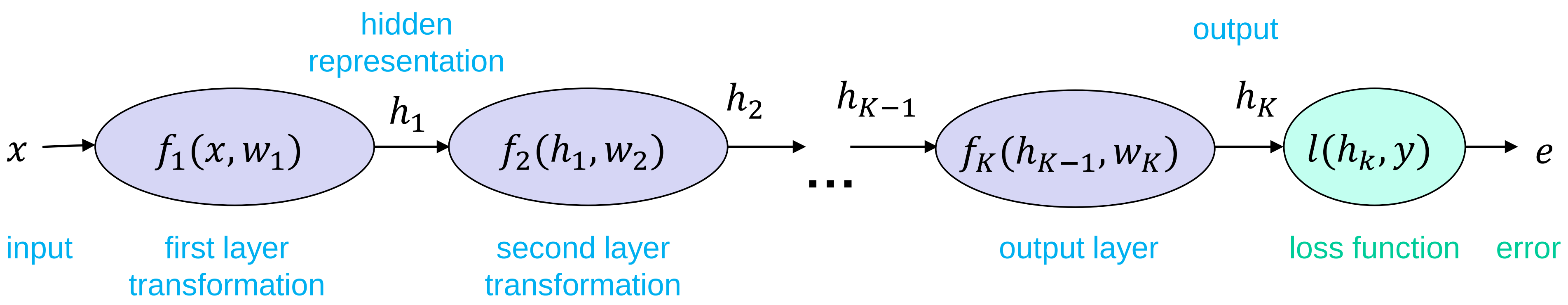


http://playground.tensorflow.org/

How to train a multi-layer network?



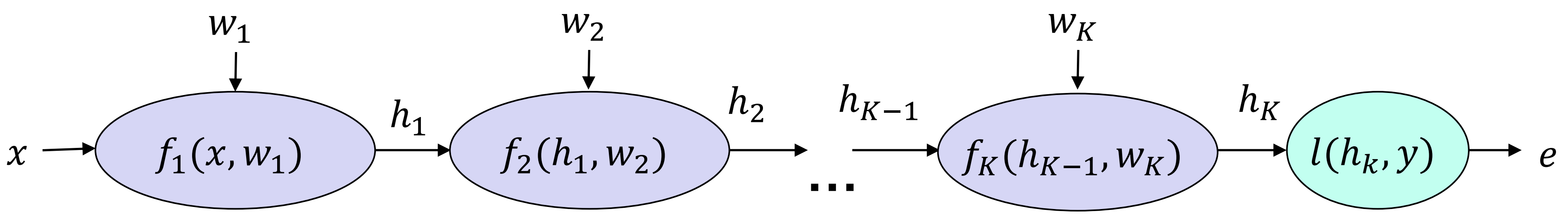
How to train a multi-layer network?



- We need to find the gradient of the error w.r.t. the parameters of each layer, $\frac{\partial e}{\partial w_k}$, to perform updates

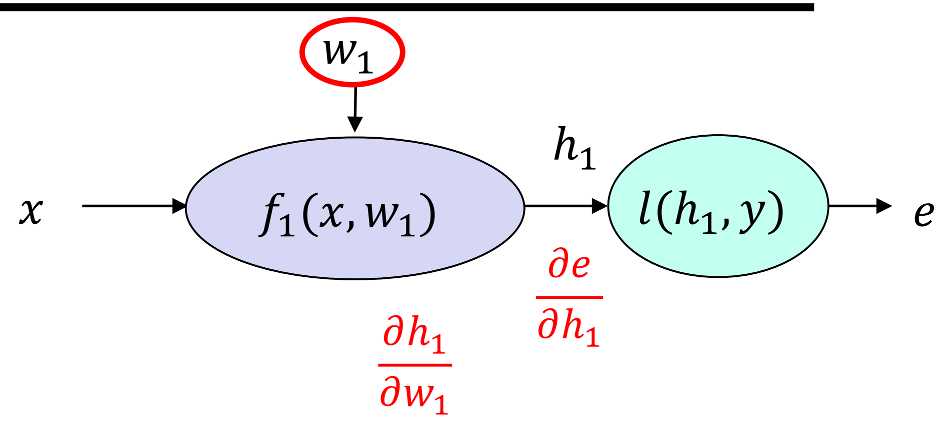
$$w_k \leftarrow w_k - \eta \frac{\partial e}{\partial w_k}$$

Computation graph



Chain rule

Let's start with $k = 1$



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

$$\frac{\partial}{\partial w_1} l(f_1(x, w_1), y) =$$

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

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

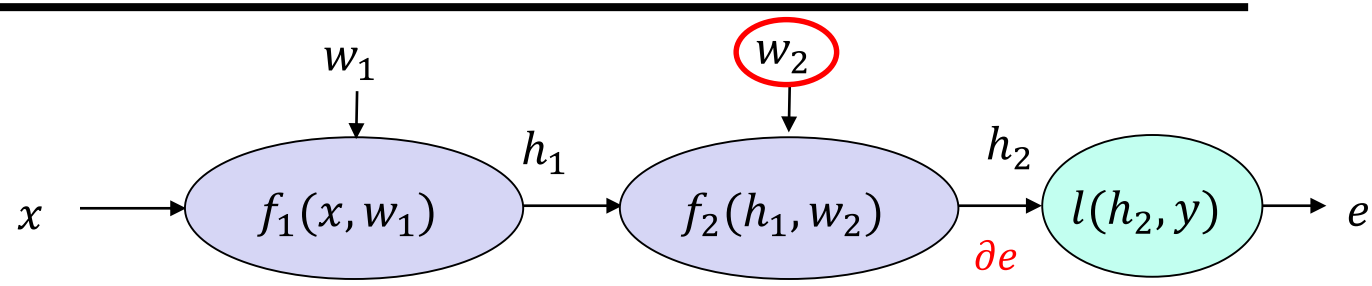
$$e = l(h_1, y) = (y - h_1)^2$$

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

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

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

Chain rule

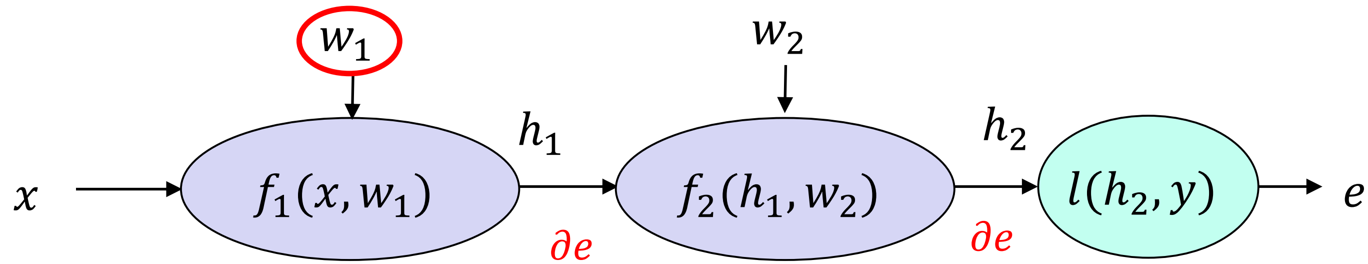


$k = 2$

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

$$\frac{\partial e}{\partial w_2} =$$

Chain rule



$k = 2$

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

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

$$\frac{\partial e}{\partial w_2} = \frac{\partial e}{\partial h_2} \frac{\partial h_2}{\partial w_2}$$

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

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

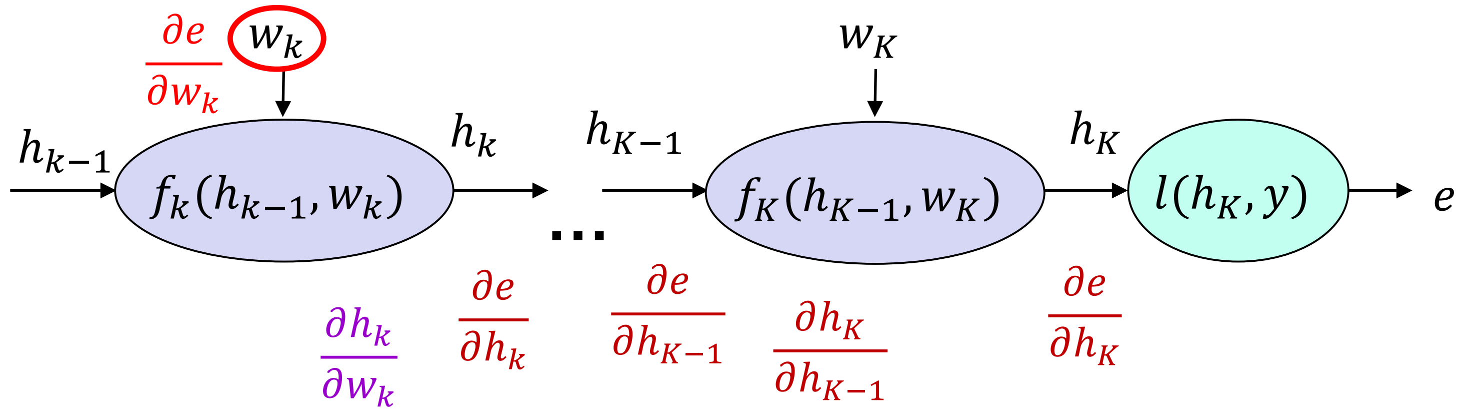
$$\frac{\partial h_1}{\partial w_1} =$$

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

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

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

Chain rule



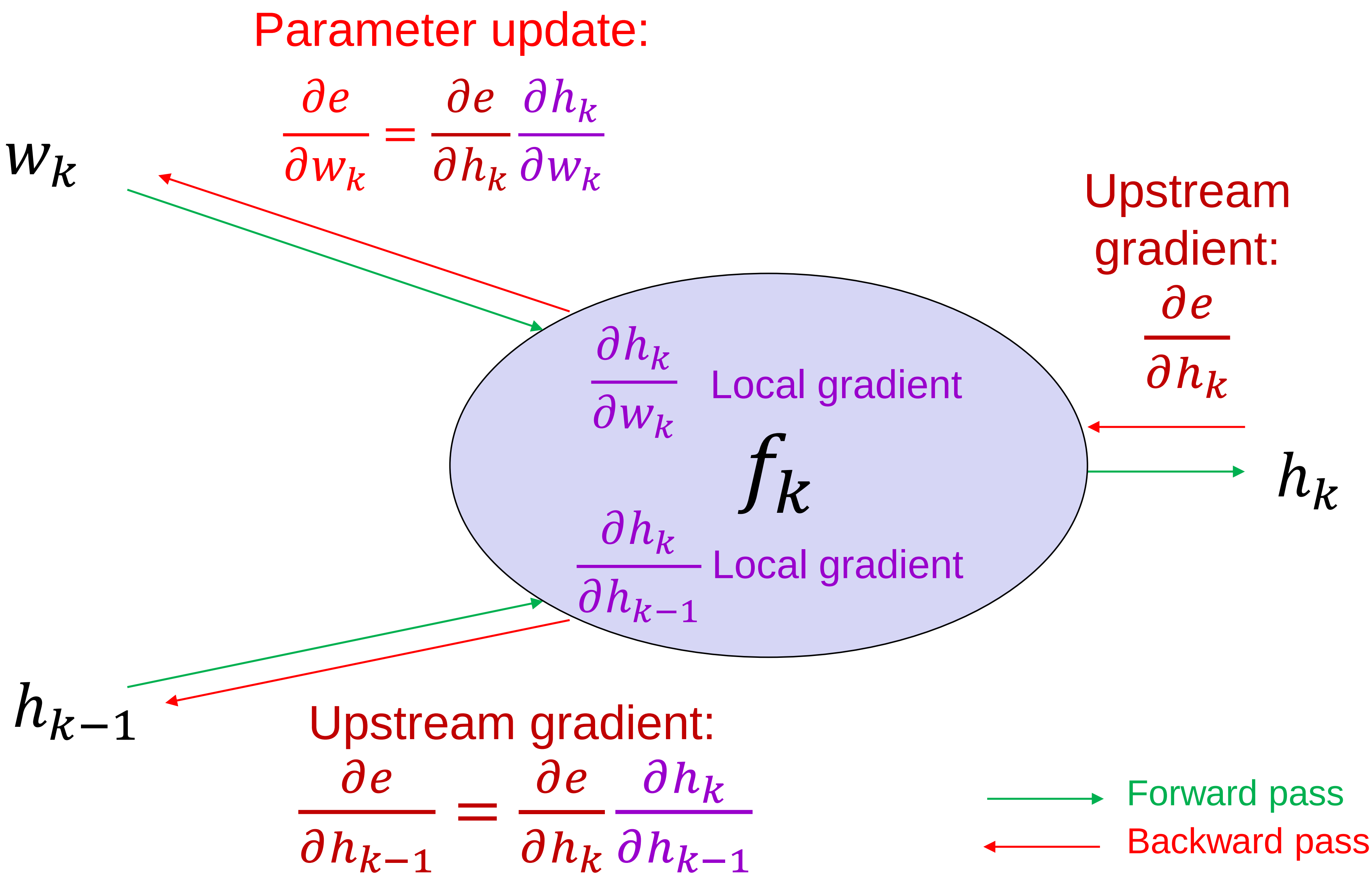
General case:

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

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

Local gradient

Backpropagation summary



What about more general computation graphs?

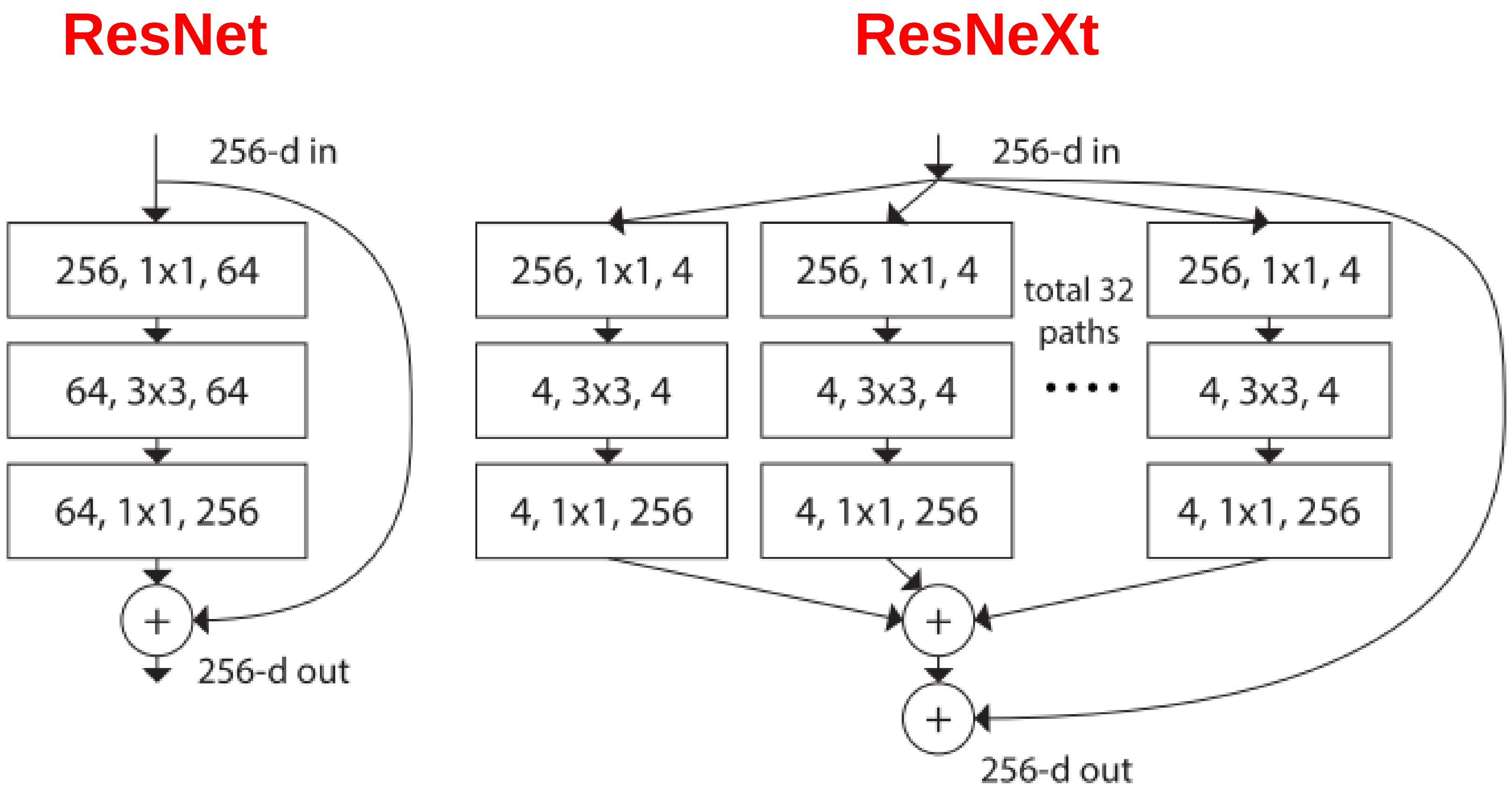
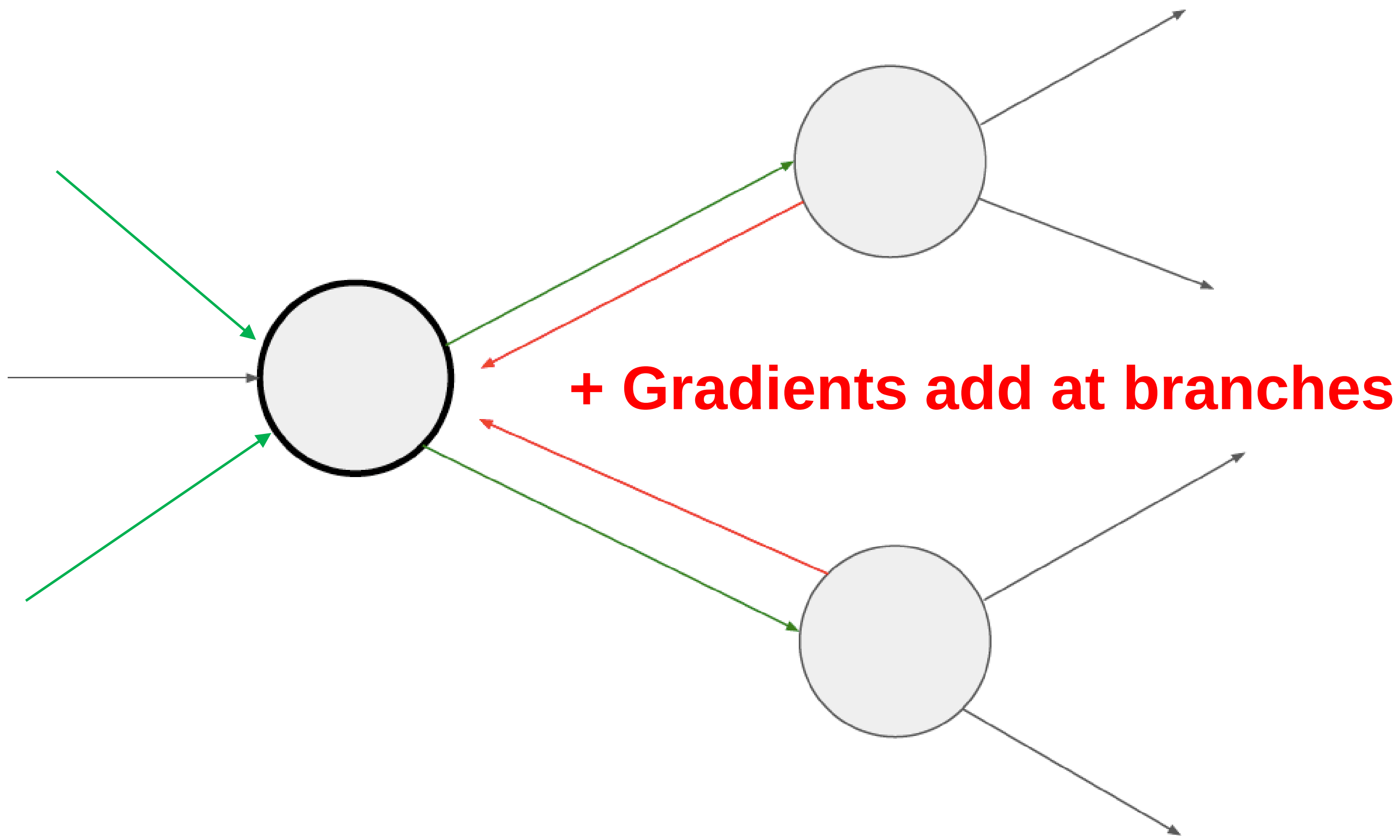


Figure source

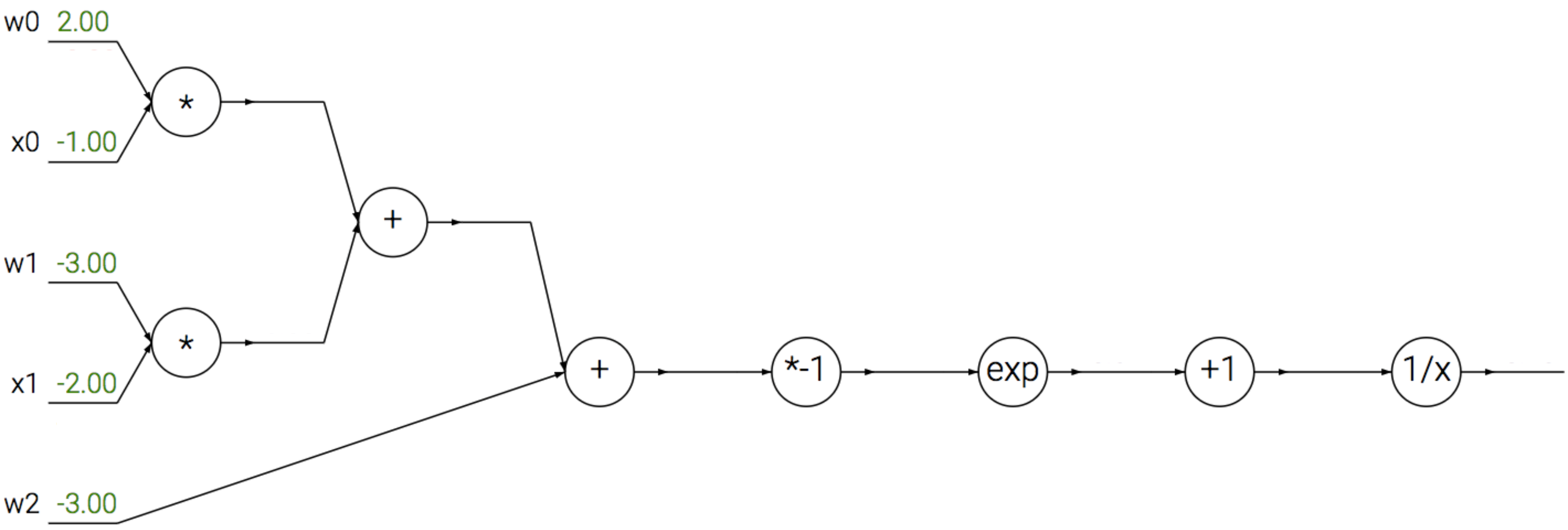
What about more general computation graphs?



Source: [Stanford 231n]

A detailed example

$$f(x,w) = \frac{1}{1+\exp[-(w_0x_0 + w_1x_1 + w_2)]}$$



Source: [Stanford 231n]()

A detailed example

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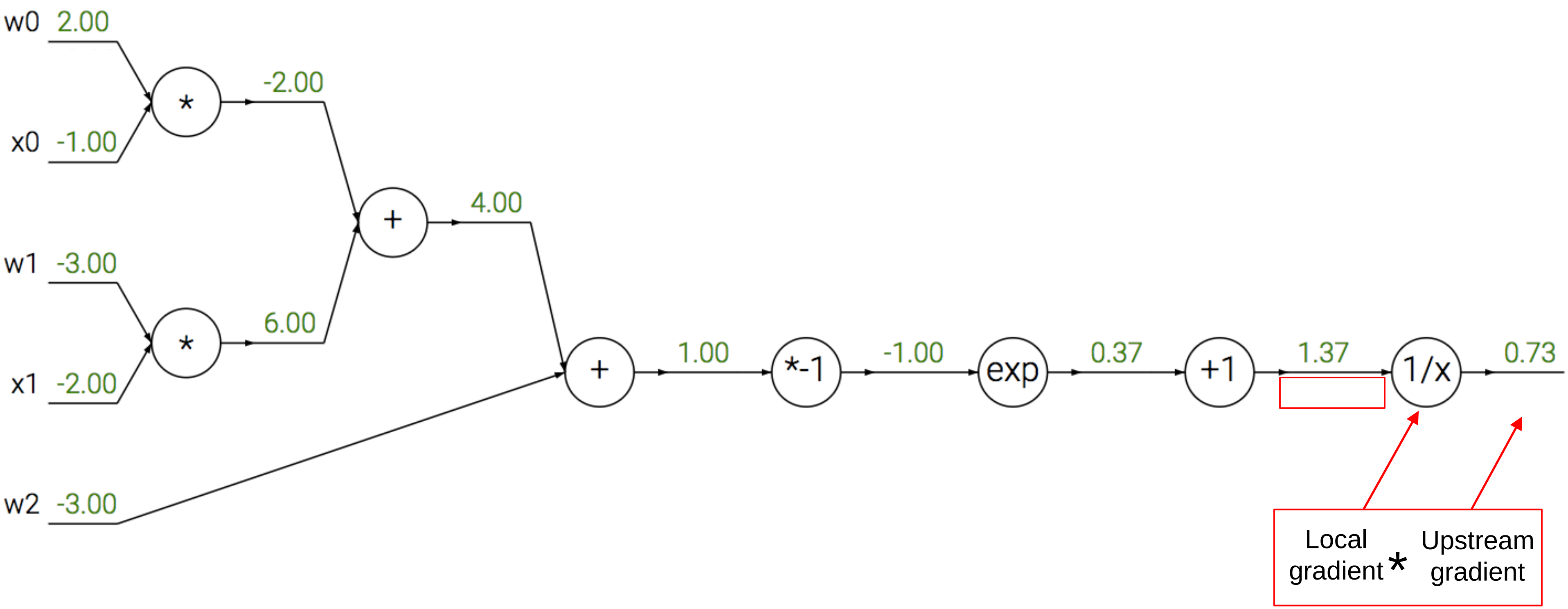


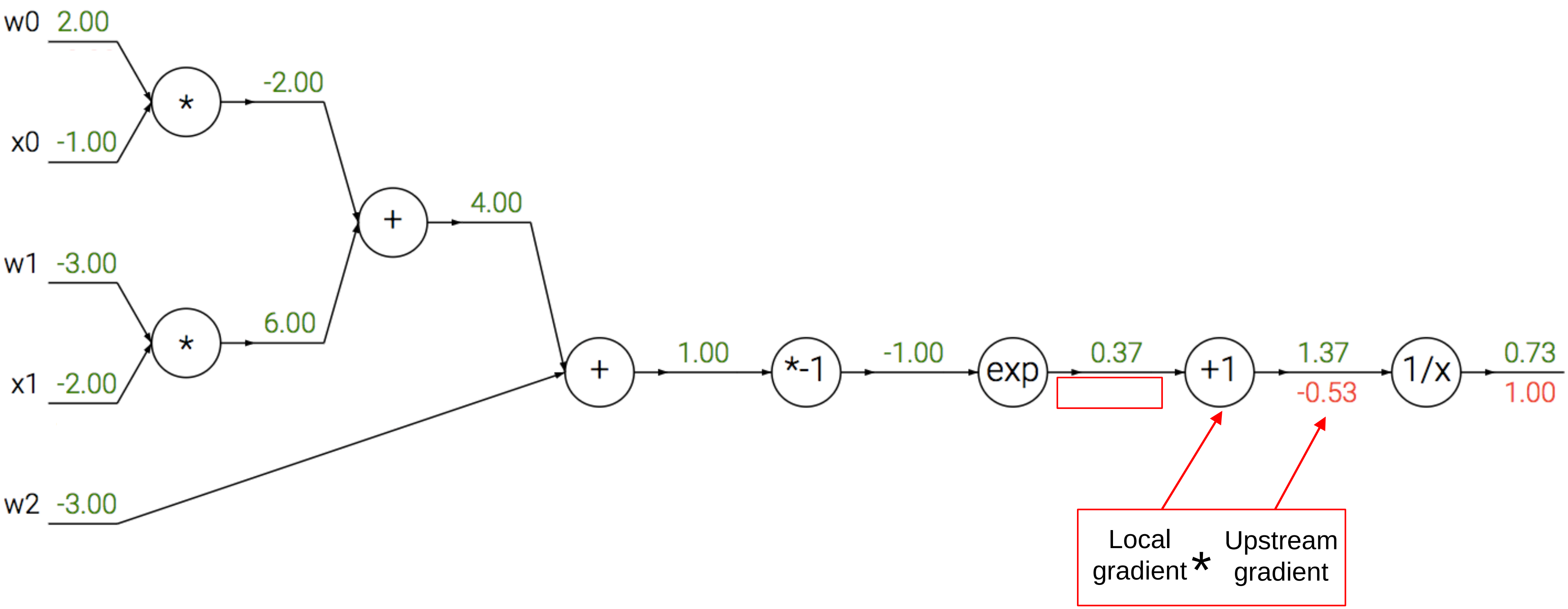
$$(1/x)' = -1/x^2$$

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

Source: [Stanford 231n]

A detailed example

$$f(x,w) = \frac{1}{1+\exp[-(w_0x_0+w_1x_1+w_2)]}$$



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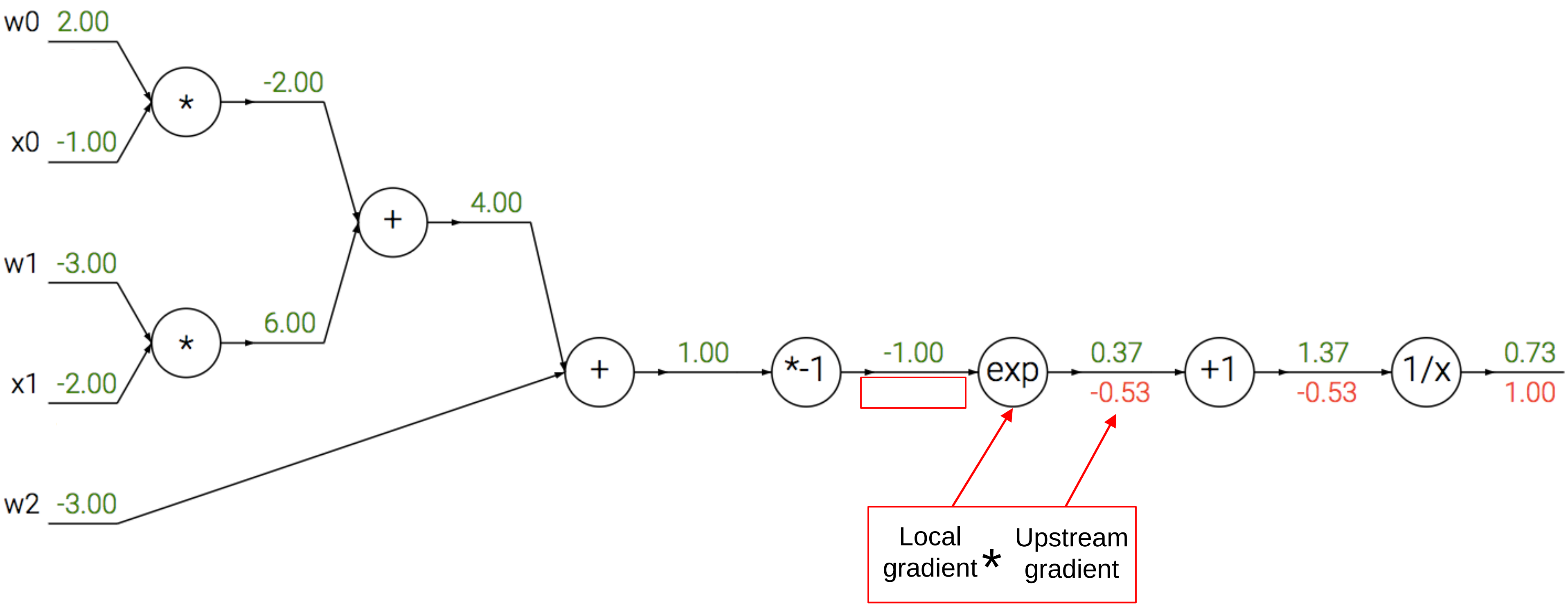
A detailed example

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

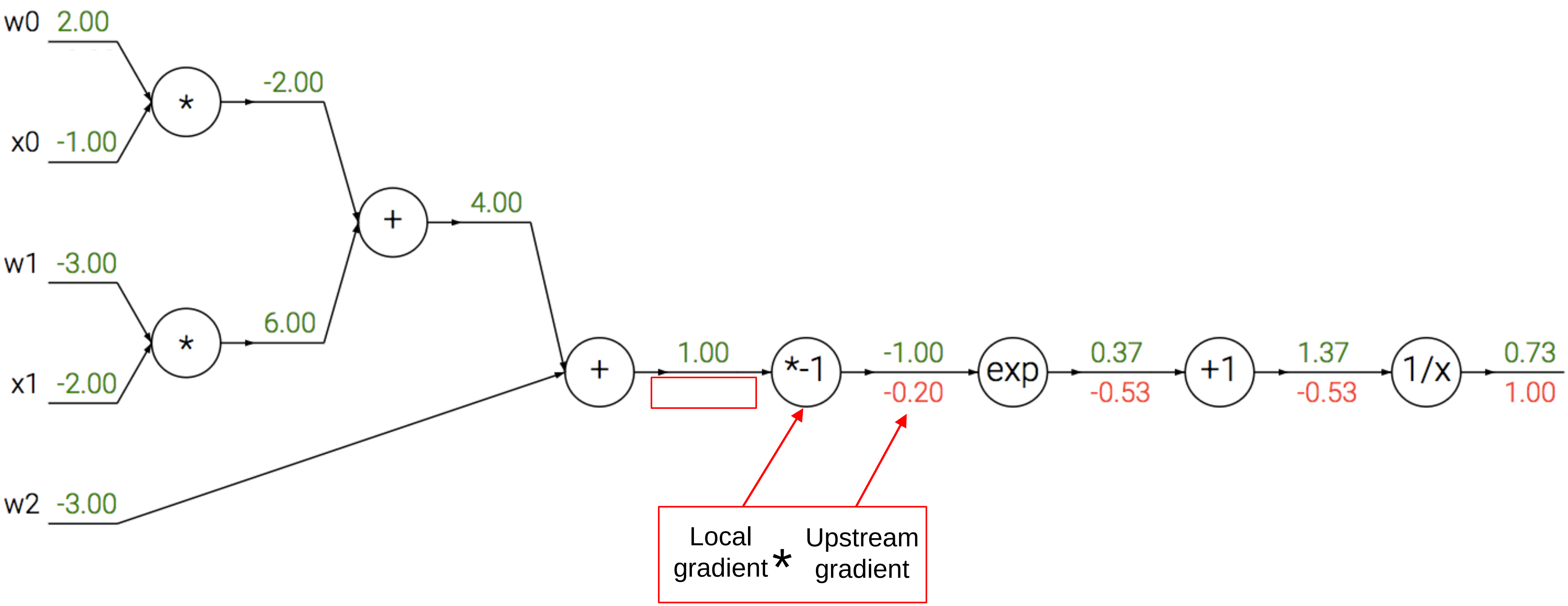


$$\exp(-1) * (-0.53) = -0.20$$

Source: [Stanford 231n]()

A detailed example

$$f(x,w) = \frac{1}{1 + \exp[-(w_0x_0 + w_1x_1 + w_2)]}$$



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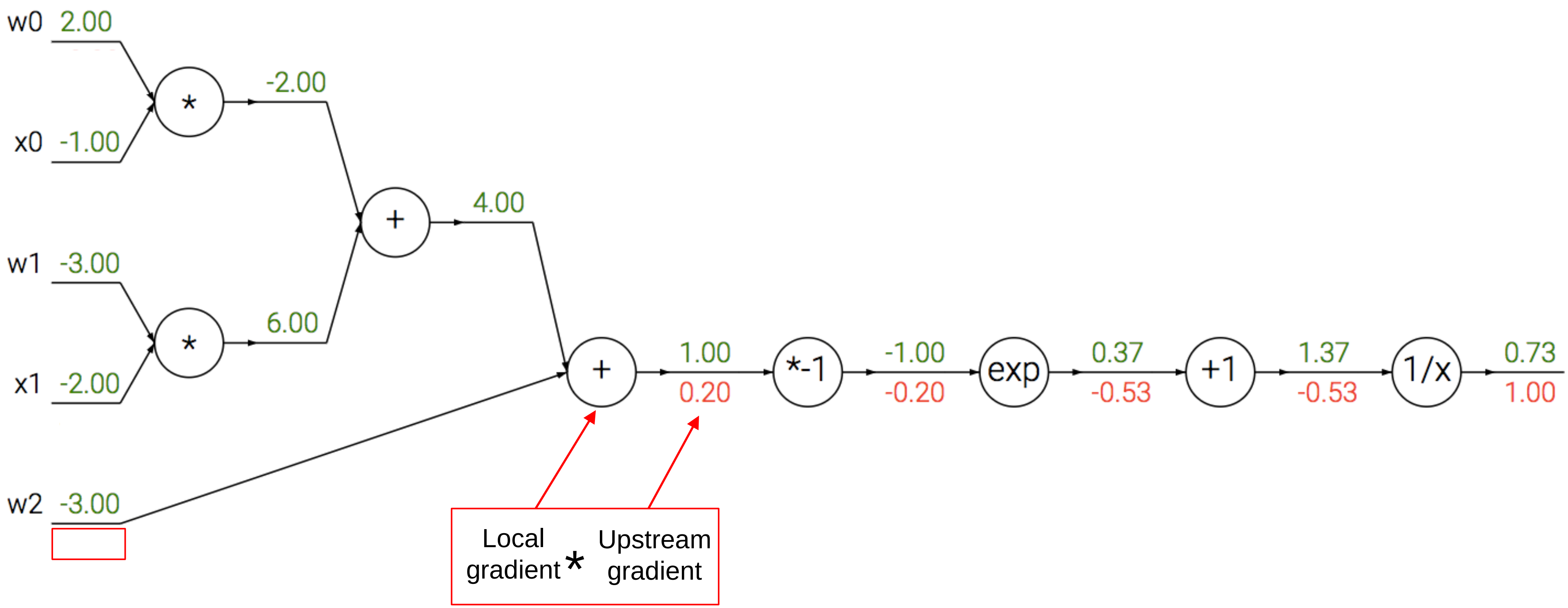

Source: [Stanford 231n]()

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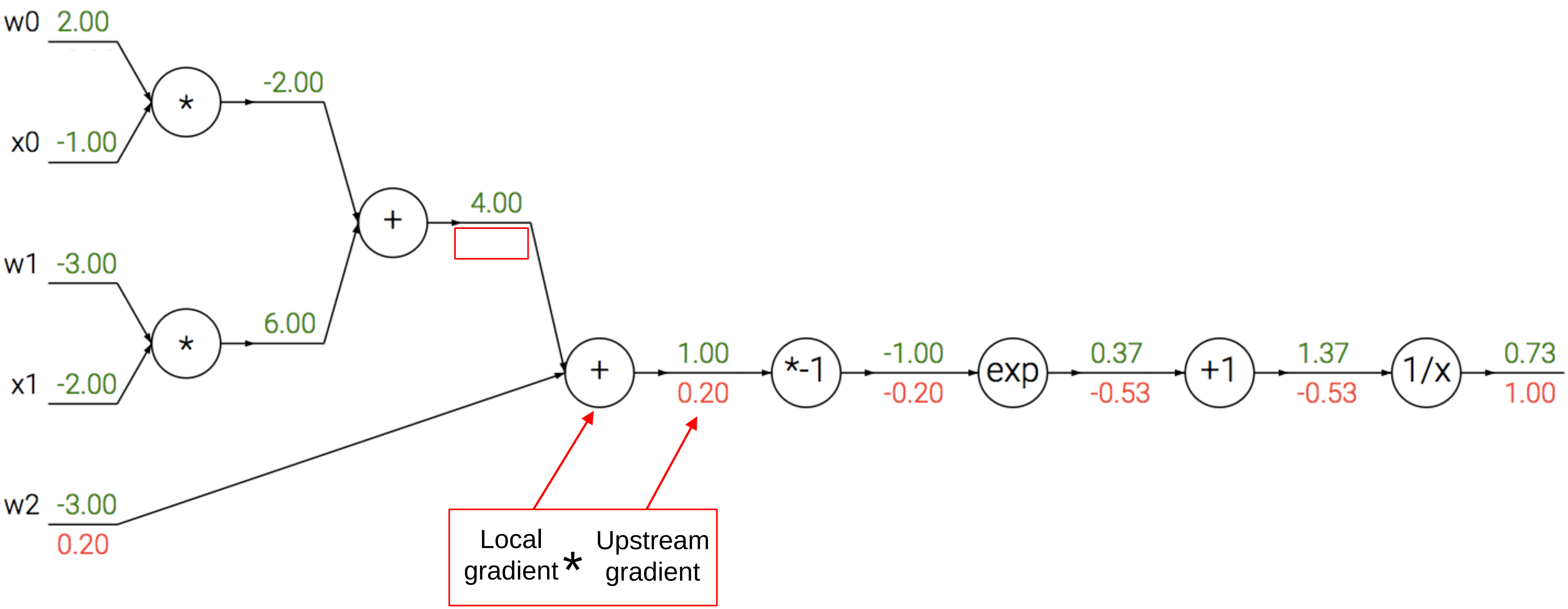

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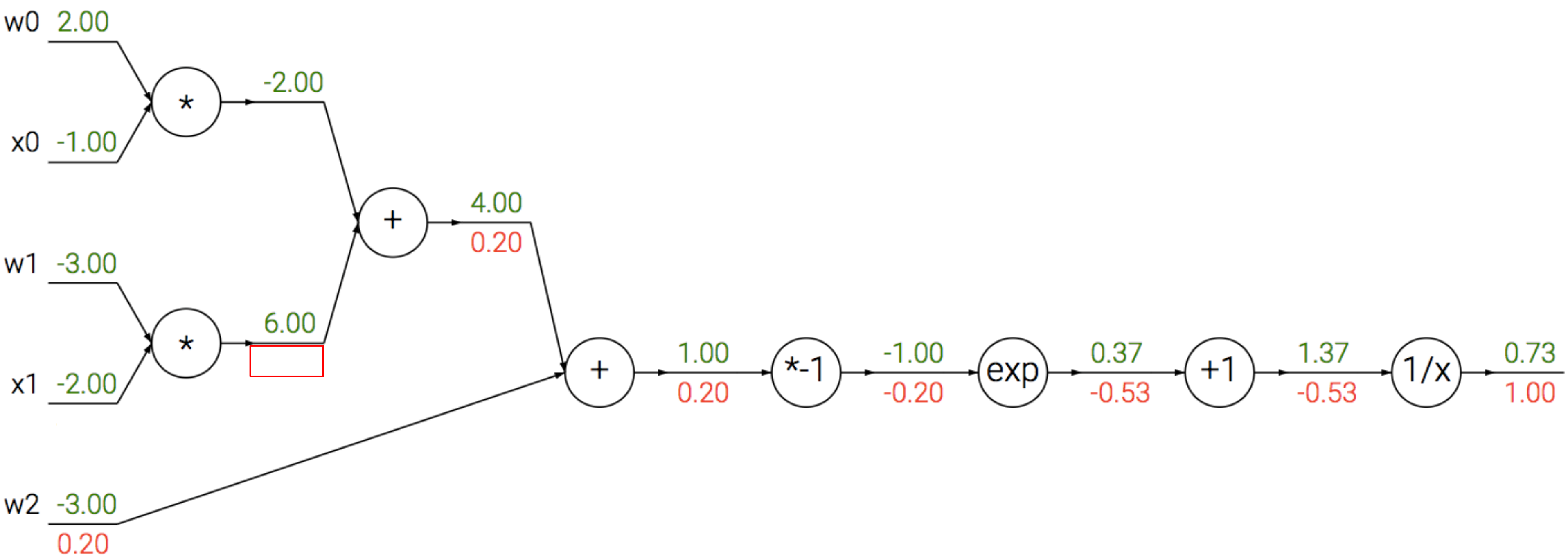

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A detailed example

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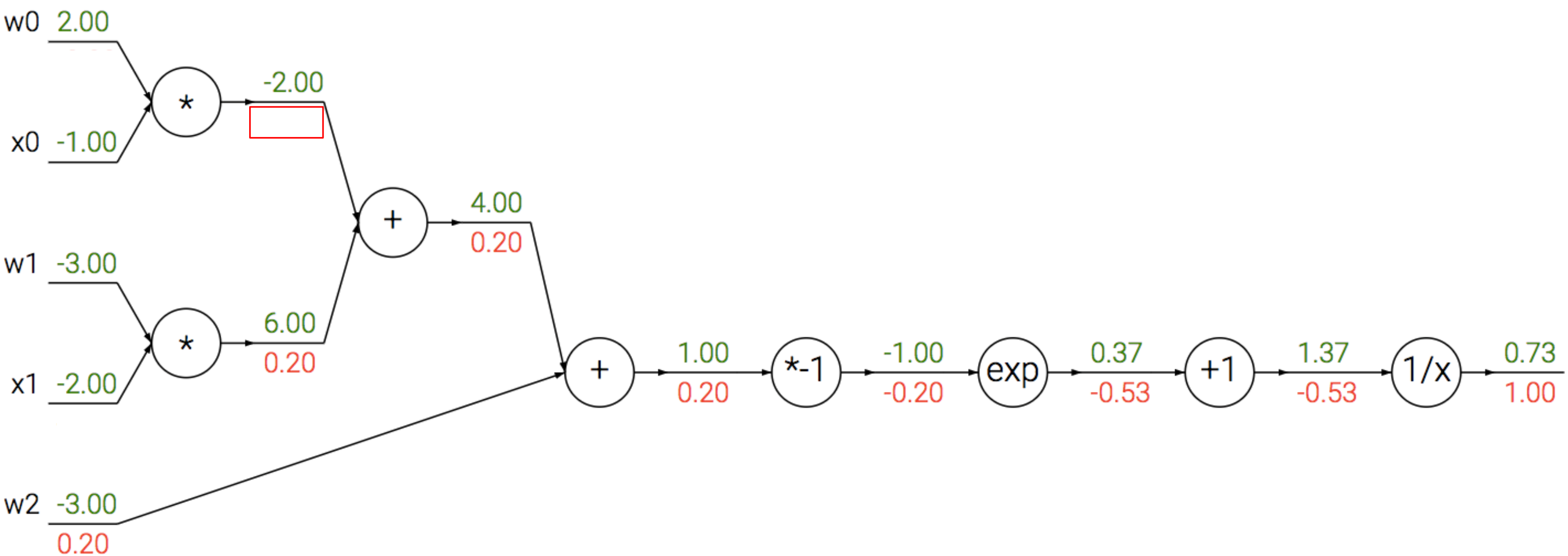

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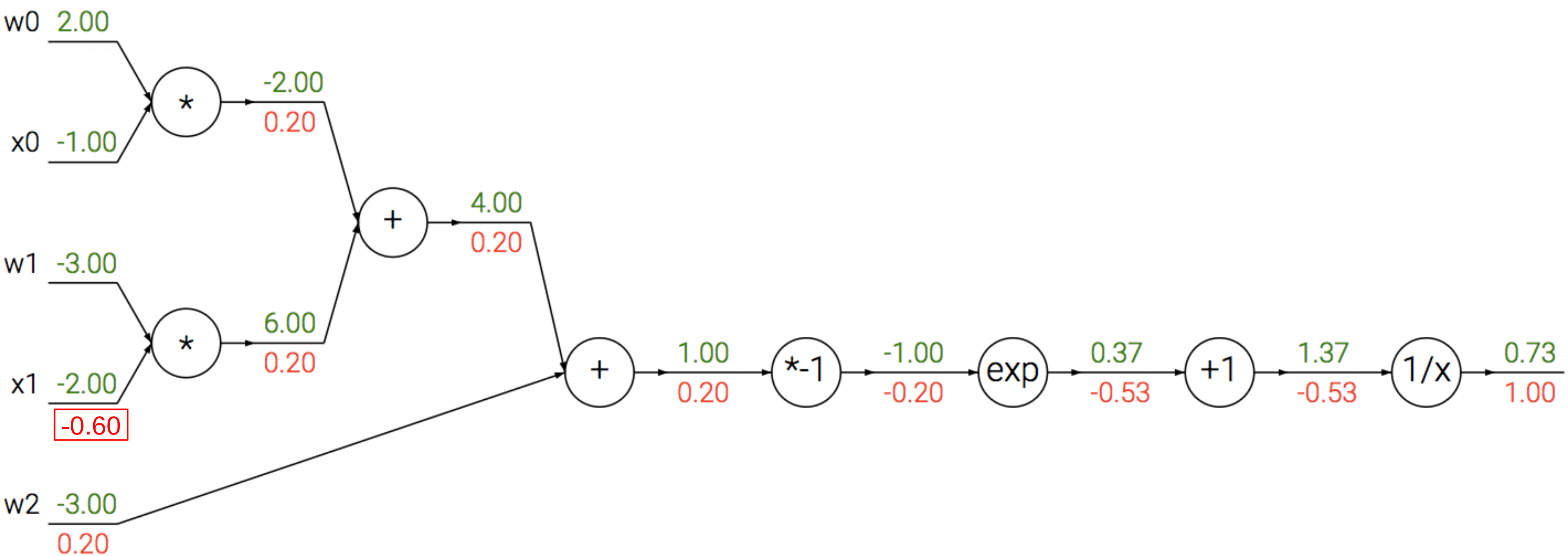

Source: [Stanford 231n]()

A detailed example

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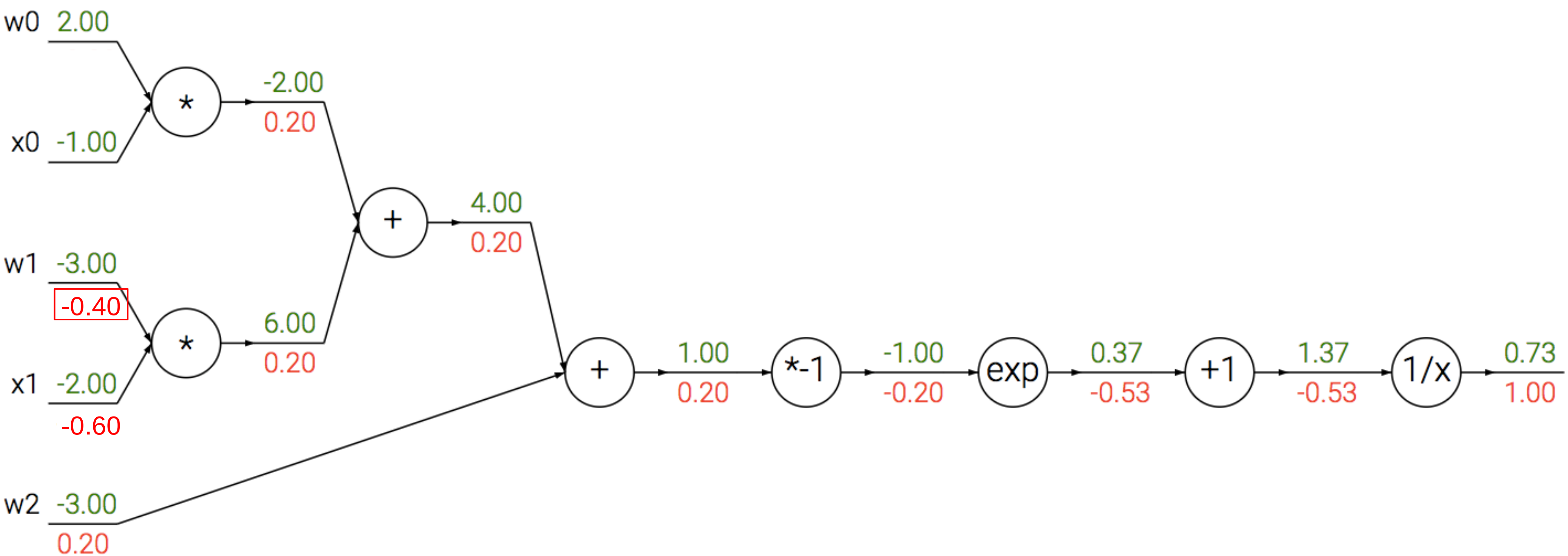

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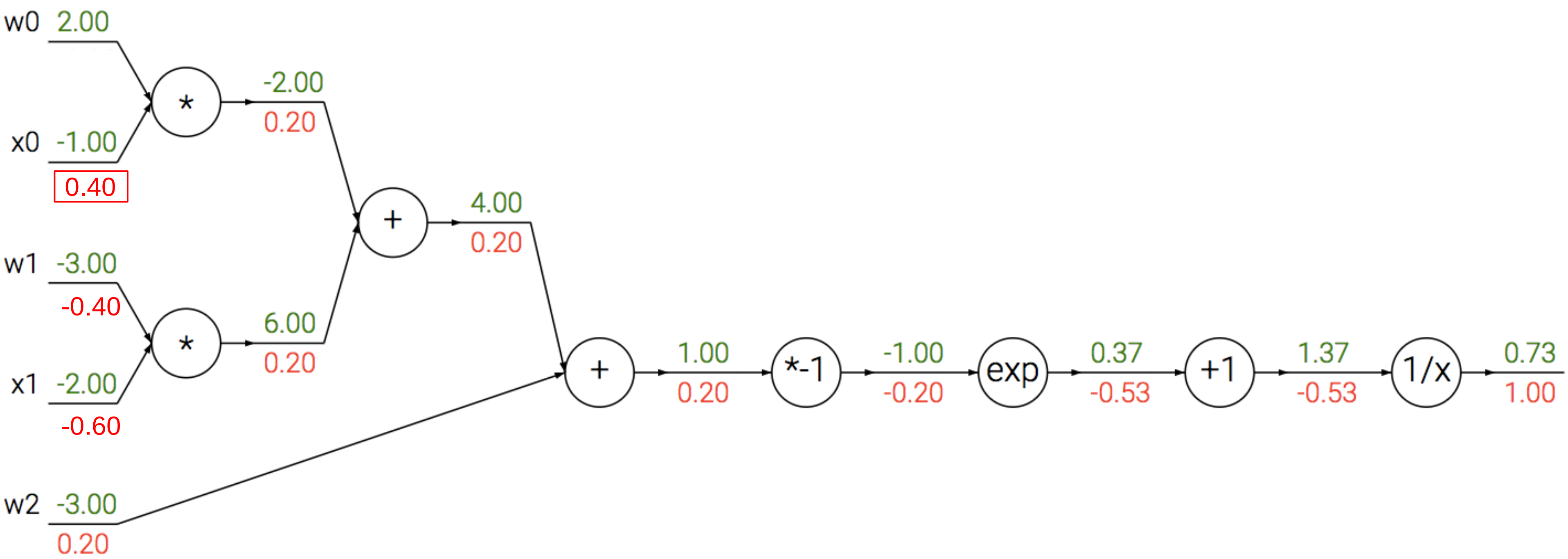

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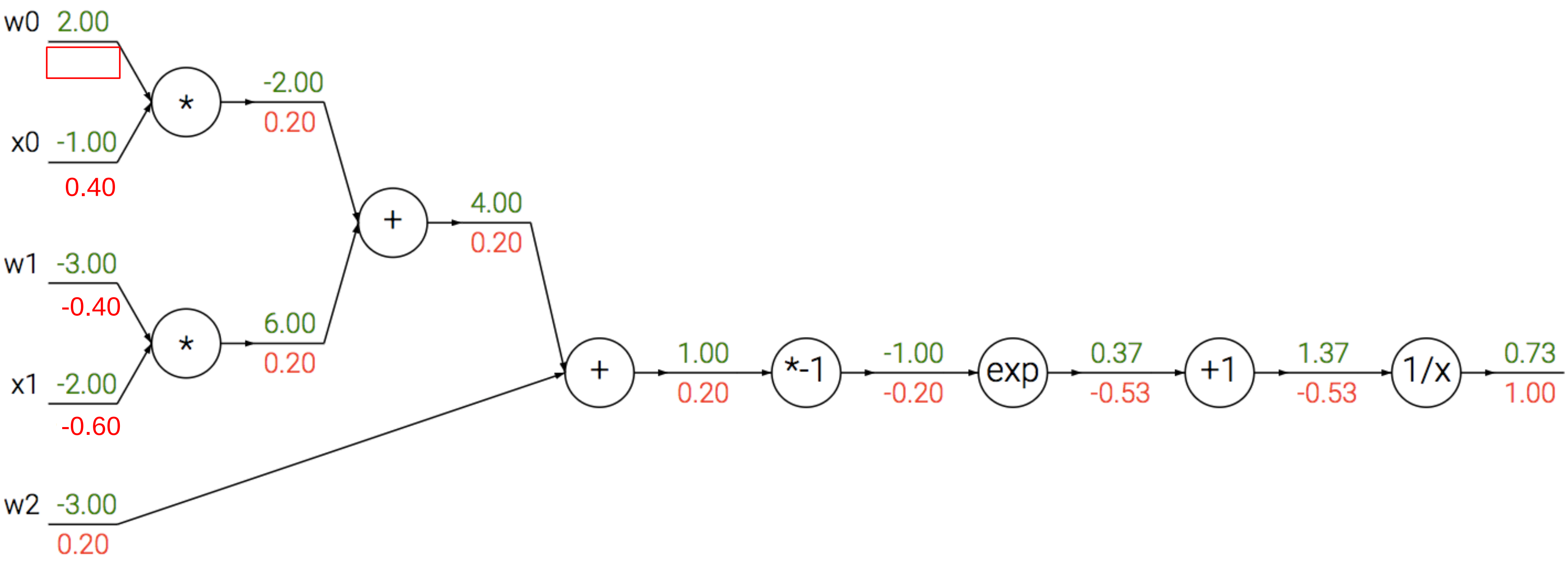

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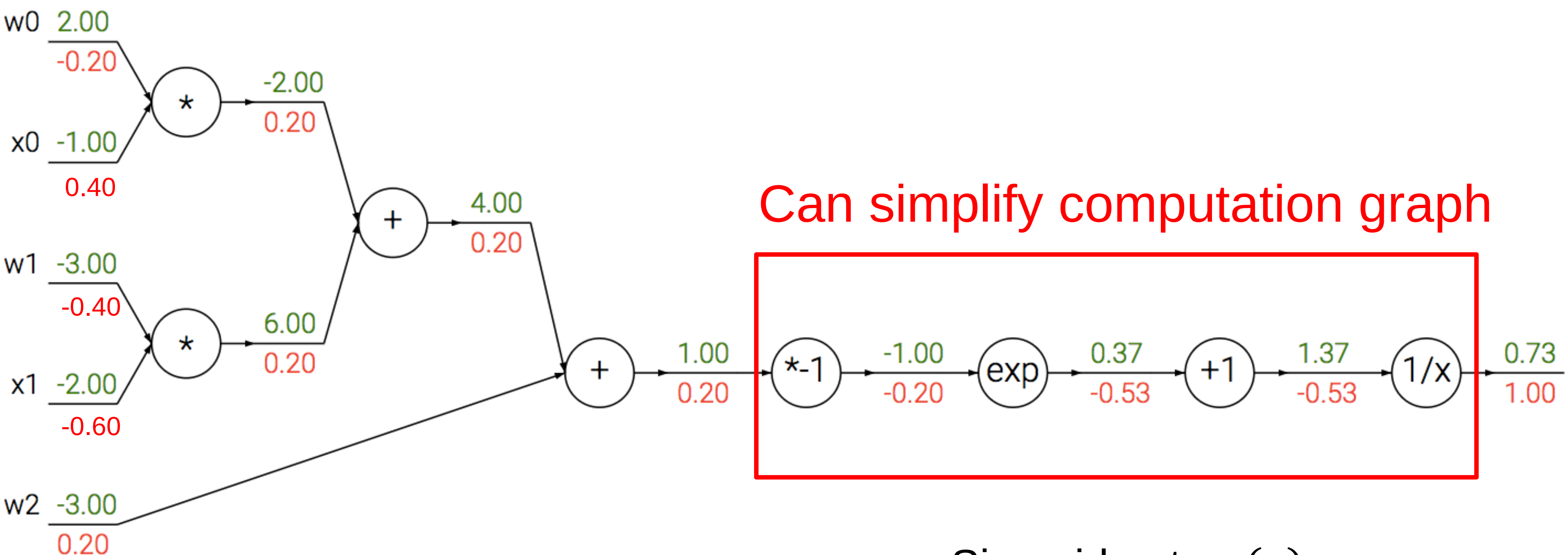


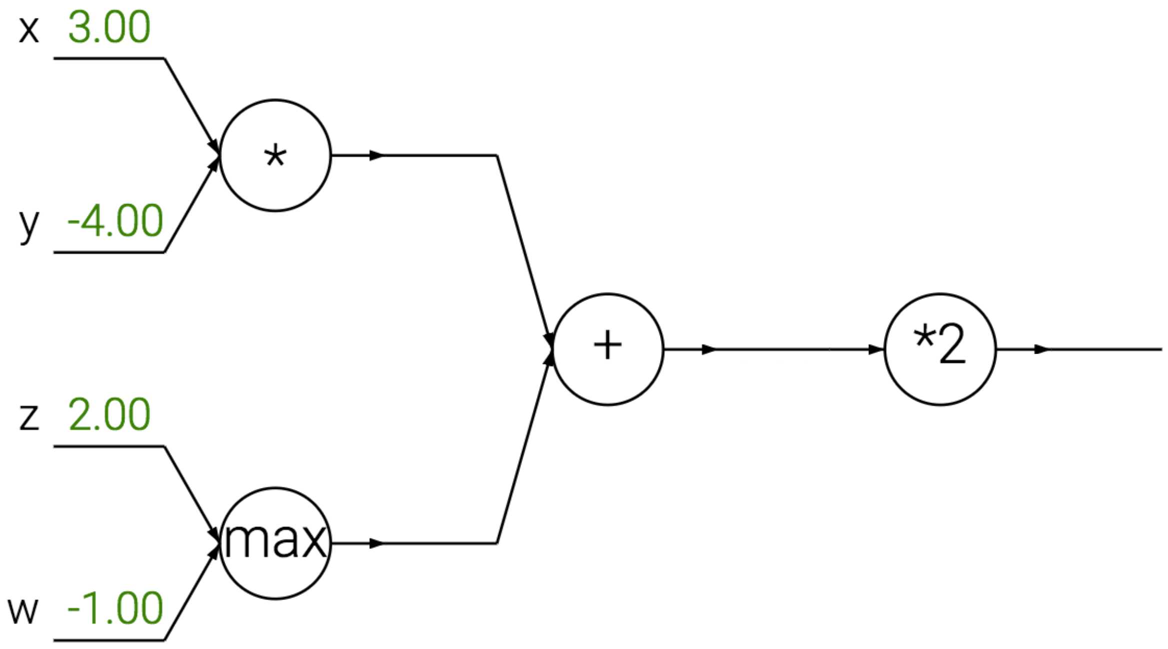
Sigmoid gate $\sigma(x)$

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

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

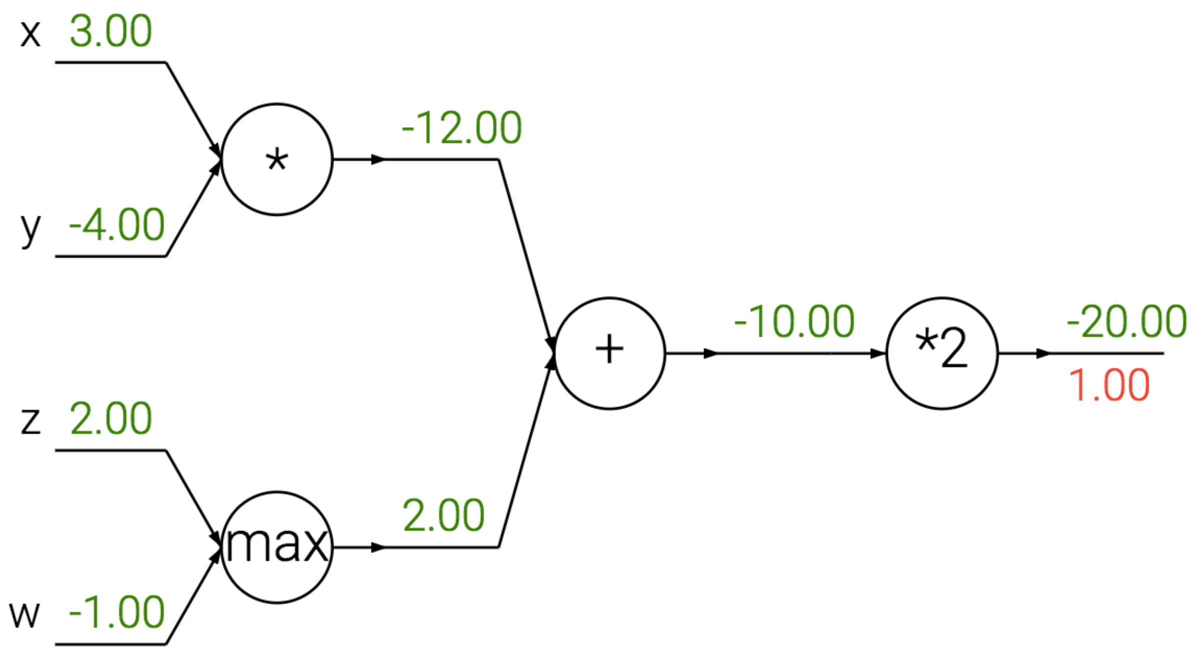
Source: [Stanford 231n]()

Patterns in gradient flow



Source: [Stanford 231n]

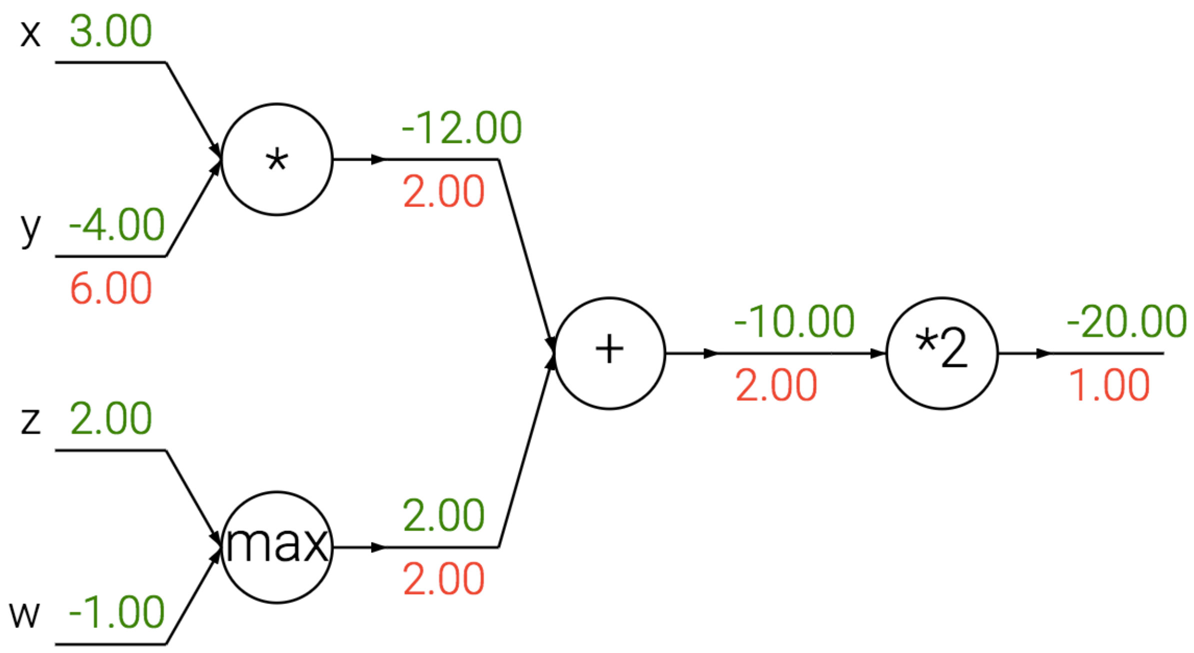
Patterns in gradient flow



Add gate: “gradient distributor”

Source: [Stanford 231n]()

Patterns in gradient flow

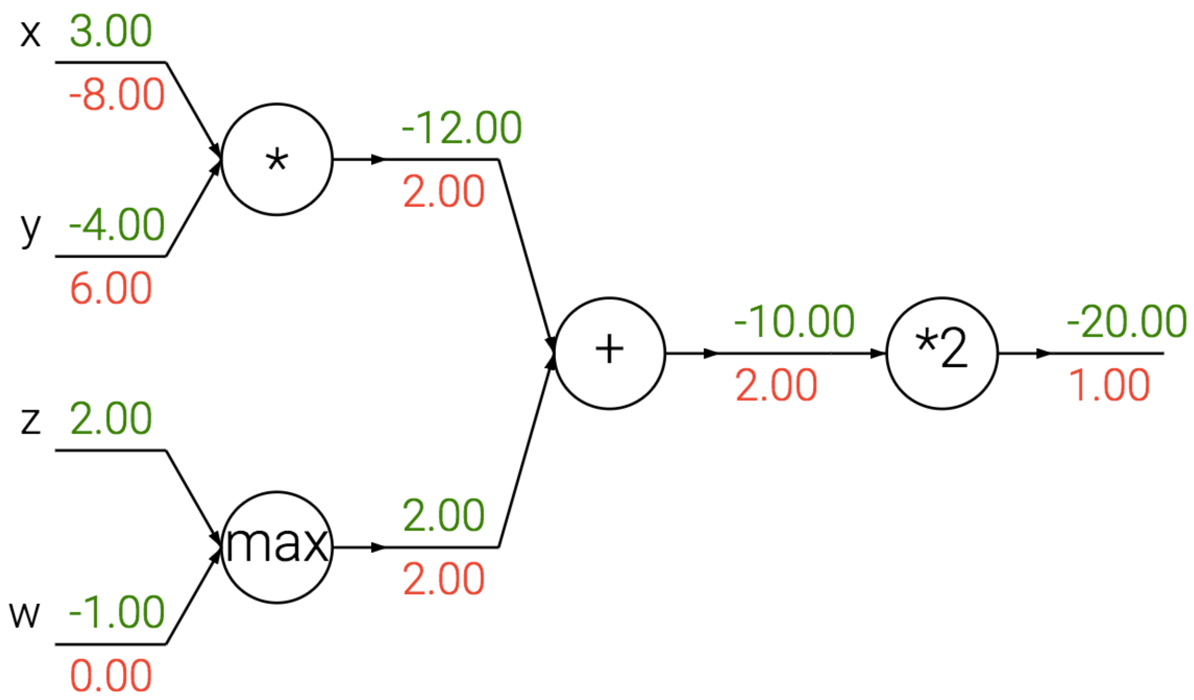


Add gate: “gradient distributor”

Multiply gate: “gradient switcher”

Source: [Stanford 231n]

Patterns in gradient flow



Add gate: “gradient distributor”

Multiply gate: “gradient switcher”

Max gate: “gradient router”

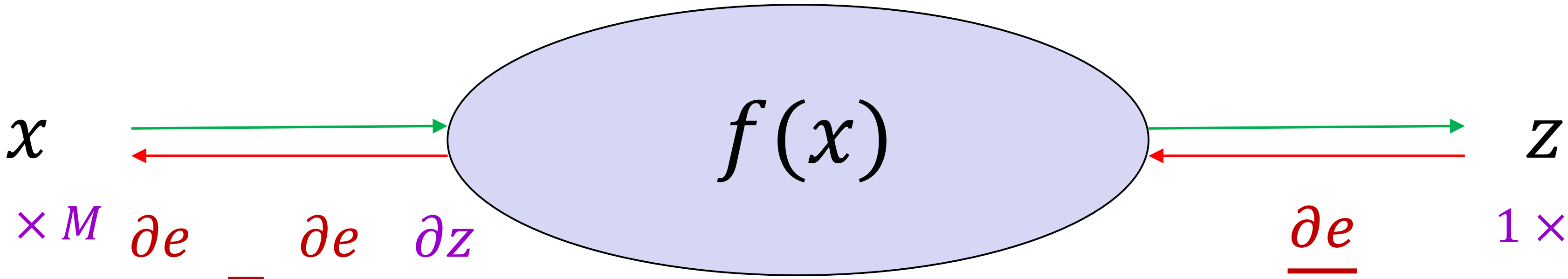
Source: [Stanford 231n]()

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



$1 \times M$

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

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

$1 \times N$

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

$1 \times N$

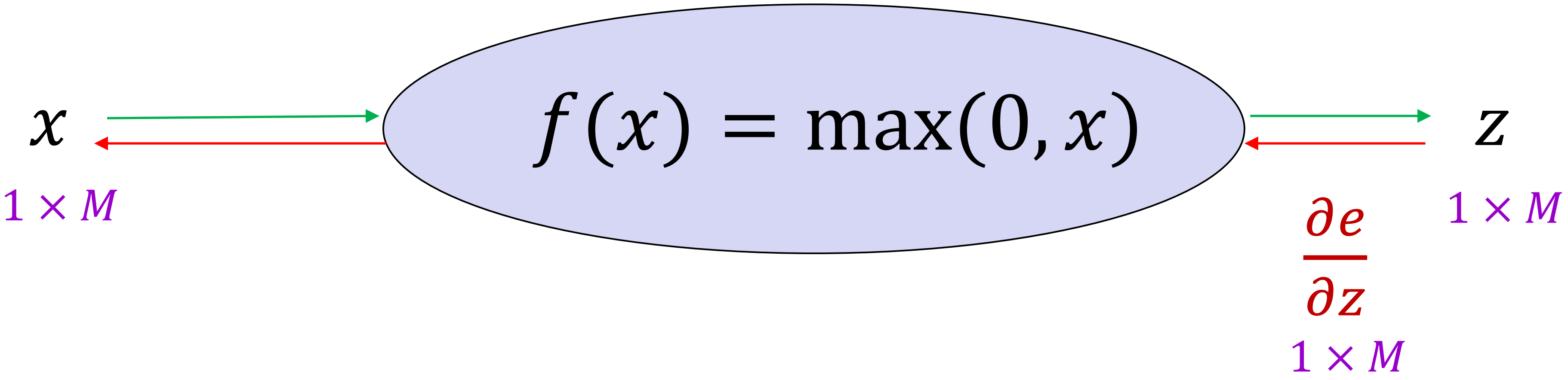
Simple case: Elementwise operation

Simple case: Elementwise operation

$$\frac{\partial z}{\partial x} = \begin{pmatrix} \frac{\partial z_1}{\partial x_1} & \cdots & \frac{\partial z_1}{\partial x_M} \\ \vdots & \ddots & \vdots \\ \frac{\partial z_M}{\partial x_1} & \cdots & \frac{\partial z_M}{\partial x_M} \end{pmatrix}$$

$M \times M$

Jacobian

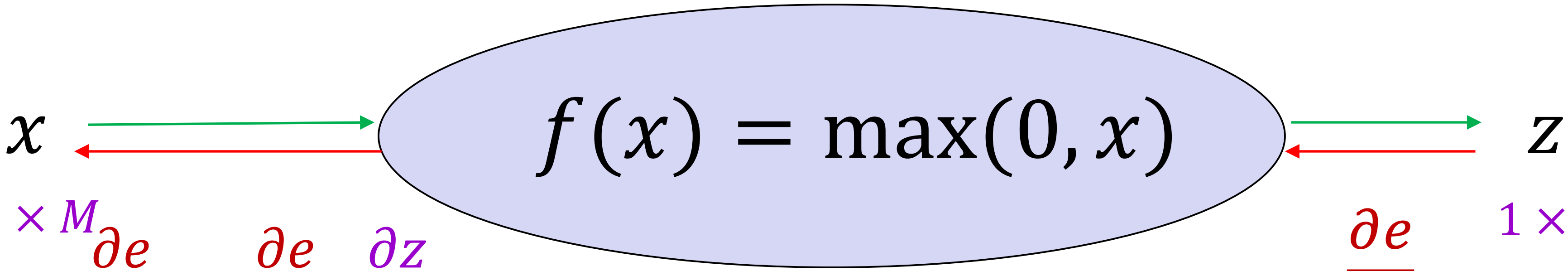


Simple case: Elementwise operation

$$\frac{\partial z}{\partial x} = \begin{pmatrix} \mathbb{I}[x_1 > 0] & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \mathbb{I}[x_M > 0] \end{pmatrix}$$

$M \times M$

Jacobian



$1 \times M$

$1 \times M$

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

$1 \times M$

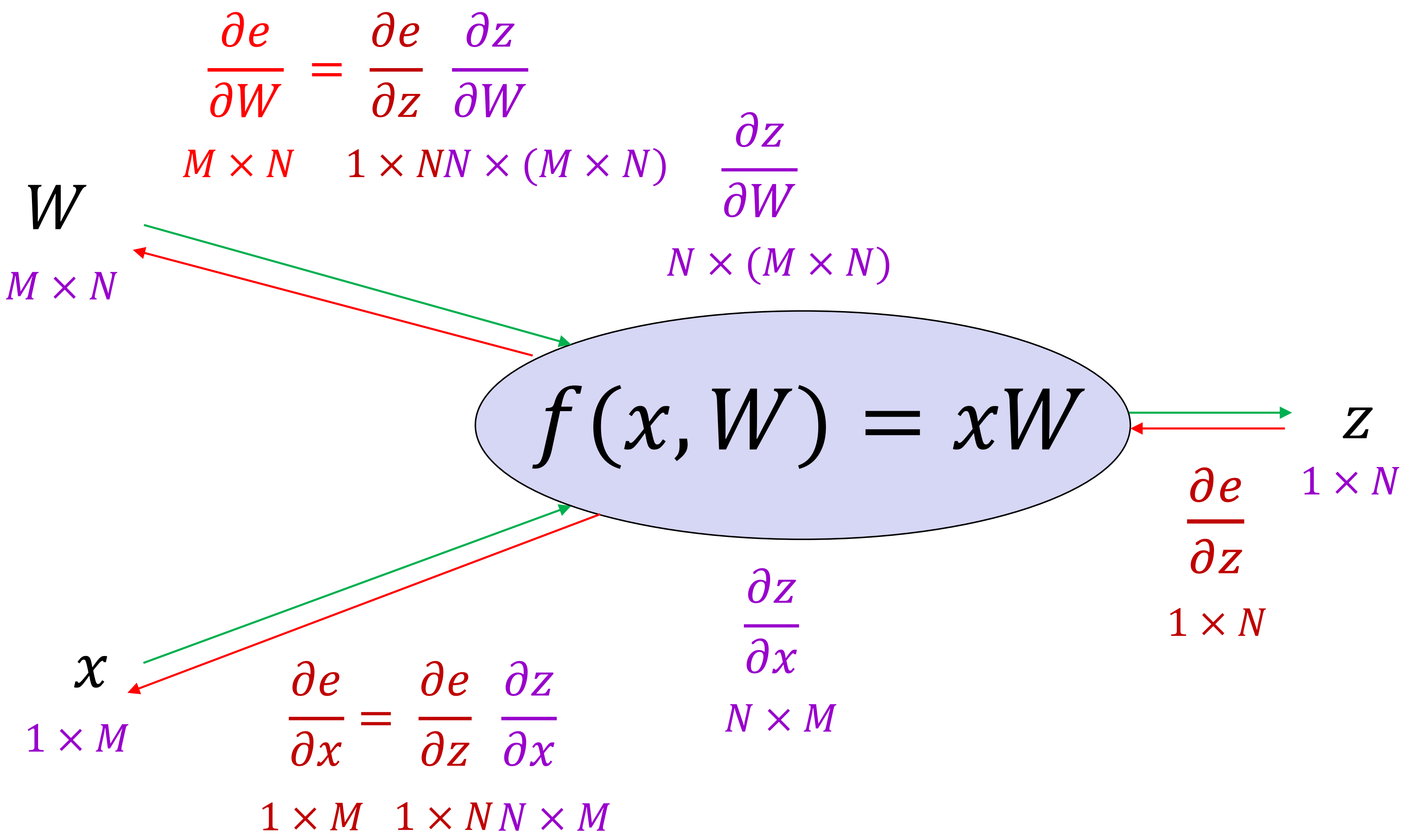
$$\frac{\partial e}{\partial x} = \frac{\partial e}{\partial z} \frac{\partial z}{\partial x}$$

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

$$\frac{\partial e}{\partial x_i} = \mathbb{I}[x_i > 0] \frac{\partial e}{\partial z_i}$$

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

Matrix-vector multiplication



Matrix-vector multiplication

$$(z_1 \quad \cdots \quad z_N) = (x_1 \quad \cdots \quad x_M)\begin{pmatrix} W_{11} & \cdots & W_{1N} \\ \vdots & \ddots & \vdots \\ W_{M1} & \cdots & W_{MN} \end{pmatrix} \qquad z_j = \sum_{i=1}^{M} x_i W_{ij}$$

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

$$\frac{\partial z_j}{\partial x_i} =$$

jth row, ith column of Jacobian

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

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

Matrix-vector multiplication

$$(z_1 \quad \cdots \quad z_N) = (x_1 \quad \cdots \quad x_M)\begin{pmatrix} W_{11} & \cdots & W_{1N} \\ \vdots & \ddots & \vdots \\ W_{M1} & \cdots & W_{MN} \end{pmatrix} \qquad z_j = \sum_{i=1}^{M} x_i W_{ij}$$

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

$$\frac{\partial e}{\partial W_{ij}} =$$

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

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

- **Useful resource:** see Lecture 4 of Stanford 231n and associated links in the syllabus