Multi-Layer Networks & Back-Propagation

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Deep Learning

Sharif University of Technology

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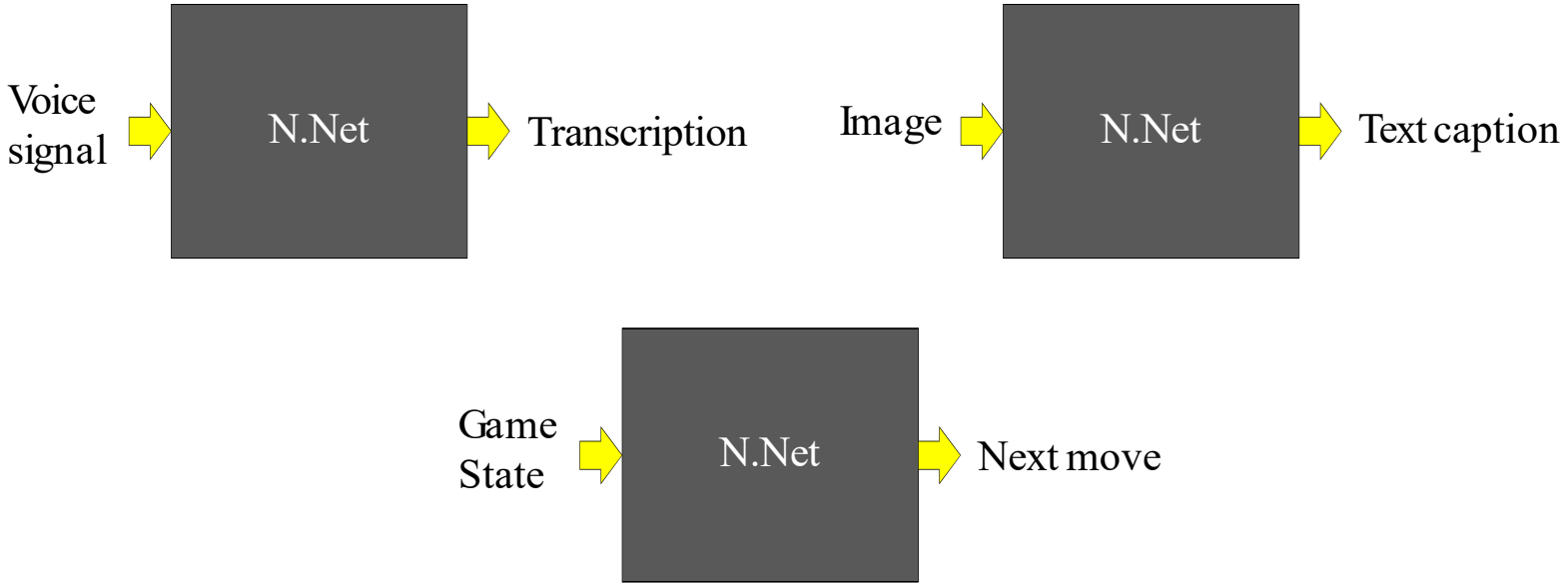
Most slides have been adapted from Bhiksha Raj, 11-785
and some from Fei Fei Li et. al, cs231n, Stanford

These boxes are functions



- Take an input
- Produce an output
- Can be modeled by a neural network!
- How do we compose the network that performs the requisite function?

Problem setup

- Given: the architecture of the network
- Training data: A set of input-output pairs

$$\left(x^{(1)}, y^{(1)}\right), \left(x^{(2)}, y^{(2)}\right), \ldots, \left(x^{(N)}, y^{(N)}\right)$$

- We want to find the function f
  - We consider a neural network as a parametric function $f(x; W)$
- We need a loss function to show how penalizes the obtained output $f(x; W)$ when the desired output is y

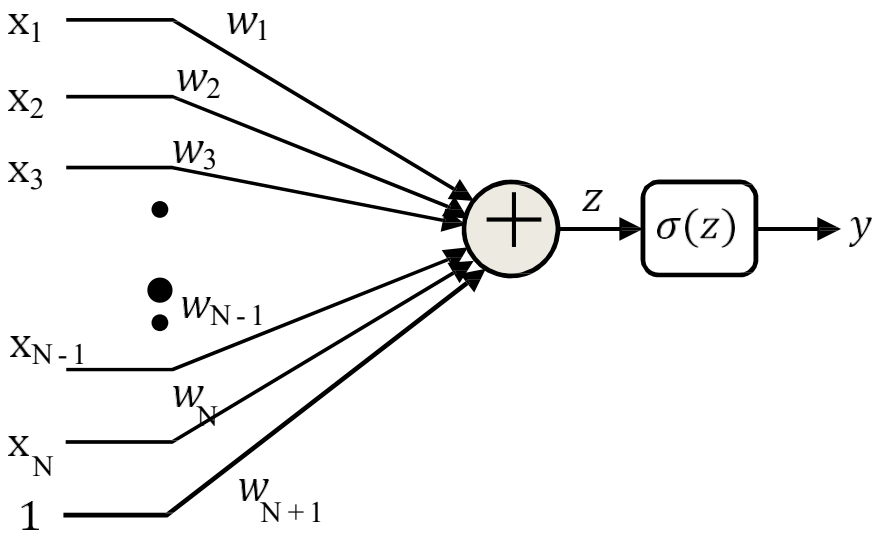
$$E(W) = \frac{1}{N} \sum_{n=1}^{N} loss\left(f\left(x^{(n)}; W\right), y^{(n)}\right)$$

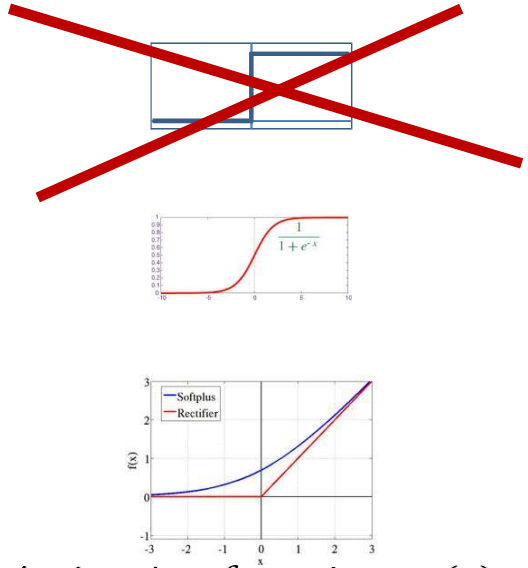
- Minimize the cost function

Training an MLP

- We define differentiable loss or divergence between the output of the network and the desired output for the training instances
  - And a total error, which is the average divergence over all training instances
- We use continuous activation functions to enables us to estimate network parameters
- We optimize network parameters to minimize the total error

Activation function

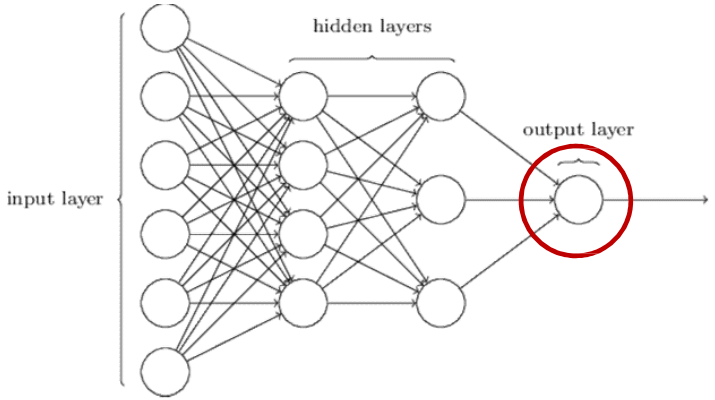


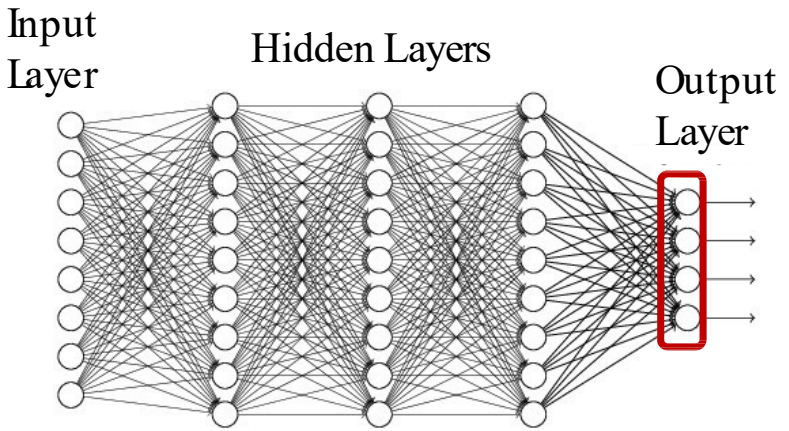


Activation functions $\sigma(z)$

- Makes the neuron differentiable, with non-zero derivatives over much of the input space
  - Small changes in weight can result in non-negligible changes in output
  - This enables us to estimate the parameters using gradient descent techniques..

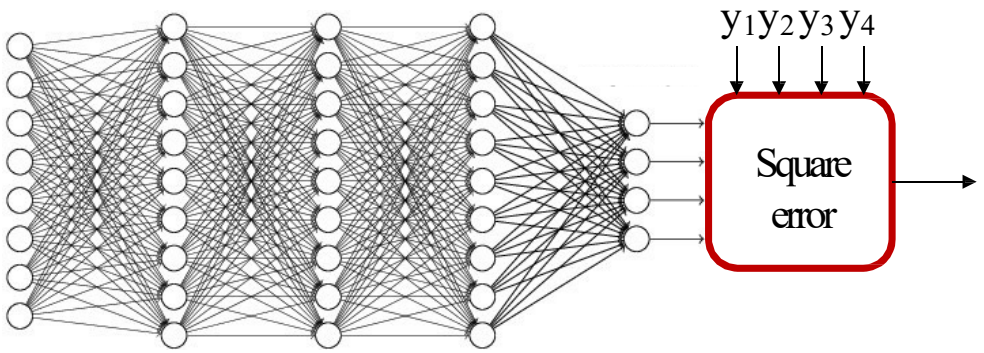
Representing the output





- If the desired output is real-valued, no special tricks are necessary
  - Scalar Output : single output neuron
    - o = scalar (real value)
  - Vector Output : as many output neurons as the dimension of the desired output
    - $\boldsymbol{o} = [o_1, o_2, \ldots, o_K]^T$ (vector of real values)

Examples of loss functions

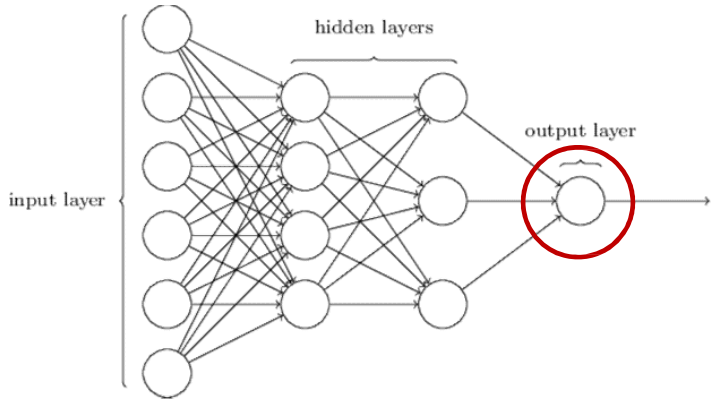


- For real-valued output vectors, the (scaled) L_2 divergence is popular

$$loss(\boldsymbol{y}, \boldsymbol{o}) = \frac{1}{2}\|\boldsymbol{y} - \boldsymbol{o}\|^2 = \frac{1}{2}\sum_k (y_k - o_k)^2$$

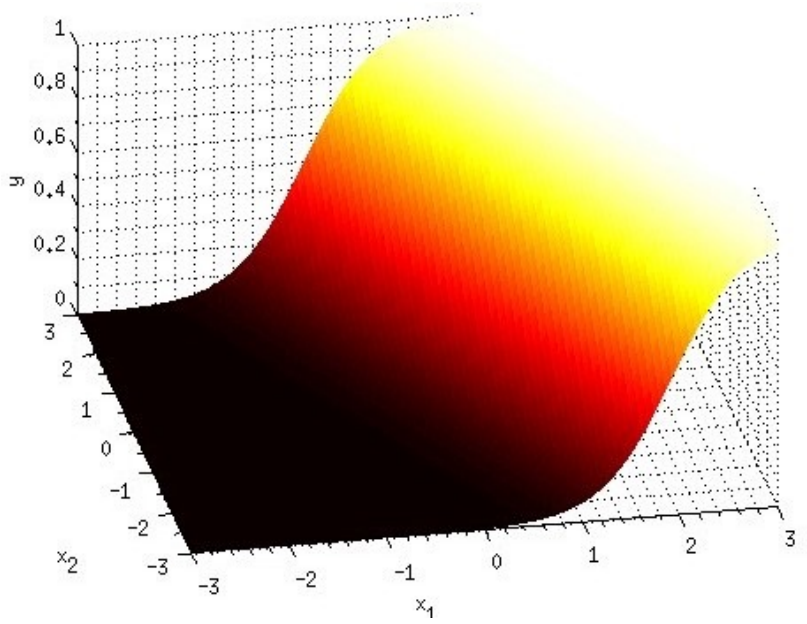
  - Squared Euclidean distance between true and desired output
  - Note: this is differentiable

Representing the output

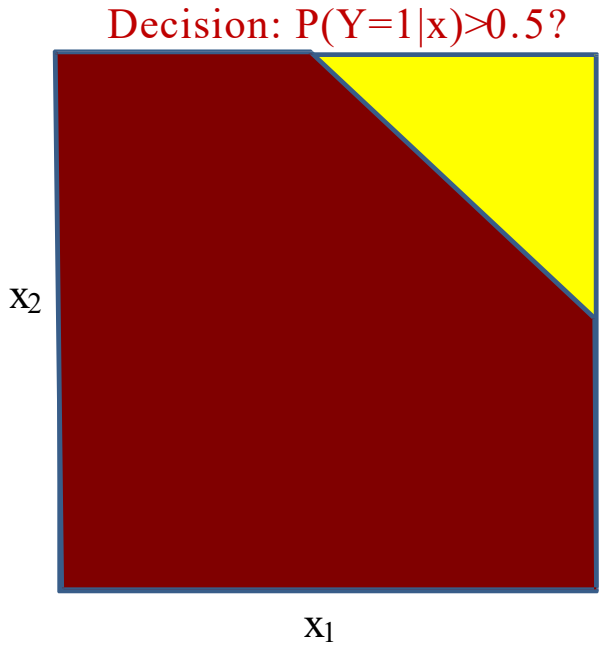


- If the desired output is binary (is this a cat or not), use a simple 1/0 representation of the desired output
  - 1 =YES it's a cat
  - 0 = NO it's not a cat.

Logistic regression



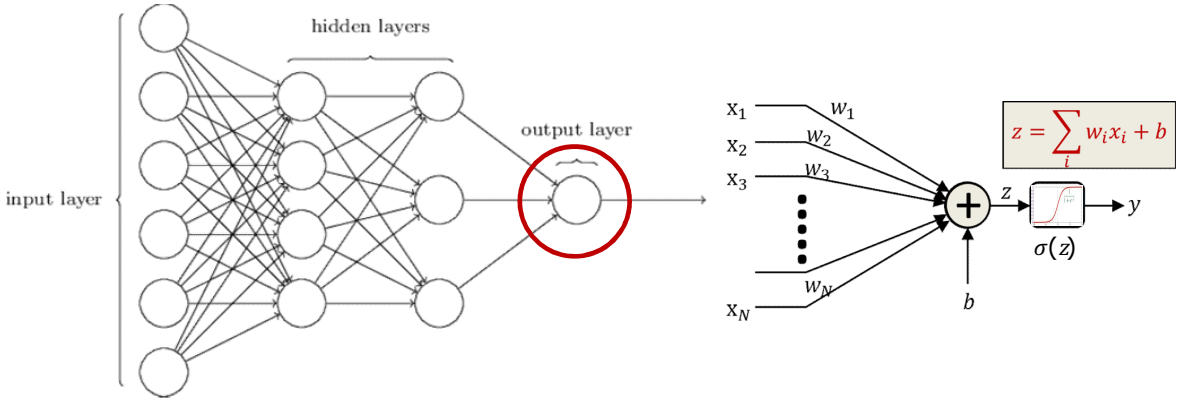
When X is a 2-D variable



$$P(Y = 1|X) = \frac{1}{1 + \exp\left(-\sum_i w_i x_i - b\right)}$$

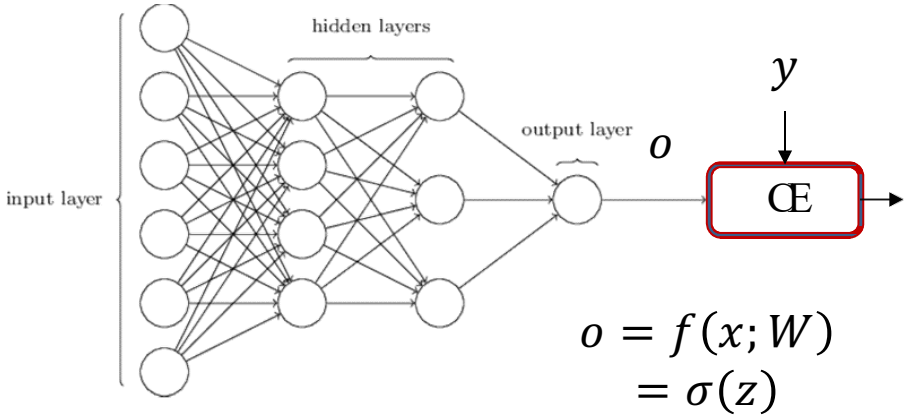
- This the perceptron with a sigmoid activation
  - It actually computes the probability that the input belongs to class 1

Representing the output



- If the desired output is binary, use a simple 1/0 representation of the desired output
- Output activation: Typically a sigmoid
  - Viewed as the probability $P(Y = 1|\boldsymbol{x})$ of class value 1
    - Indicating the fact that for actual data, in general a feature vector may occur for both classes, but with different probabilities
    - Is differentiable

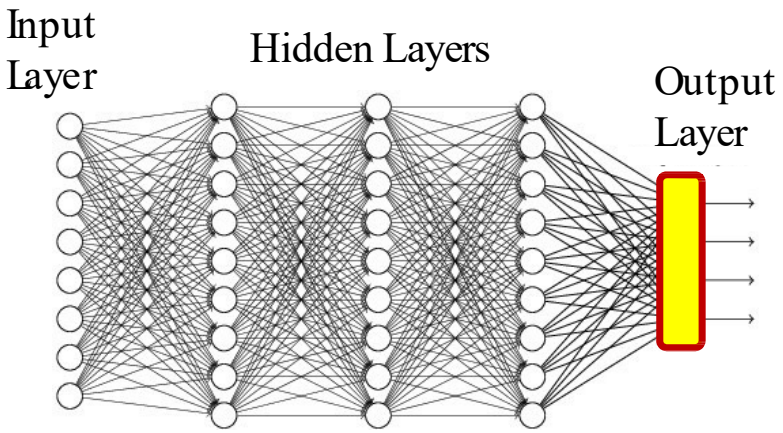
For binary classifier: Logistic regression



- For binary classifier with scalar output $o \in (0,1)$, y is 0/1:

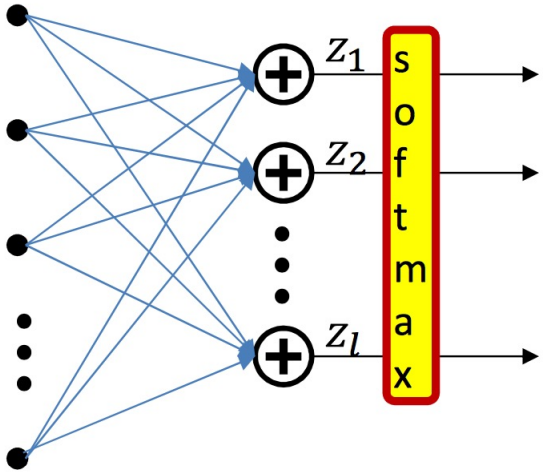
$$loss(y, o) = -ylogo\ -(1-y)\log(1-o)$$

Multi-class networks



- For a multi-class classifier with K classes, the one-hot representation for the desired output y
  - The neural network's output too must ideally be binary (K-1 zeros and a single 1 in the right place)
- The network's output will be a probability vector
  - K probability values that sum to 1.

Vector activation example: Softmax



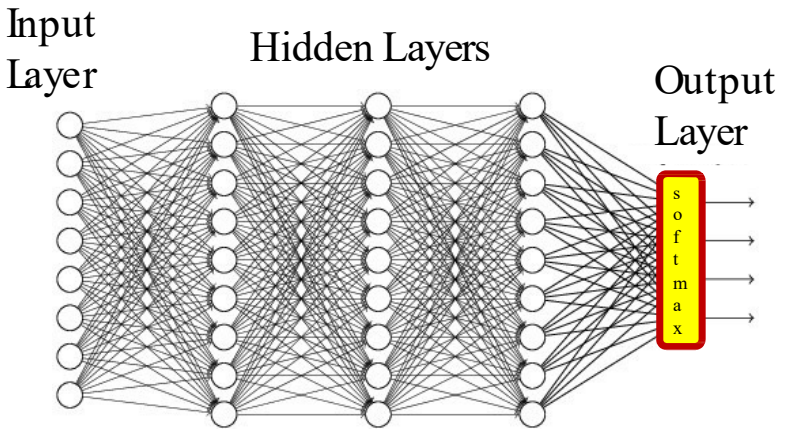
- Example: Softmax vector activation

$$z_i = \sum_j w_{ji} x_j + b_i$$

Parameters are weights w_{ji} and bias b_i

$$o_i = \frac{exp(z_i)}{\sum_j exp(z_j)}$$

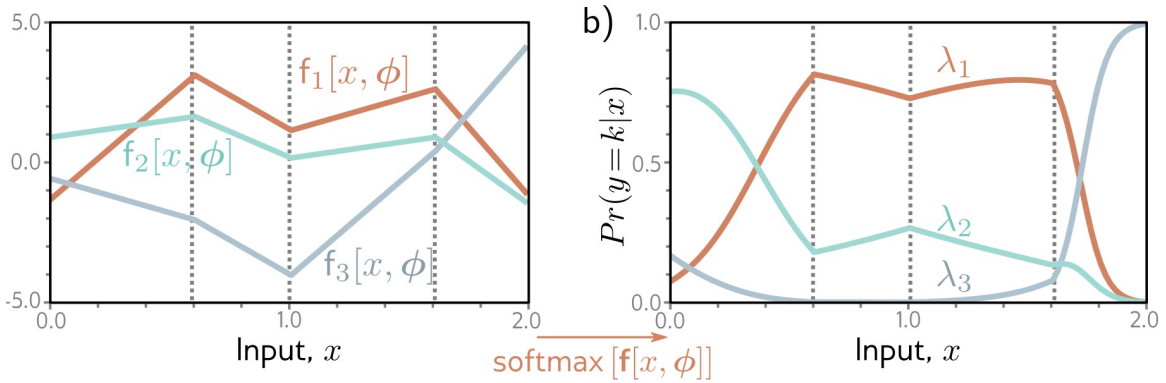
Multi-class classification: Output



- Softmax vector activation is often used at the output of multi-class classifier nets

$$z_i = \sum_j w_{ji}^{(l)} a_j^{(n-1)}$$

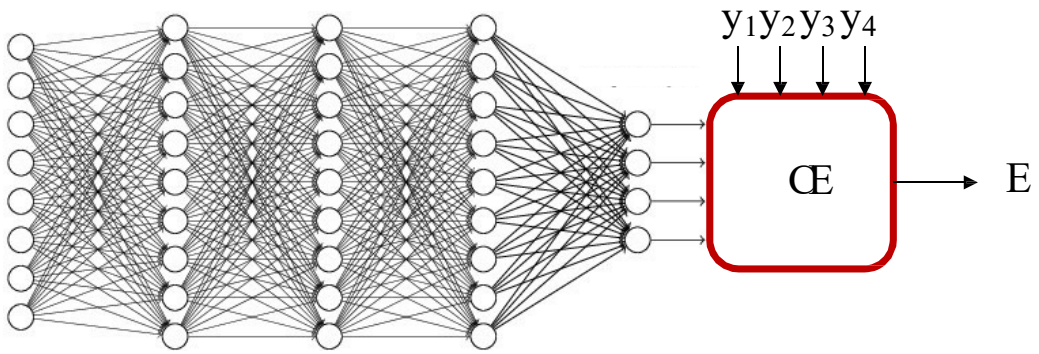
$$o_i = \frac{\exp(z_i)}{\sum_j \exp(z_j)}$$



[Understanding Deep Learning, 2023]

- This can be viewed as the probability $o_i = P(class = i|\boldsymbol{x})$

For multi-class classification

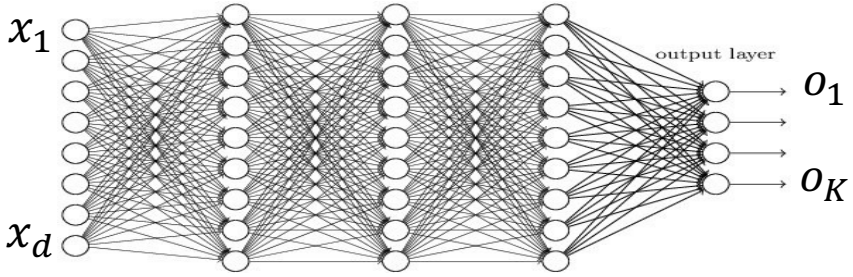


- Desired output y is one-hot vector $[0\ 0\ \ldots 1\ \ldots 0\ 0\ 0]^T$ with the 1 in the c-th position (for class c)
- Actual output will be probability distribution $[o_1, o_2, \ldots, o_K]^T$
- The cross-entropy between the desired one-hot output and actual class c

$$loss(y, o) = -\sum_{i=1}^{K} y_i \log o_i = -\log o_c$$

Choosing cost function: Examples

- Regression problem
  - SSE



$$E = \sum_{n=1}^{N} E_n$$

$$E_n = \frac{1}{2}\left\|\boldsymbol{o}^{(n)} - \boldsymbol{y}^{(n)}\right\|^2 = \sum_{k=1}^{K}\left(o_k^{(n)} - y_k^{(n)}\right)^2$$ Multi-dimensional output

- Classification problem
  - Cross-entropy
    - Binary classification

$$loss_n = -y^{(n)} \log o^{(n)} - (1 - y^{(n)}) \log(1 - o^{(n)}) \qquad o = \sigma(z) = \frac{1}{1 + e^{-z}}$$

Output layer uses sigmoid activation function

    - Multi-class classification

$$loss_n = -\log o_{y^{(n)}}$$

Output is found by a softmax layer $o_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$

Likelihood Objective

- Likelihood

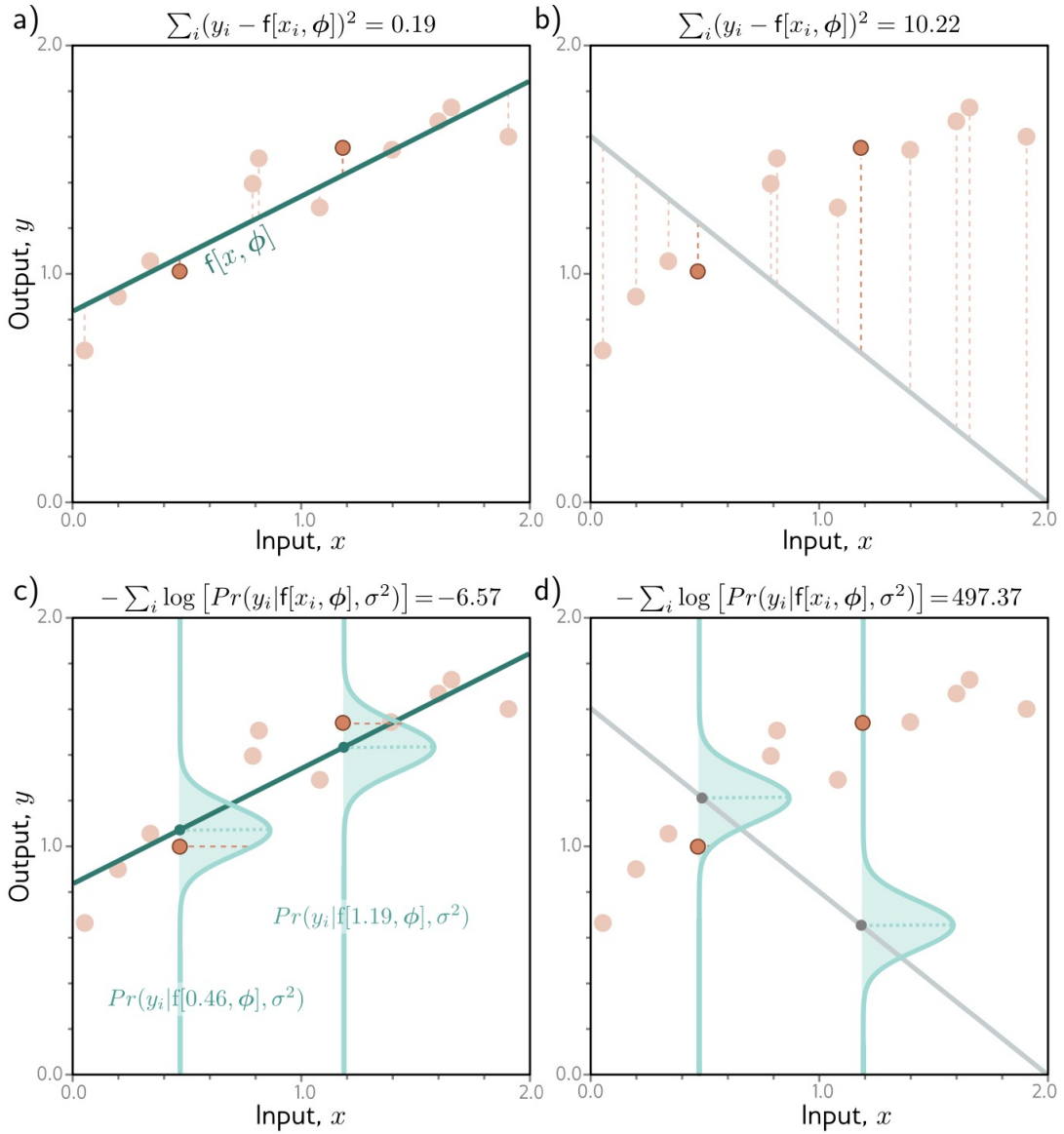
$$p\left(y^{(1)}, y^{(2)}, \ldots, y^{(N)} | x^{(1)}, x^{(2)}, \ldots, x^{(N)}\right) = \prod_{n=1}^{N} p\left(y^{(n)} | x^{(n)}\right) = \prod_{n=1}^{N} p\left(y^{(n)} | f(x^{(n)}; W)\right)$$

- Log-likelihood

$$\log \prod_{n=1}^{N} p\left(y^{(n)} | f(x^{(n)}; W)\right) = \sum_{n=1}^{N} \log p\left(y^{(n)} | f(x^{(n)}; W)\right)$$

- Maximizing likelihood corresponds to loss function $-\log p\left(y^{(n)} | f(x^{(n)}; W)\right)$

Probabilistic Viewpoint of Sum of Squares Error (SSE)



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$$p(y|f(x;\phi)) = N(y|\, f(x;\phi), \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2\sigma^2}\left(y - f(x;\phi)\right)^2}$$

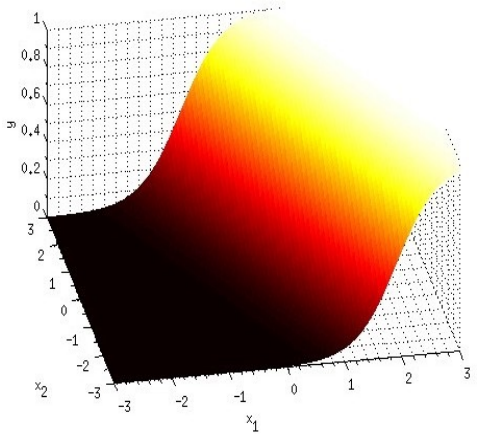
$$\log p(y|f(x;\phi)) = -\log\sqrt{2\pi}\,\sigma - \frac{1}{2\sigma^2}\left(y - f(x;\phi)\right)^2$$

$$\underset{\phi}{\text{argmax}} \sum_{n=1}^{N} \log p\left(y^{(n)}\middle|f\left(x^{(n)};\phi\right)\right)$$

$$= \underset{\phi}{\text{argmin}} \sum_{n=1}^{N} \left(y^{(n)} - f\left(x^{(n)};\phi\right)\right)^2$$

Probabilistic Viewpoint of Cost Functions

- Binary classification: $Bern(y|\theta) = \theta^{y}(1-\theta)^{(1-y)}$ $\theta = P(Y=1)$



$$-\log p(y|f(x;W)) = -\log Bern(y|f(x;W))$$

$$= -\log f(x;W)^{y^{(n)}}\left(1-f(x;W)\right)^{1-y(n)}$$

$$= -y^{(n)}\log f(x;W) - \left(1-y(n)\right)\log\left(1-f(x;W)\right)$$

- Multi-class classification: $Multi(\boldsymbol{y}|\boldsymbol{\theta}) = \prod_{k=1}^{K}\theta_k^{y_k}$ $\theta_k = P(y_k=1)$

$$-\log p(y|f(x;W)) = -\log Muti(y|f(x;W)) = -\sum_{k=1}^{K} y_k^{(n)}\log f_k(x;W)$$

Cross Entropy Loss

$$D_{KL}[q||p] = \int q(z) \log \frac{q(z)}{p(z)} dz = \int q(z) \log q(z)\, dz - \int q(z) \log p(z)\, dz$$

- For multi-class classification problem:
  - $q(y|x)$ is a one-hot vector shows the target class of x
  - $p_\theta(y|x)$ shows the output of the parametric model

$$D_{KL}[q||p] = \sum_z q(z) \log \frac{q(z)}{p(z)}$$

$$\underset{\theta}{\operatorname{argmin}}\, D_{KL}[q||p_\theta] = -\sum_{k=1}^{K} y_k \log p_\theta(y = k|x)$$

Problem setup

- Given: the architecture of the network

- Training data: A set of input-output pairs

$$\left(x^{(1)}, y^{(1)}\right), \left(x^{(2)}, y^{(2)}\right), \ldots, \left(x^{(N)}, y^{(N)}\right)$$

- We need a loss function to show how penalizes the obtained output $o = f(x; W)$ when the desired output is y

$$E(W) = \sum_{n=1}^{N} loss\left(o^{(n)}, y^{(n)}\right) = \frac{1}{N} \sum_{n=1}^{N} loss\left(f\left(x^{(n)}; W\right), y^{(n)}\right)$$

- Minimize E w.r.t. W that containts $\left\{w_{i,j}^{[k]}, b_j^{[k]}\right\}$

Recap: Iterative optimization of cost function

- Cost function: $E(\boldsymbol{w})$
- Optimization problem: $\hat{\boldsymbol{w}} = \underset{\boldsymbol{w}}{\operatorname{argmin}} E(\boldsymbol{w})$

- Steps:
  - Start from $\boldsymbol{w}^0$
  - Repeat
    - Update $\boldsymbol{w}^t$ to $\boldsymbol{w}^{t+1}$ in order to reduce E
    - $t \leftarrow t + 1$
  - until we hopefully end up at a minimum

Recap: How to compute the slope?

- In 1-dimension, the derivative of a function:

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

  - the slope of the error surface can be calculated by taking the derivative of the error function at that point

- In multiple dimensions, the **gradient** is the vector of (partial derivatives) along each dimension

- The direction of steepest descent is the **negative gradient**

Recap: Gradient descent (or steepest descent)

- In each step, takes steps proportional to the negative of the gradient vector of the function at the current point $\boldsymbol{w}^t$:

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \gamma_t \nabla J(\boldsymbol{w}^t)$$

  - $J(\boldsymbol{w})$ decreases fastest if one goes from $\boldsymbol{w}^t$ in the direction of $-\nabla J(\boldsymbol{w}^t)$
  - Assumption: $J(\boldsymbol{w})$ is defined and differentiable in a neighborhood of a point $\boldsymbol{w}^t$

Learning rate: The amount of time he travels before taking another measurement is the learning rate of the algorithm.

Recap: Gradient descent

- Minimize $J(\boldsymbol{w})$

Step size
(Learning rate parameter)

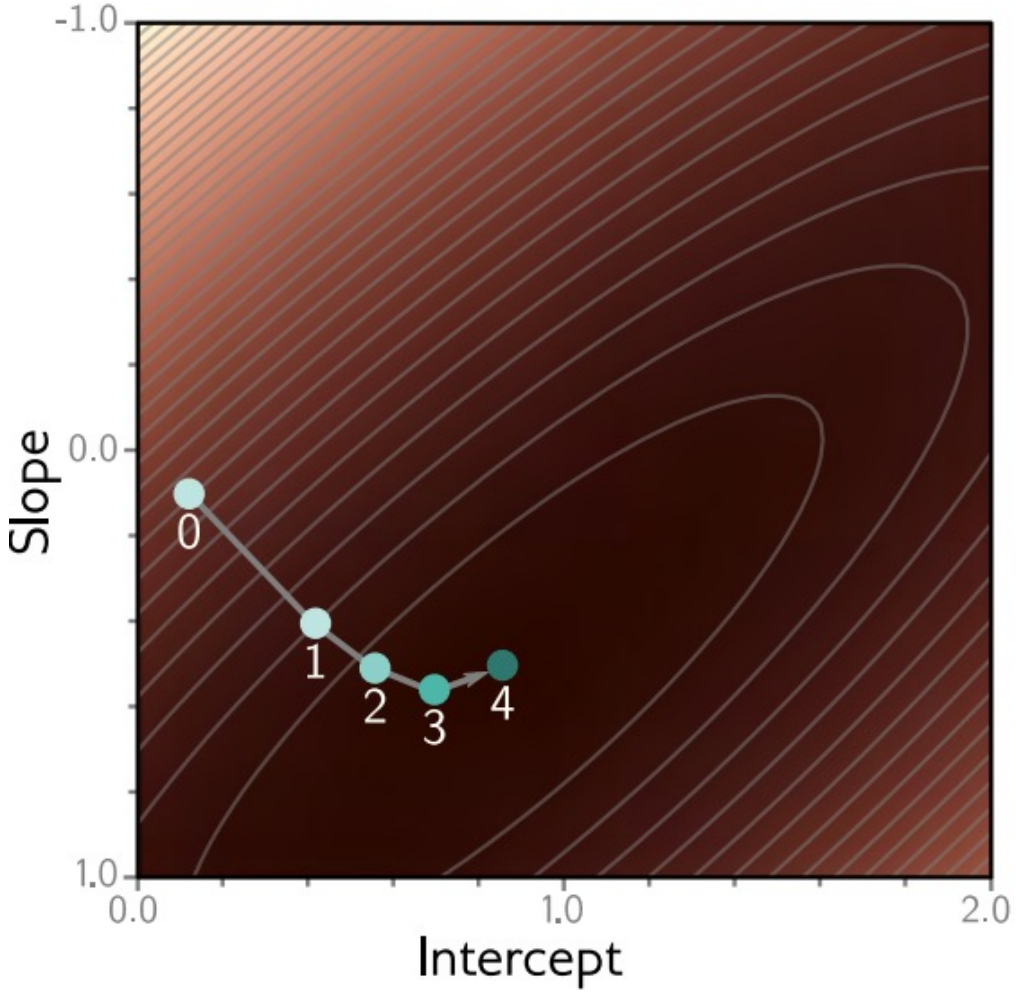
$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} - \eta \nabla_{\boldsymbol{w}} J(\boldsymbol{w}^{t})$$

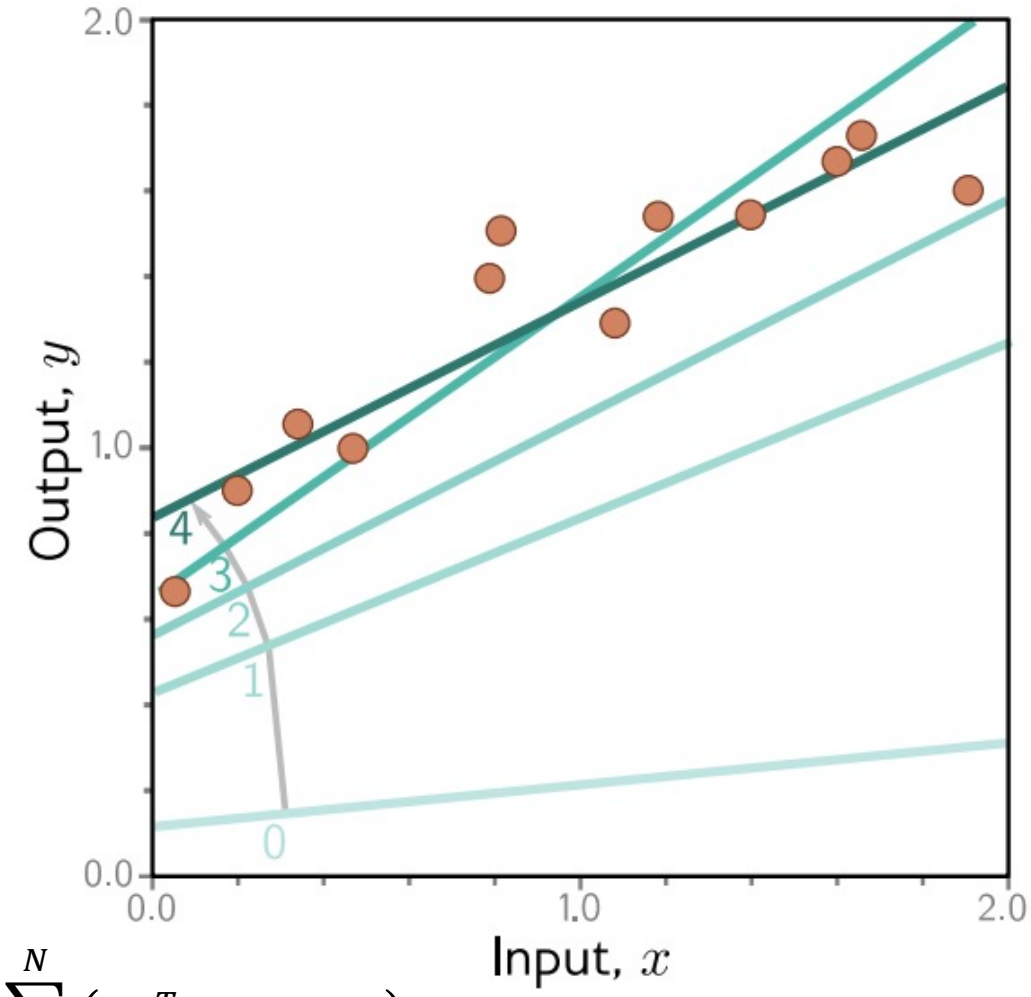
$$\nabla_{\boldsymbol{w}} J(\boldsymbol{w}) = \left[\frac{\partial J(\boldsymbol{w})}{\partial w_0}, \frac{\partial J(\boldsymbol{w})}{\partial w_2}, \ldots, \frac{\partial J(\boldsymbol{w})}{\partial w_d} \right]^T$$

- If η is small enough, then $J(\boldsymbol{w}^{t+1}) \leq J(\boldsymbol{w}^{t})$.
- η can be allowed to change at every iteration as η_t.

Recap: SSE optimization by gradient descent

$J(w_0, w_1)$ (function of the parameters w_0, w_1)





$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} - \eta \sum_{i=1}^{N} \left(\boldsymbol{w}^{t^T} \boldsymbol{x}^{(i)} - y^{(i)} \right) \boldsymbol{x}^{(i)}$$

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How to adjust weights for multi layer networks?

- We need multiple layers of adaptive, non-linear hidden units. But how can we train such nets?
  - We need an efficient way of adapting all the weights, not just the last layer.
  - This is difficult because nobody is telling us directly what the hidden units should do.

Training multi-layer networks

- Back-propagation
  - Training algorithm that is used to adjust weights in multi-layer networks (based on the training data)
  - The back-propagation algorithm is based on gradient descent
  - Use chain rule and dynamic programming to efficiently compute gradients

Training Neural Nets through Gradient Descent

Total training error:

$$E = \sum_{n=1}^{N} loss\left(\boldsymbol{o}^{(n)}, \boldsymbol{y}^{(n)}\right)$$

- Gradient descent algorithm
- Initialize all weights and biases $\left\{w_{ij}^{[k]}\right\}$

Assuming the bias is also represented as a weight

  - Using the extended notation : the bias is also weight
- Do :
  - For every layer k for all i, j update:
    - $w_{i,j}^{[k]} = w_{i,j}^{[k]} - \eta \frac{dE}{dw_{i,j}^{[k]}}$
- Until E has converged

The derivative

Total training error:

$$E = \sum_{n=1}^{N} loss\left(\boldsymbol{o}^{(n)}, \boldsymbol{y}^{(n)}\right)$$

- Computing the derivative

Total derivative:

$$\frac{dE}{dw_{i,j}^{[k]}} = \sum_{n=1}^{N} \frac{loss\left(\boldsymbol{o}^{(n)}, \boldsymbol{y}^{(n)}\right)}{dw_{i,j}^{[k]}}$$

Training by gradient descent

- Initialize all weights $\left\{w_{ij}^{[k]}\right\}$
- Do :
  - For all i , j , k, initialize $\frac{dE}{dw_{i,j}^{[k]}} = 0$
  - For all $n = 1{:}\, N$
    - For every layer k for all i, j:
      - Compute $\frac{d\ loss\left(o^{(n)}, y^{(n)}\right)}{dw_{i,j}^{[k]}}$
      - $\frac{dE}{dw_{i,j}^{[k]}} \mathrel{+}= \frac{d\ loss\left(o^{(n)}, y^{(n)}\right)}{dw_{i,j}^{[k]}}$
  - For every layer k for all i, j:

$$w_{i,j}^{[k]} = w_{i,j}^{[k]} - \frac{\eta}{N} \frac{dE}{dw_{i,j}^{[k]}}$$

The derivative

Total training error:

$$E = \sum_{n=1}^{N} loss\left(\boldsymbol{o}^{(n)}, \boldsymbol{y}^{(n)}\right)$$

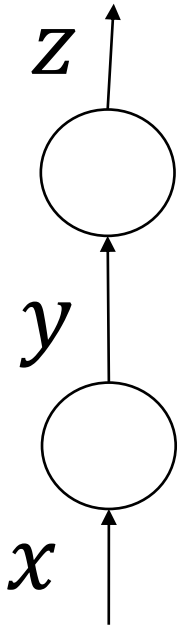
Total derivative:

$$\frac{dE}{dw_{i,j}^{[k]}} = \sum_{n=1}^{N} \frac{d\, loss\left(\boldsymbol{o}^{(n)}, \boldsymbol{y}^{(n)}\right)}{dw_{i,j}^{[k]}}$$

- So we must first figure out how to compute the derivative of divergences of individual training inputs

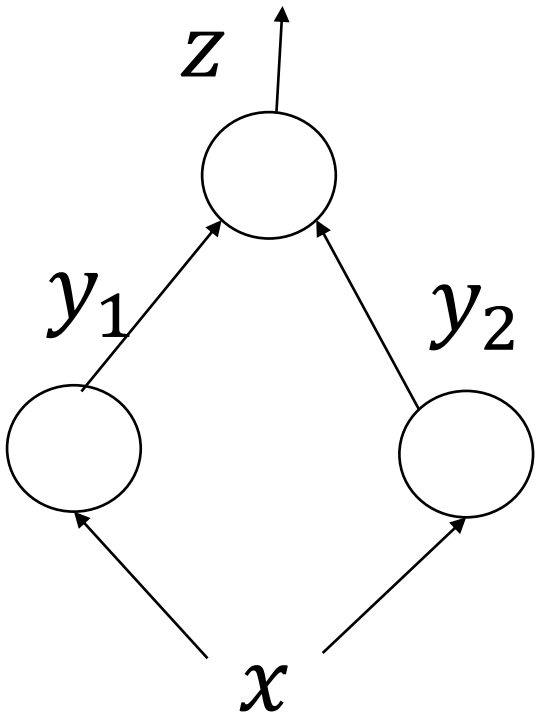
Simple chain rule

- $z = f\big(g(x)\big)$
- $y = g(x)$



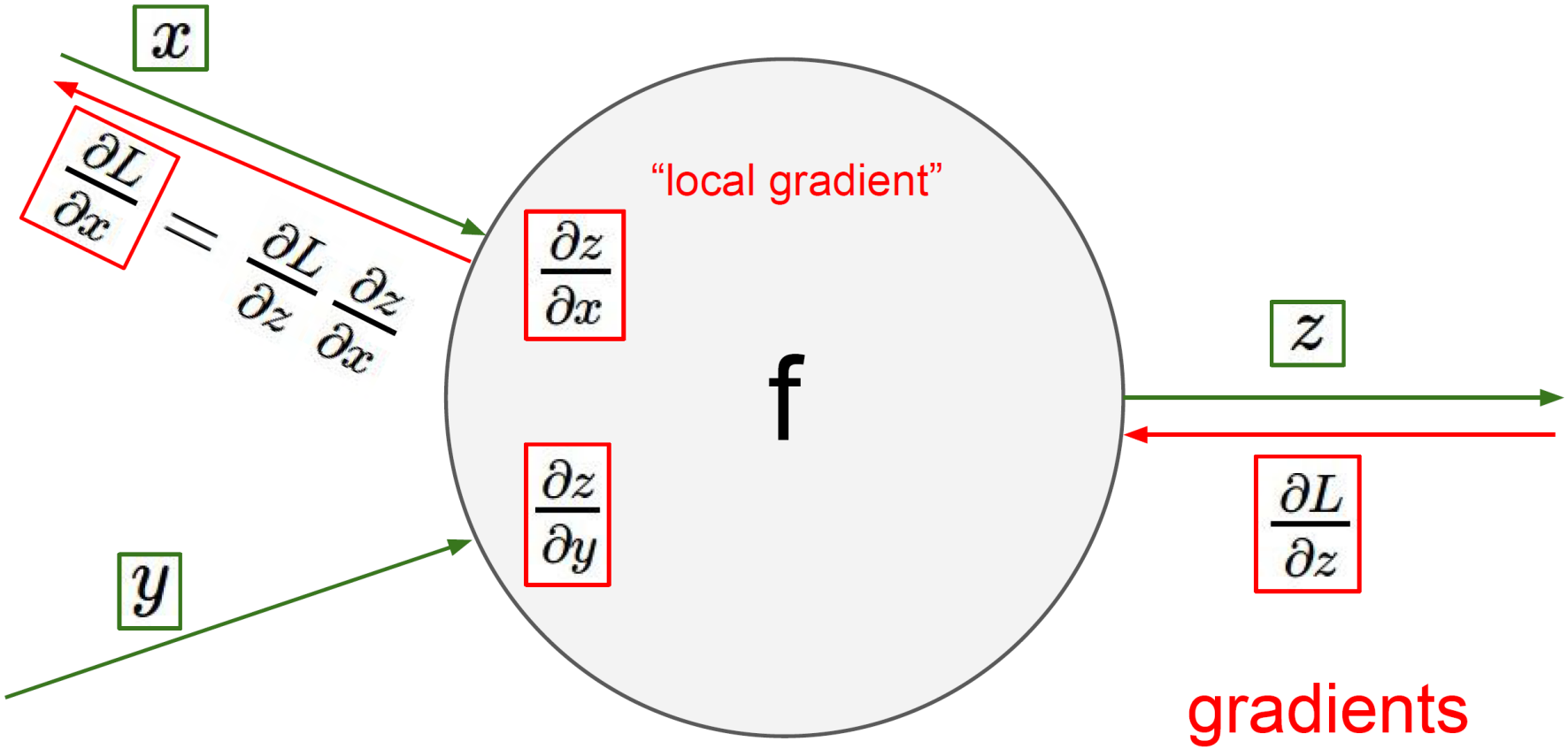
$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}$$

Multiple paths chain rule



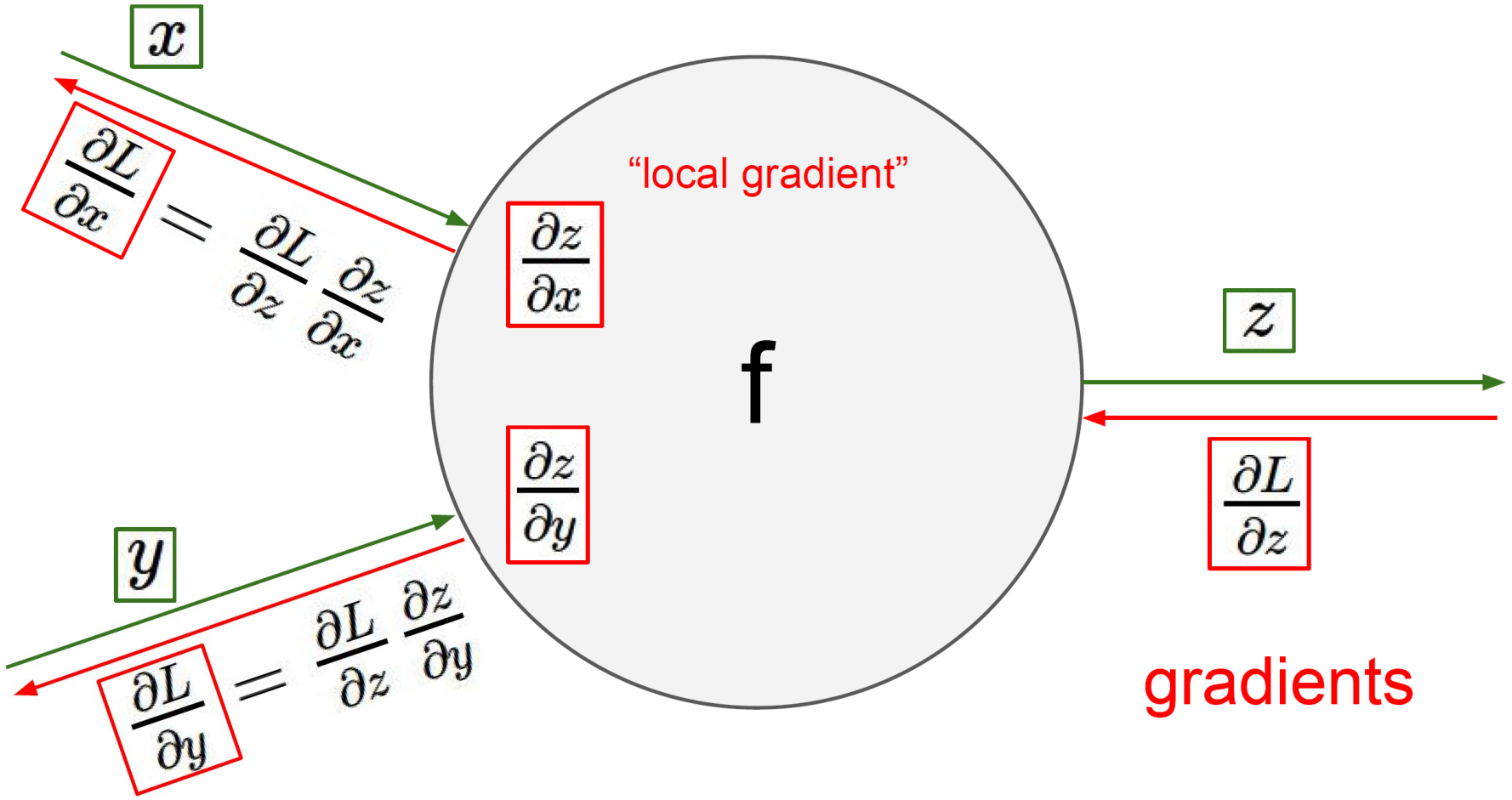
$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y_1}\frac{\partial y_1}{\partial x} + \frac{\partial z}{\partial y_2}\frac{\partial y_2}{\partial x}$$

How to propagate the gradients backward

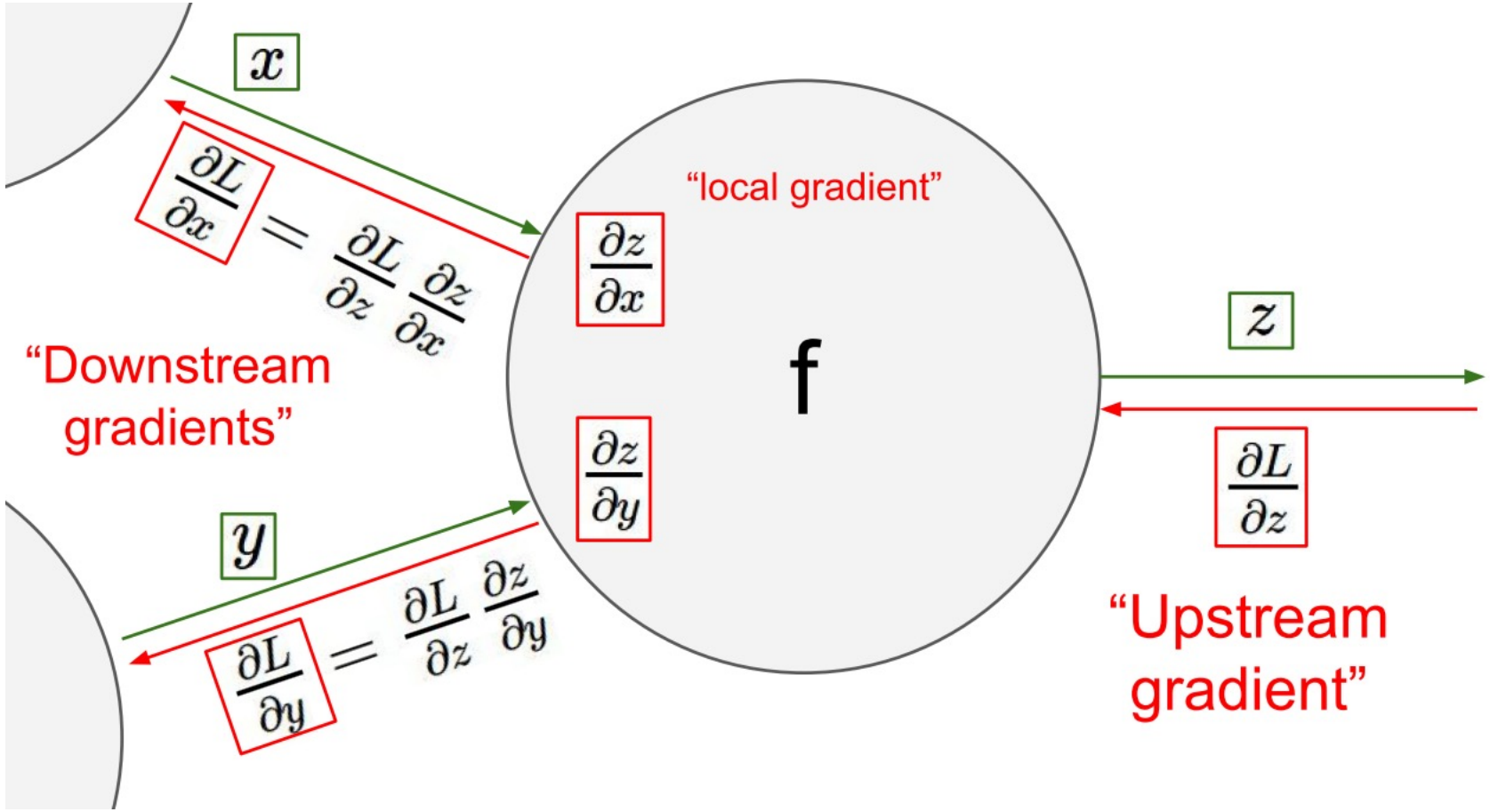


$$z = f(x, y)$$

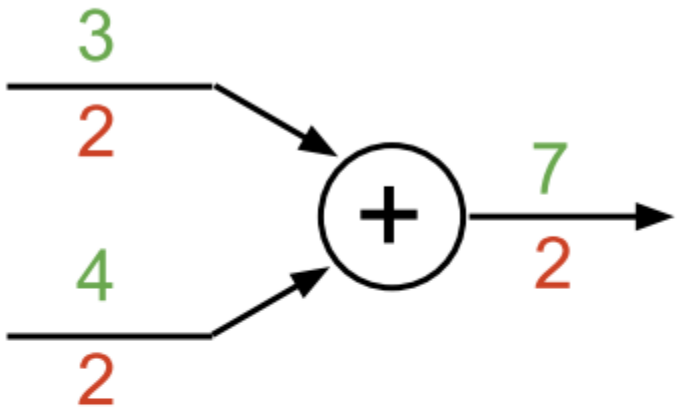
How to propagate the gradients backward



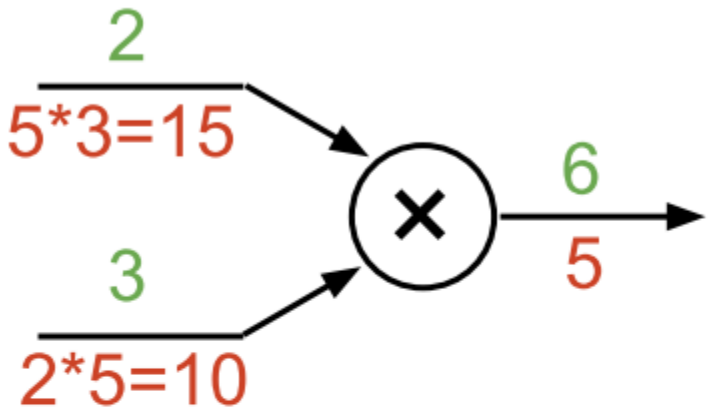
Downstream gradients from upstream ones



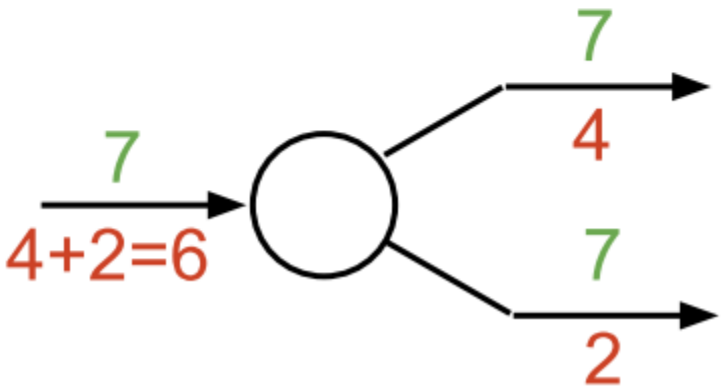
add gate: gradient distributor



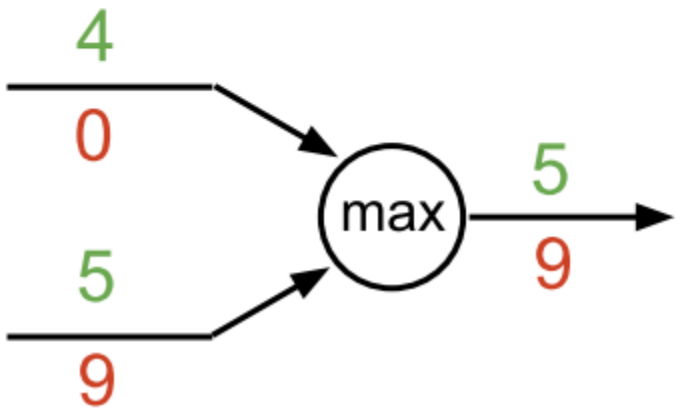
mul gate: “swap multiplier”



copy gate: gradient adder



max gate: gradient router

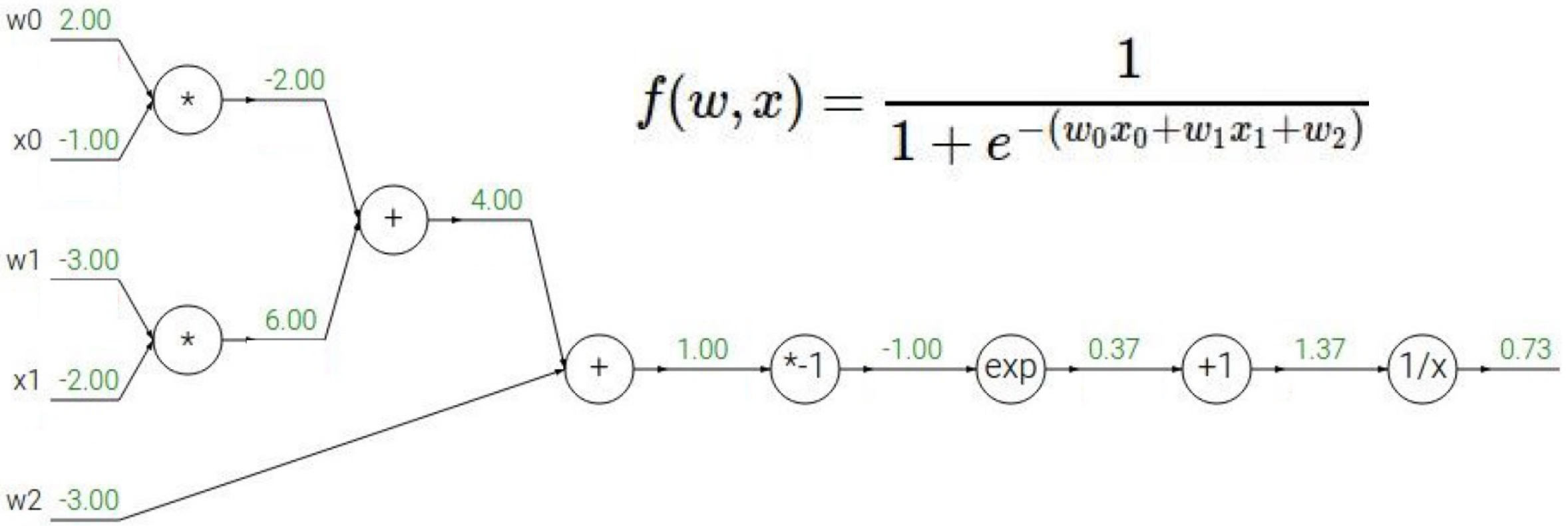


This slide has been adopted from Fei-Fei Li & Jiajun Wu & Ruohan Gao, cs231n, Stanford, Fall 2022

Returning to our problem

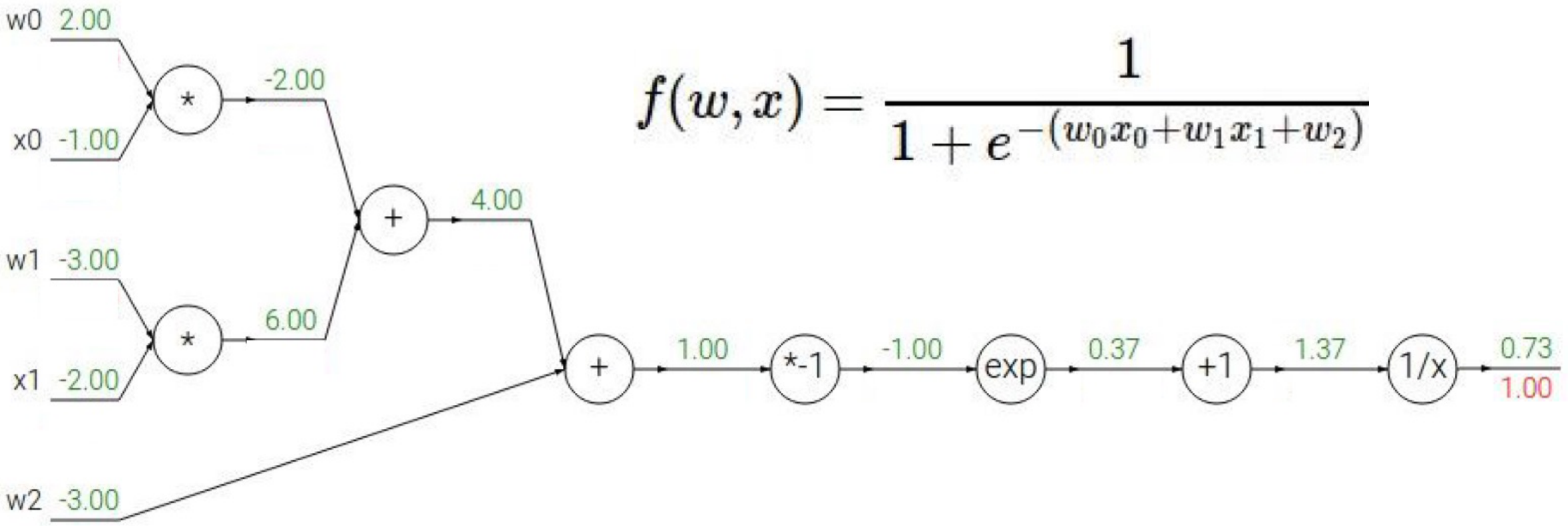
- How to compute $\frac{d\ loss(\boldsymbol{o}, \boldsymbol{y})}{dw_{i,j}^{[k]}}$

Another example



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

Another example



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

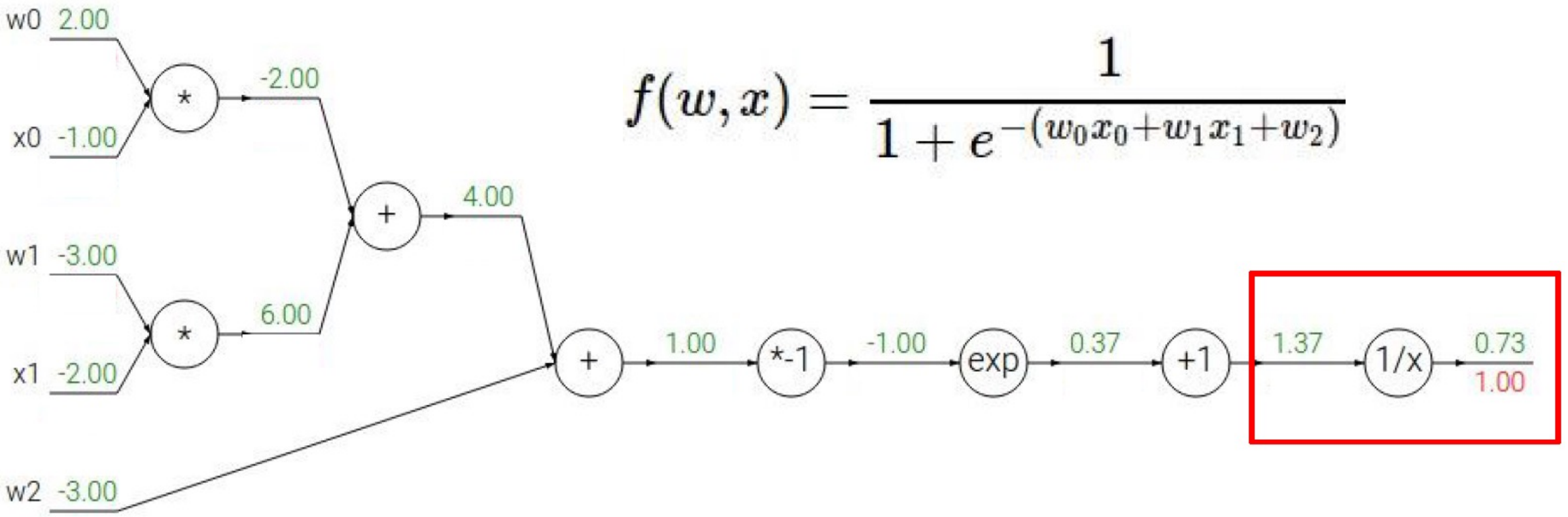
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

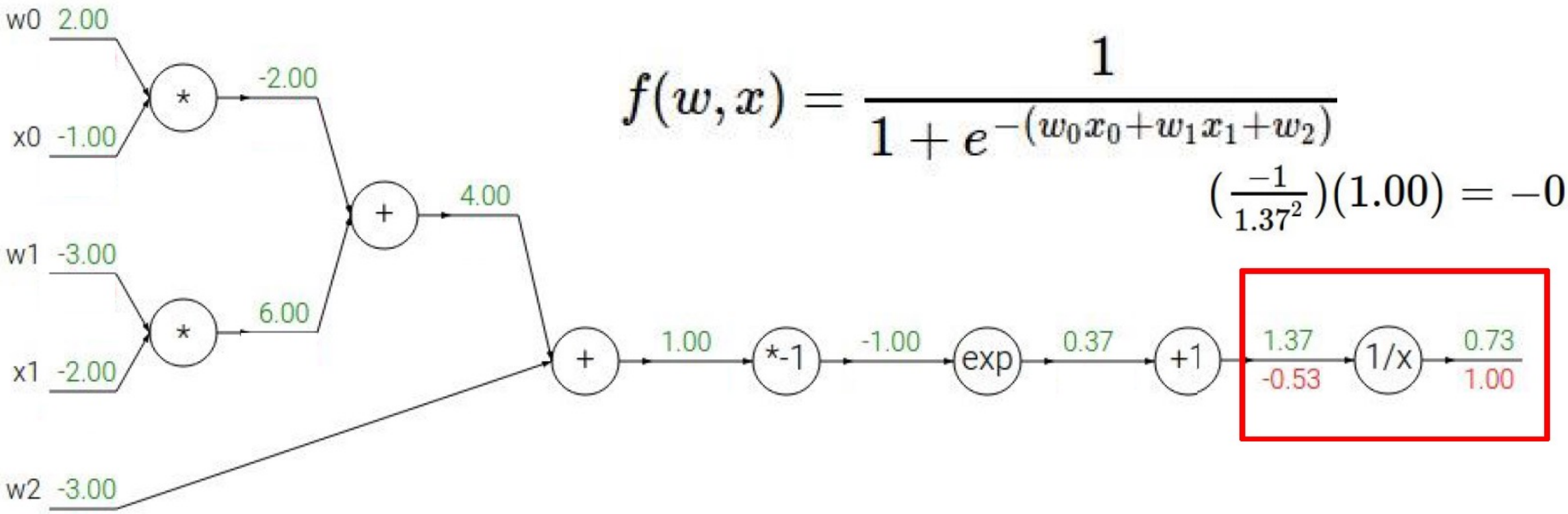
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

$$(\frac{-1}{1.37^2})(1.00) = -0.5$$

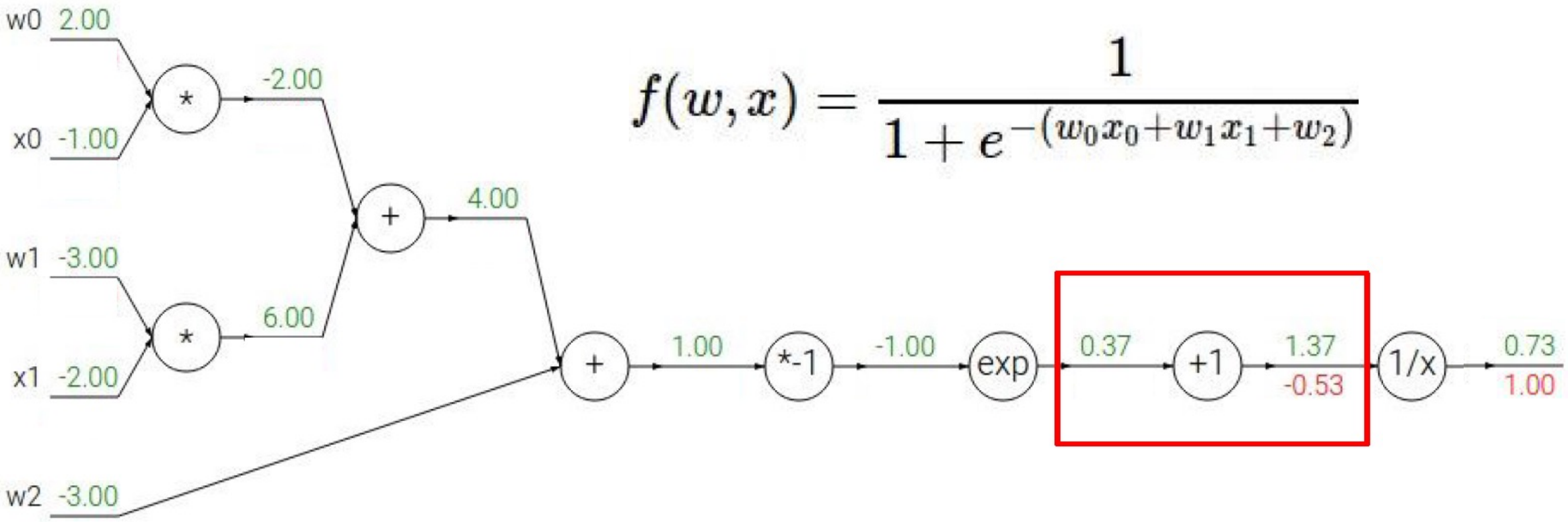
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

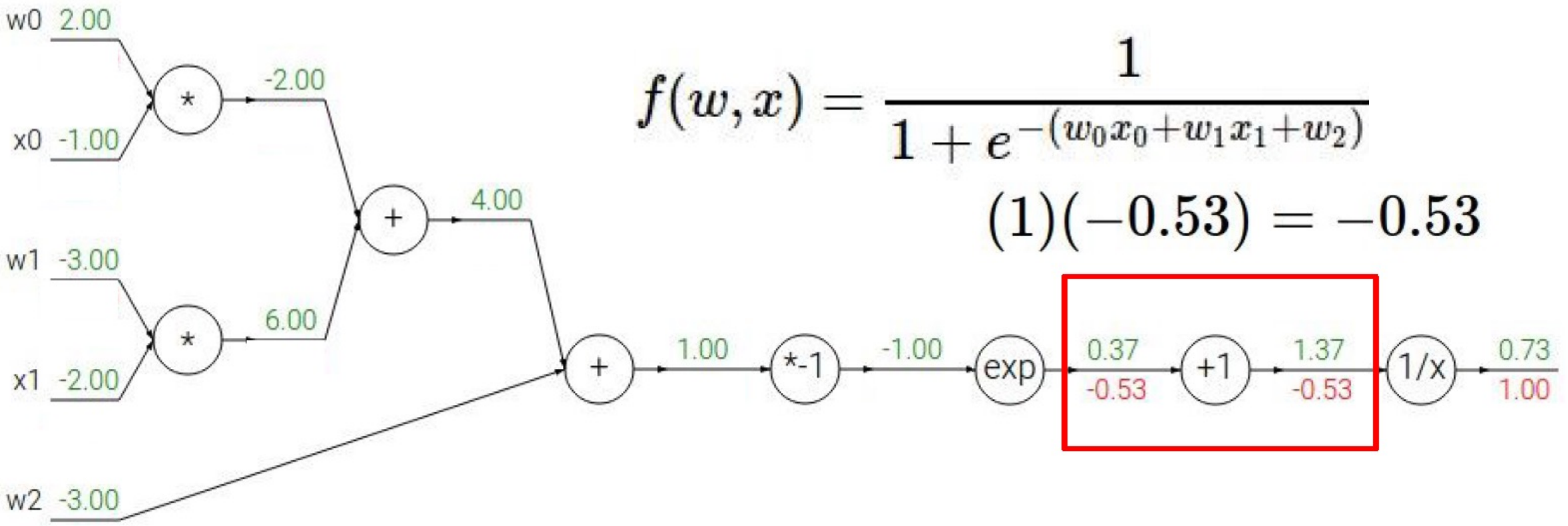
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

$$(1)(-0.53) = -0.53$$

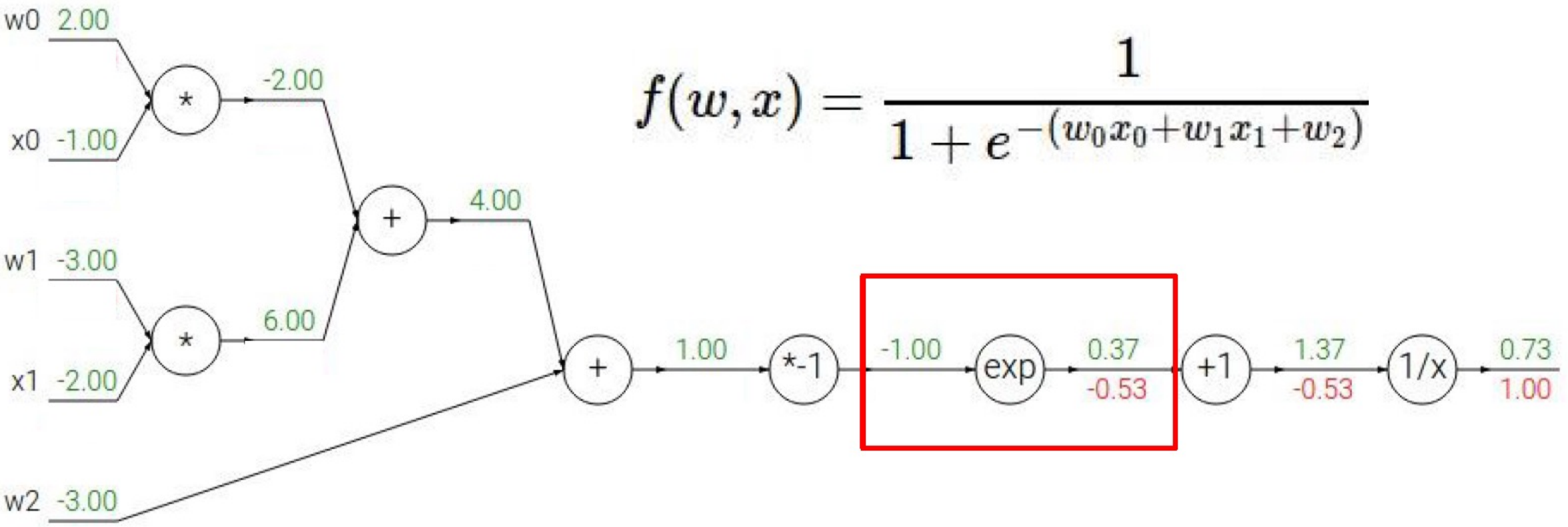
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

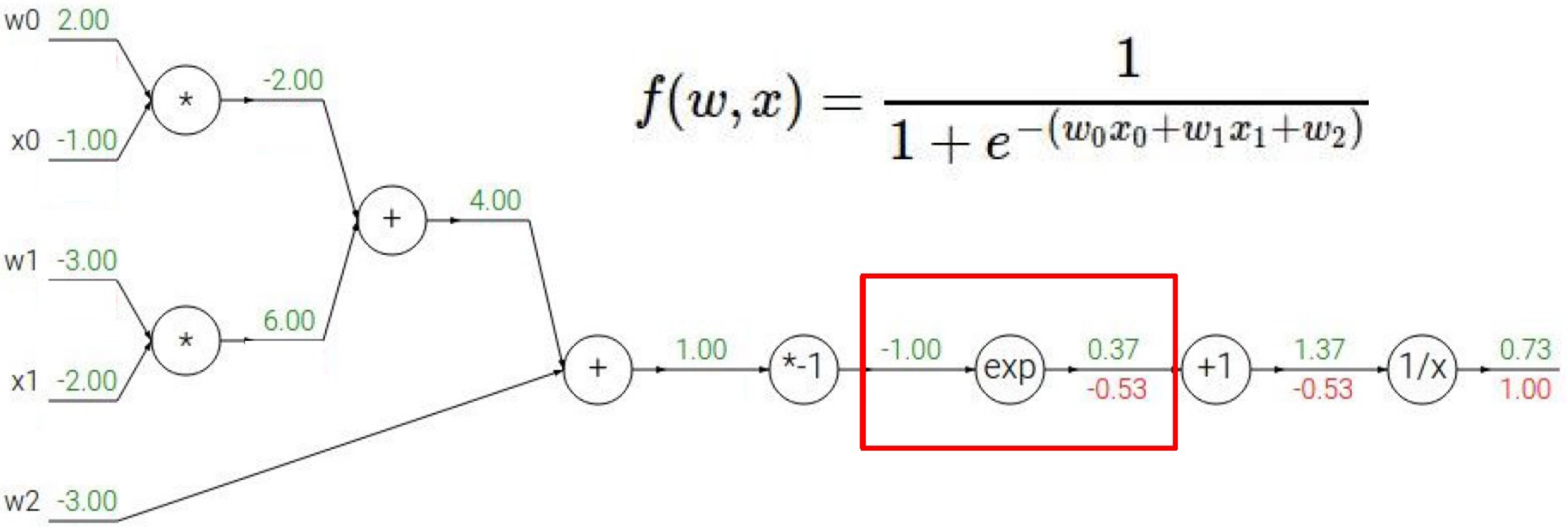
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

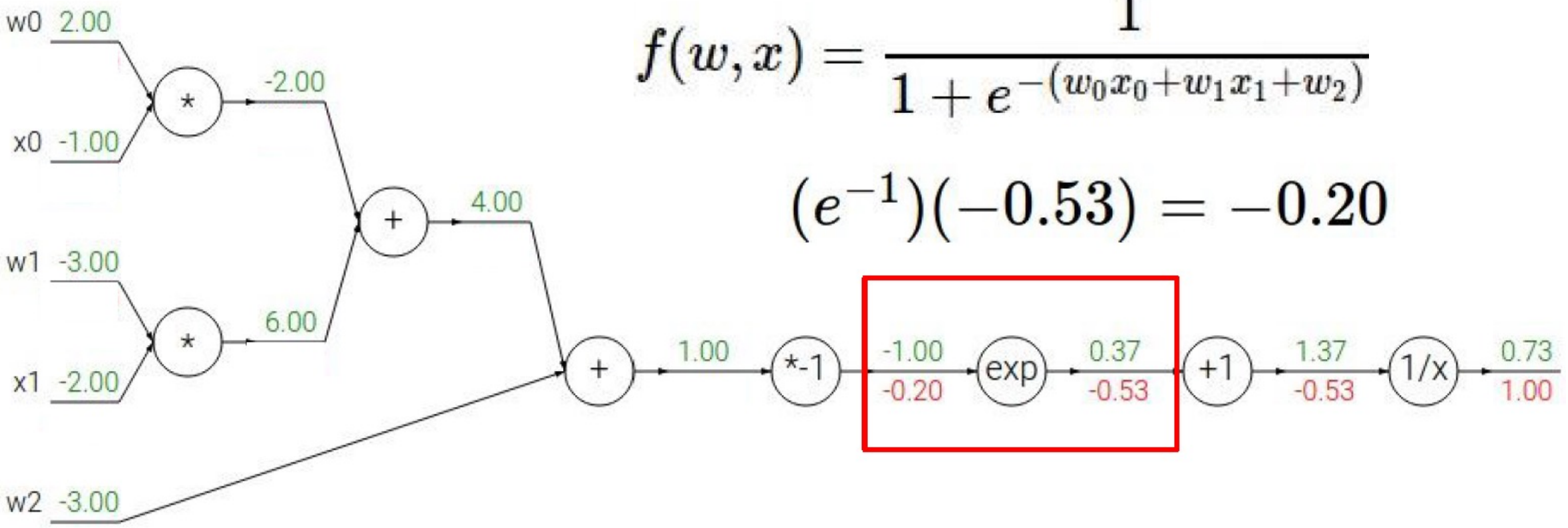
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

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

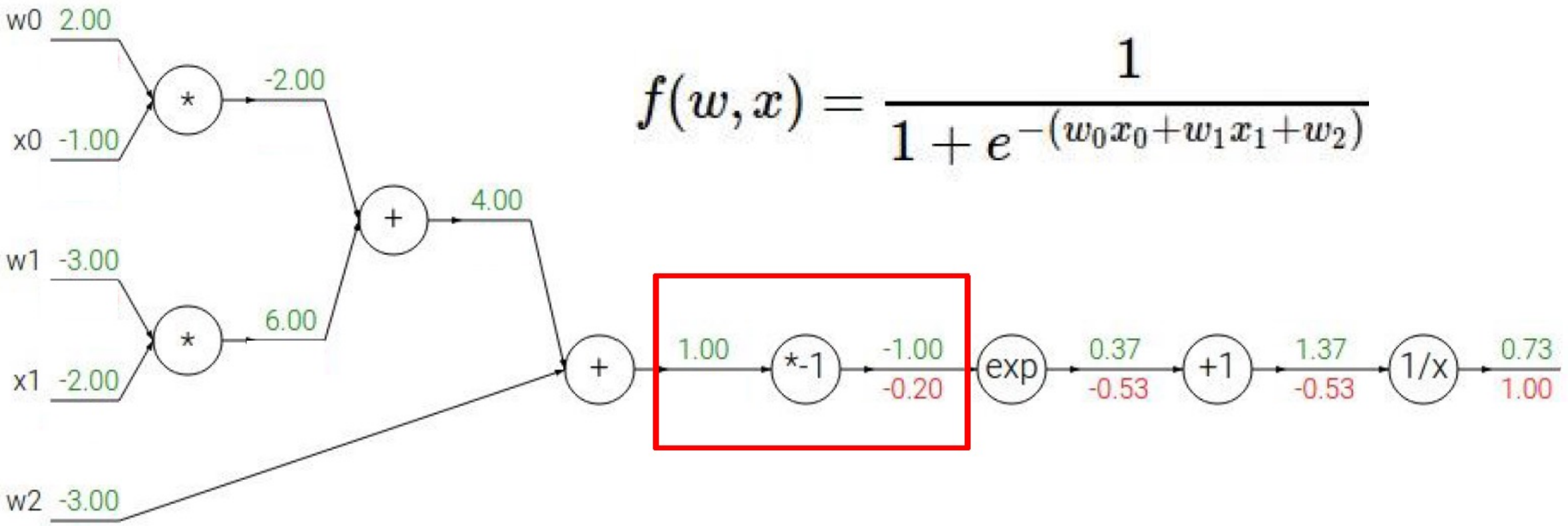
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

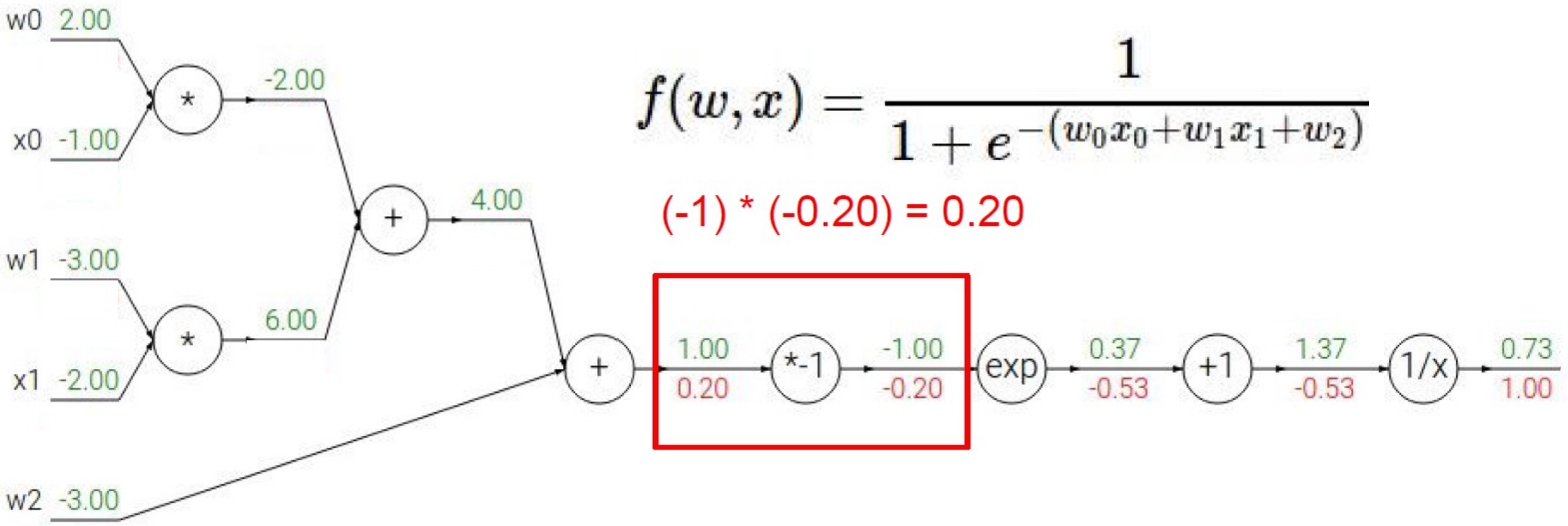
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

(-1) * (-0.20) = 0.20

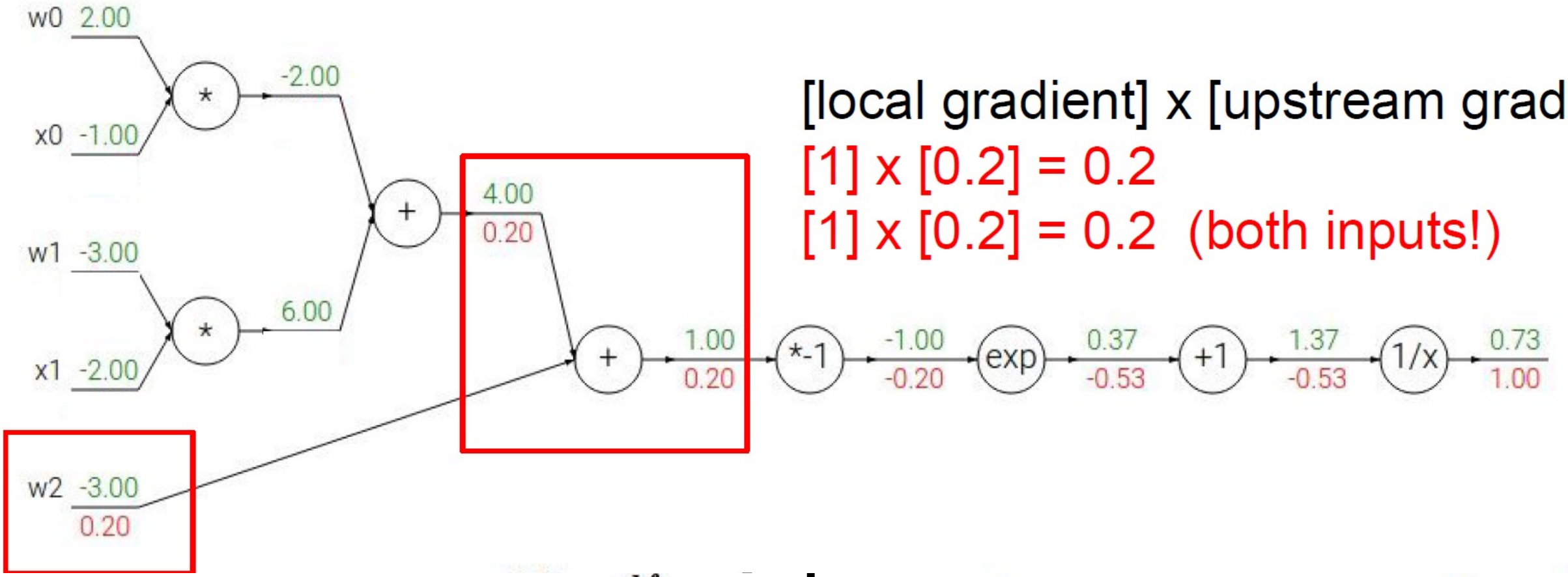
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



[local gradient] x [upstream gradient]

[1] x [0.2] = 0.2

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

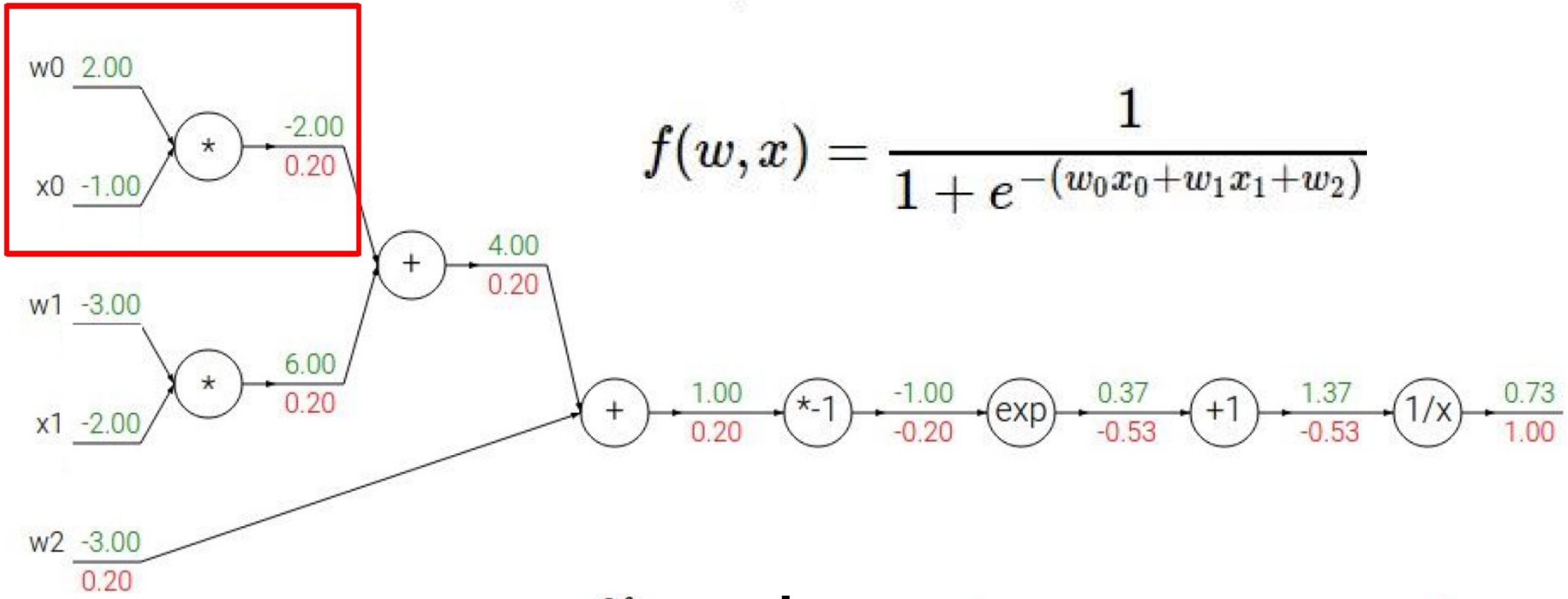
$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

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

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

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

Another example



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

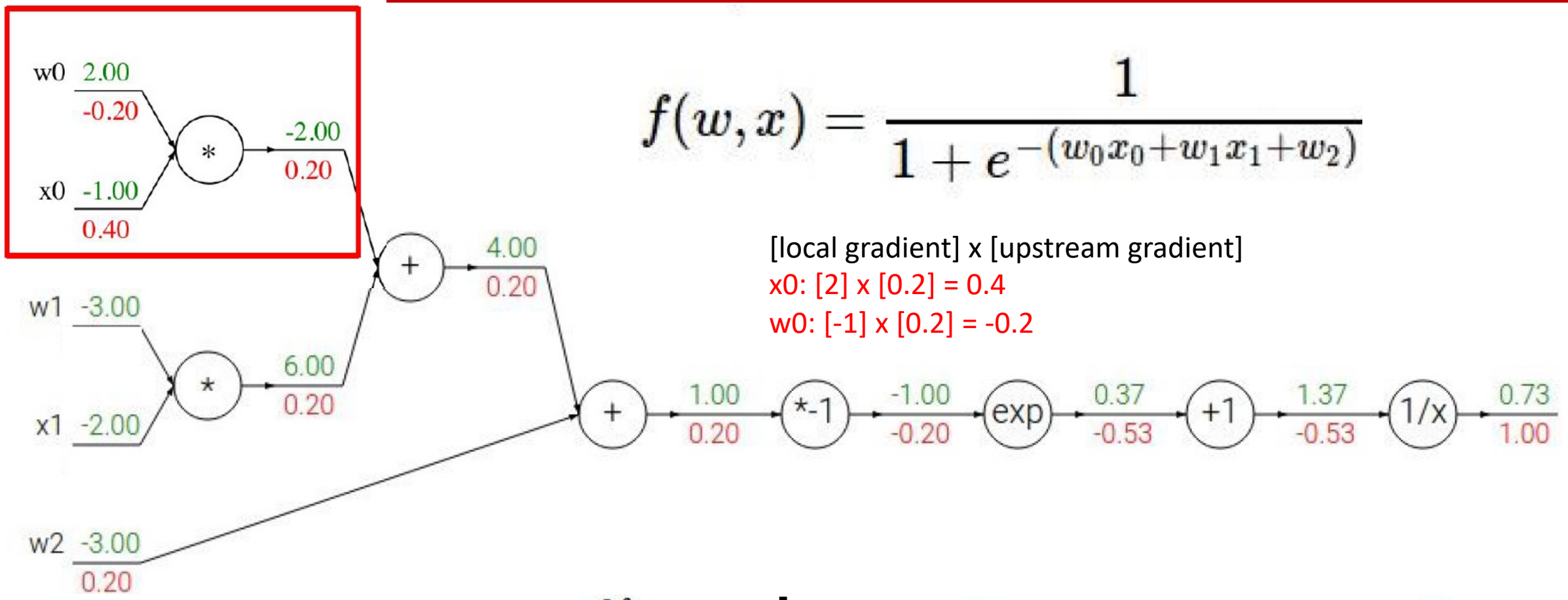
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

Another example



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

[local gradient] x [upstream gradient]

x0: [2] x [0.2] = 0.4

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

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

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

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

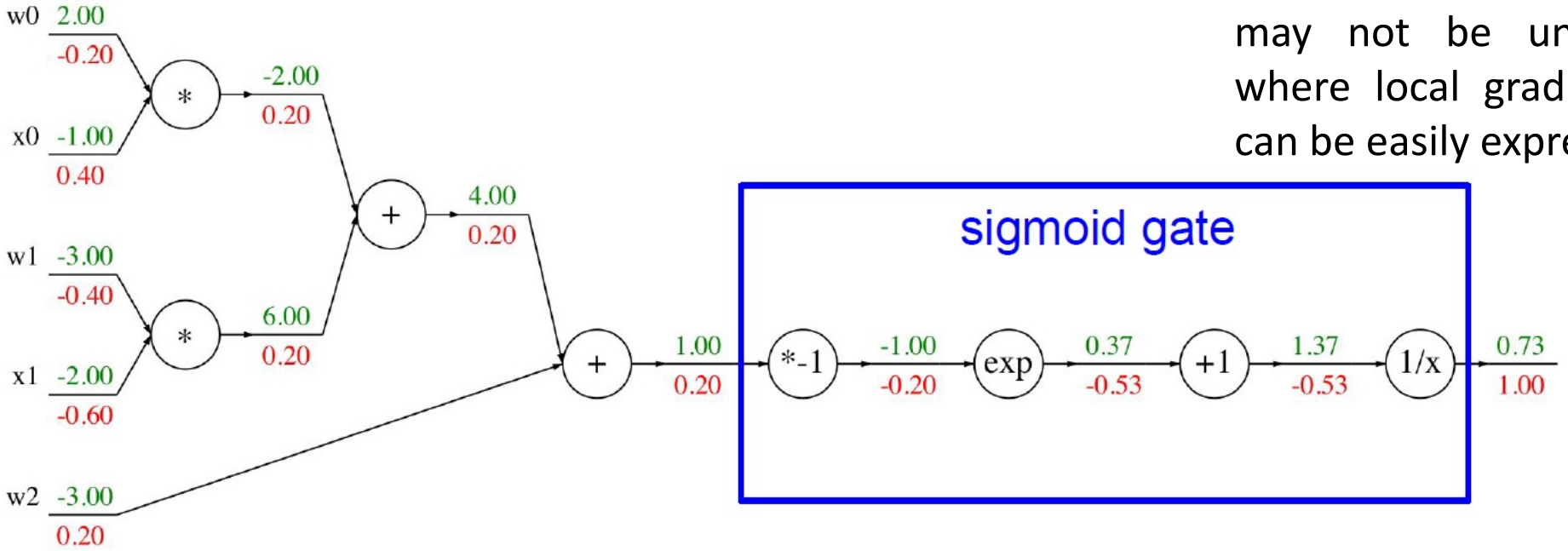
$$f_c(x) = c + x \rightarrow \frac{df}{dx} = 1$$

Another example: 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

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



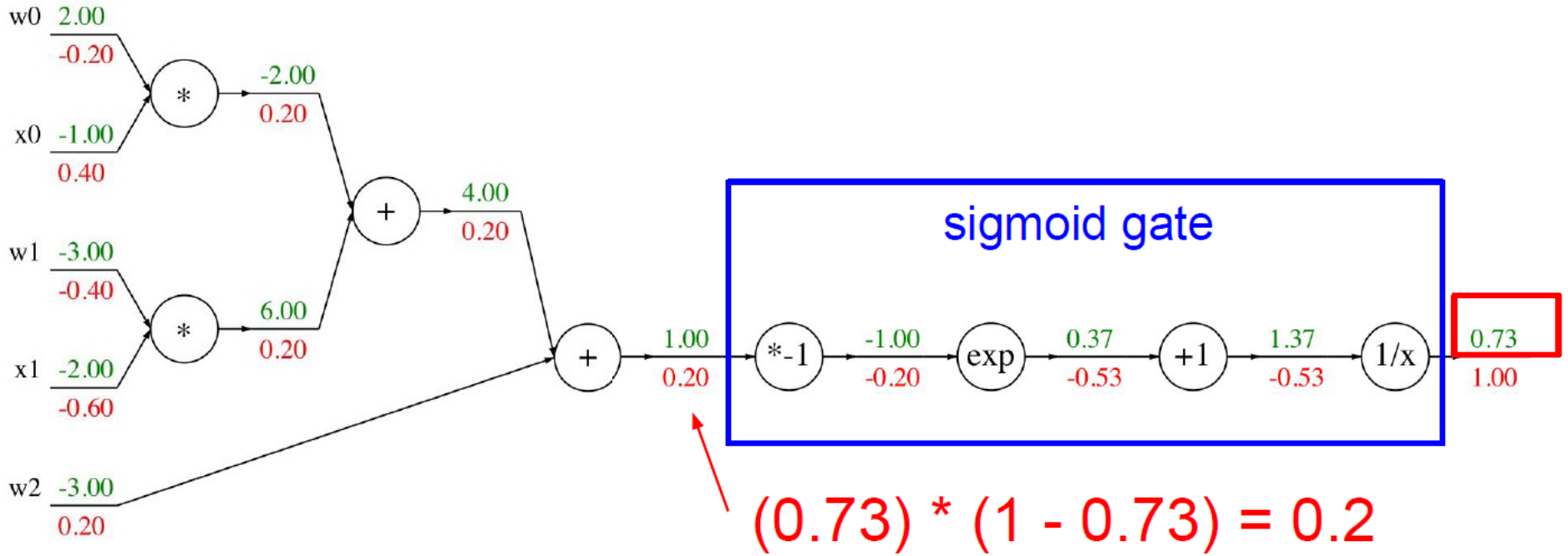
Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!

Another example: sigmoid

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

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

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

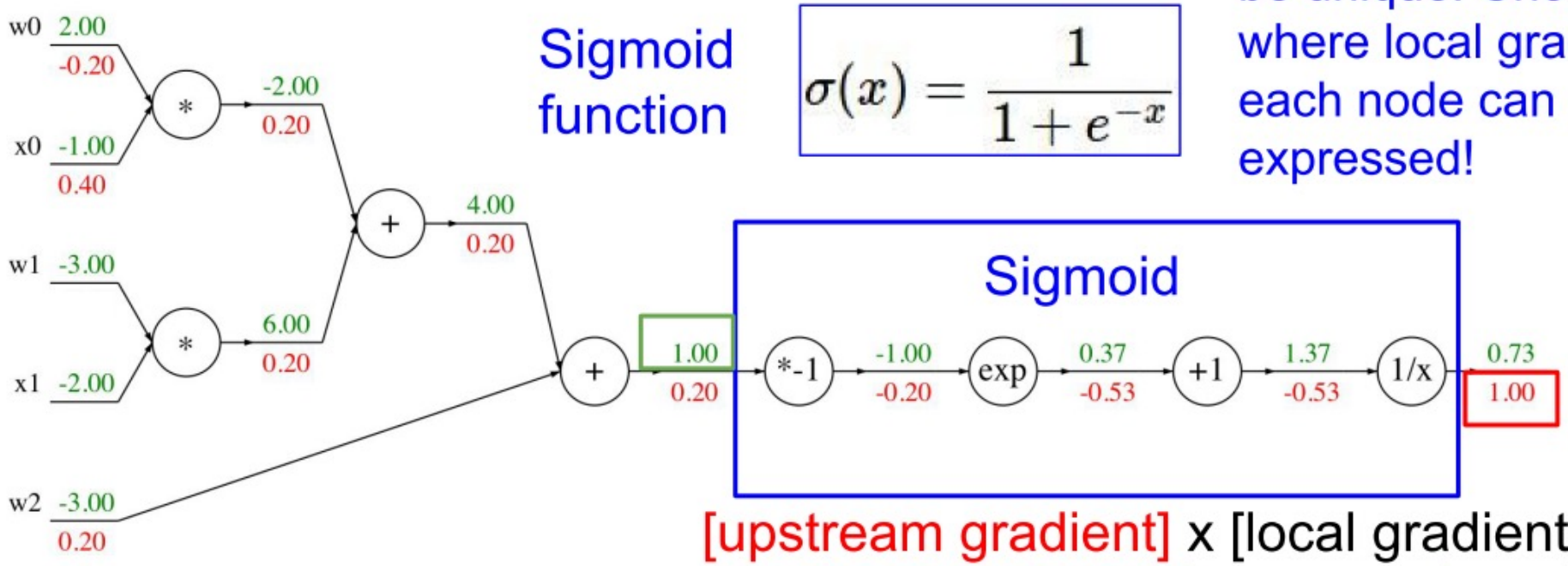


Another example: sigmoid

Another 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!

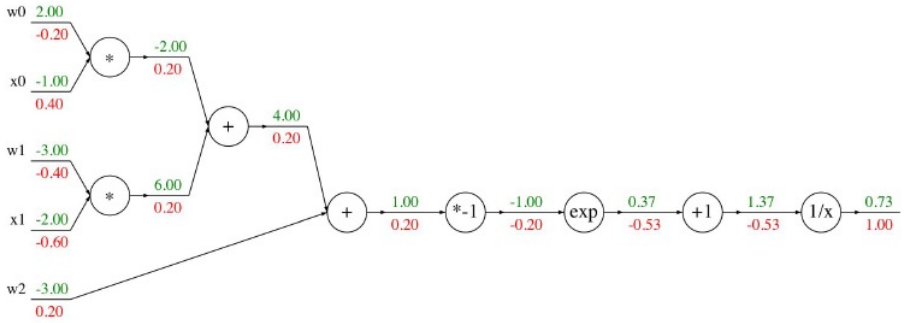
Sigmoid function $$\sigma(x) = \frac{1}{1+e^{-x}}$$



[upstream gradient] x [local gradient]

[1.00] x [(1 - $1/(1+e^{-1})$) ($1/(1+e^{-1})$)] = 0.2

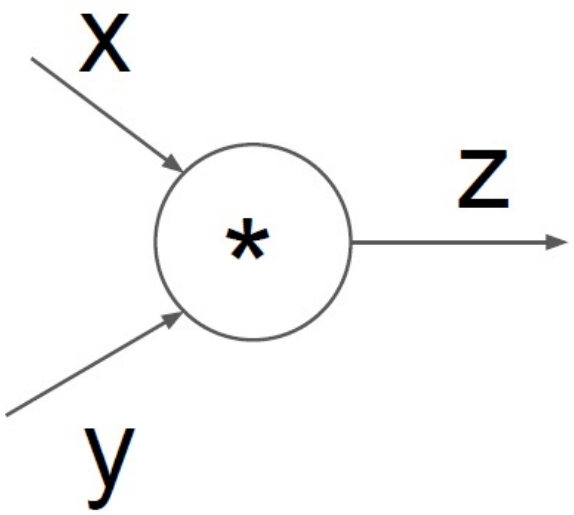
Modularized implementation: forward / backward API



Graph (or Net) object *(rough psuedo code)*

```
class ComputationalGraph(object):
    #...
    def forward(inputs):
        # 1. [pass inputs to input gates...]
        # 2. forward the computational graph:
        for gate in self.graph.nodes_topologically_sorted():
            gate.forward()
        return loss # the final gate in the graph outputs the loss
    def backward():
        for gate in reversed(self.graph.nodes_topologically_sorted()):
            gate.backward() # little piece of backprop (chain rule applied)
        return inputs_gradients
```

Modularized implementation: forward / backward API



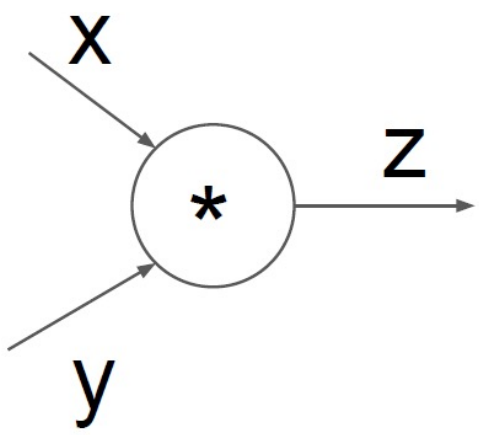
(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        return z
    def backward(dz):
        # dx = ... #todo
        # dy = ... #todo
        return [dx, dy]
```

$\frac{\partial L}{\partial z}$

$\frac{\partial L}{\partial x}$

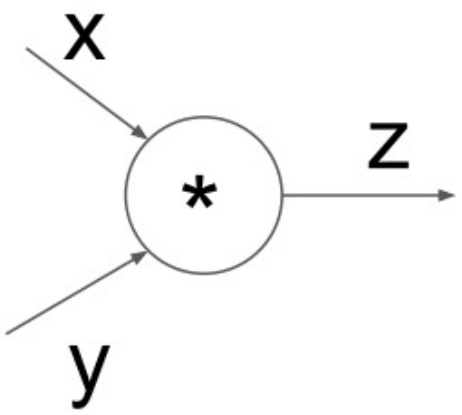
Modularized implementation: forward / backward API



(x,y,z are scalars)

```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
```

Modularized implementation: forward / backward API



(x,y,z are scalars)

Gate / Node / Function object: Actual PyTorch code

```
class Multiply(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x, y):
    ctx.save_for_backward(x, y)
    z = x * y
    return z
  @staticmethod
  def backward(ctx, grad_z):
    x, y = ctx.saved_tensors
    grad_x = y * grad_z   # dz/dx * dL/dz
    grad_y = x * grad_z   # dz/dy * dL/dz
    return grad_x, grad_y
```

Need to cash some values for use in backward

Upstream gradient

Multiply upstream and local gradients

Example: PyTorch operators

pytorch / pytorch

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Tree: 517c7c9861 ▾ pytorch / aten / src / THNN / generic / | Create new file | Upload files | Find file | History

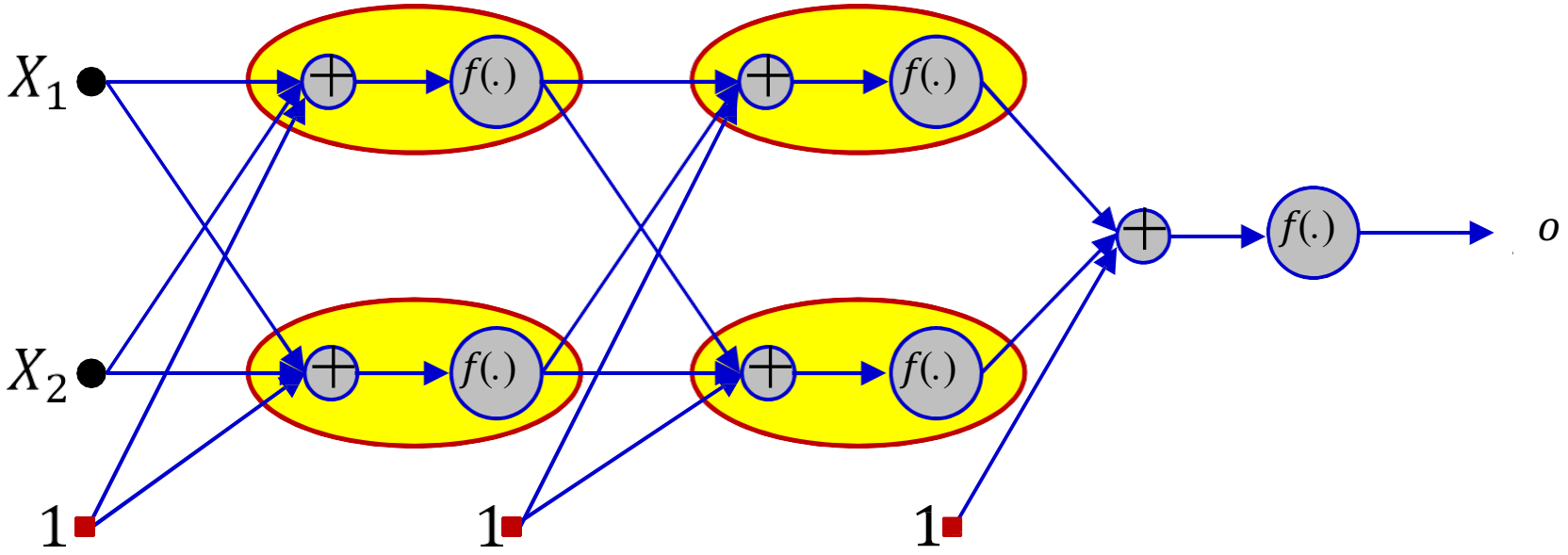
ezyang and facebook-github-bot Canonicalize all includes in PyTorch. (#14849) ··· Latest commit 517c7c9 on Dec 8, 2018

..

AbsCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
BCECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ClassNLLCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Col2Im.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ELU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
FeatureLPPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
GatedLinearUnit.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
HardTanh.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Im2Col.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
IndexLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LeakyReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LogSigmoid.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MSECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MultiLabelMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MultiMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
RReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Sigmoid.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SmoothL1Criterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago

SpatialClassNLLCriterion.c	Canonicalize all includes in PyTorch. (#14849)
SpatialConvolutionMM.c	Canonicalize all includes in PyTorch. (#14849)
SpatialDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)
SpatialDilatedMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)
SpatialFractionalMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)
SpatialFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)
SpatialMaxUnpooling.c	Canonicalize all includes in PyTorch. (#14849)
SpatialReflectionPadding.c	Canonicalize all includes in PyTorch. (#14849)
SpatialReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)
SpatialUpSamplingBilinear.c	Canonicalize all includes in PyTorch. (#14849)
SpatialUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)
THNN.h	Canonicalize all includes in PyTorch. (#14849)
Tanh.c	Canonicalize all includes in PyTorch. (#14849)
TemporalReflectionPadding.c	Canonicalize all includes in PyTorch. (#14849)
TemporalReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)
TemporalRowConvolution.c	Canonicalize all includes in PyTorch. (#14849)
TemporalUpSamplingLinear.c	Canonicalize all includes in PyTorch. (#14849)
TemporalUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)
VolumetricAdaptiveAveragePoolin...	Canonicalize all includes in PyTorch. (#14849)
VolumetricAdaptiveMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)
VolumetricAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)
VolumetricConvolutionMM.c	Canonicalize all includes in PyTorch. (#14849)
VolumetricDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)
VolumetricDilatedMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)
VolumetricFractionalMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)
VolumetricFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)

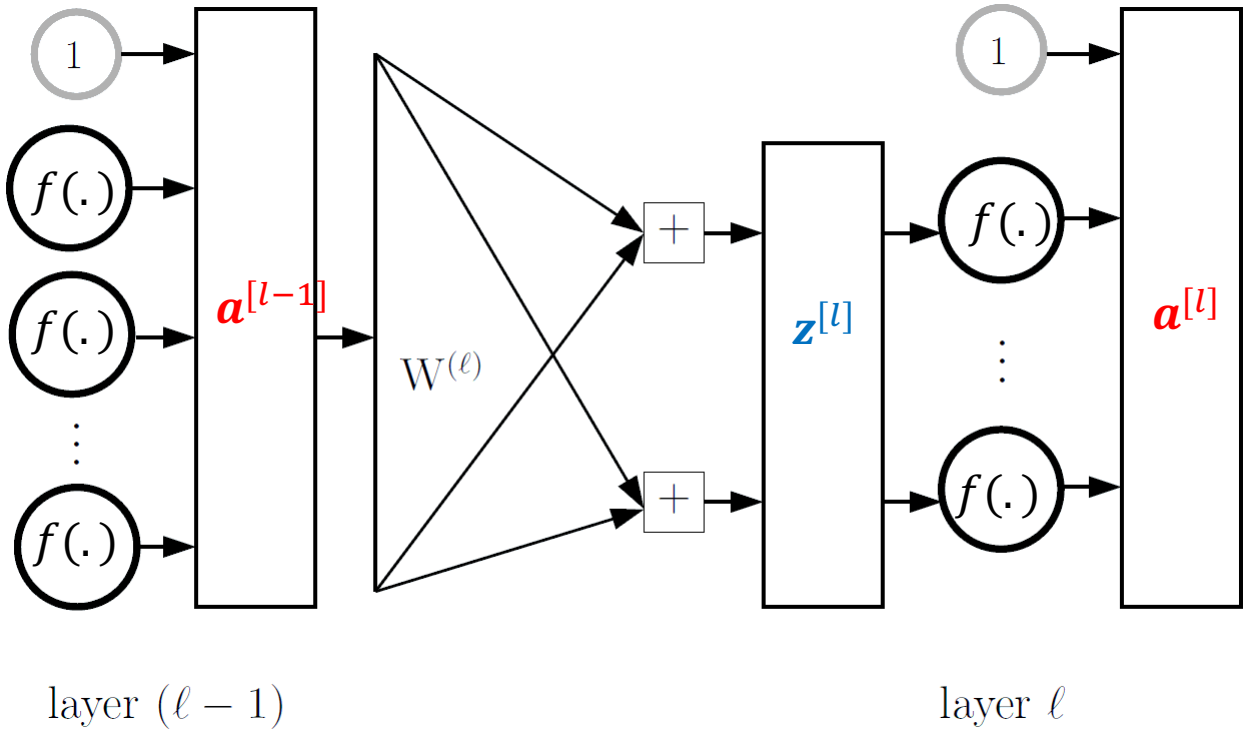
A first closer look at the network



- Showing a tiny 2-input network for illustration
  - Actual network would have many more neurons and inputs
- Explicitly separating the weighted sum of inputs from the activation

Backpropagation: Notation

- $\boldsymbol{a}^{[0]} \leftarrow Input$
- $output \leftarrow \boldsymbol{a}^{[L]}$



Backpropagation: Last layer gradient

For squared error loss:

$$loss = \frac{1}{2}\sum_j (o_j - y_j)^2$$

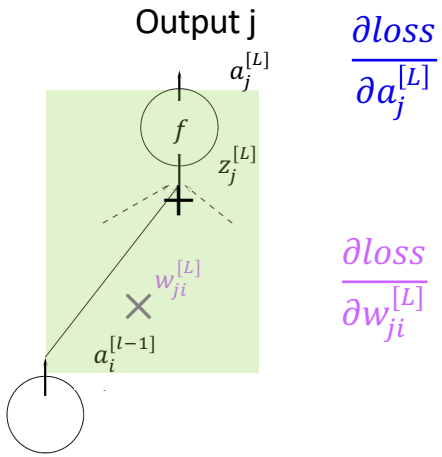
$$o_j = a_j^{[L]}$$

$$\frac{\partial loss}{\partial a_j^{[L]}} = (a_j^{[L]} - y_j)$$

$$\frac{\partial loss}{\partial w_{ji}^{[L]}} = ?$$

$$a_i^{[L]} = f\left(z_i^{[L]}\right)$$

$$z_j^{[L]} = \sum_{i=0}^{M} w_{ji}^{[L]} a_i^{[L-1]}$$



Backpropagation: Last layer gradient

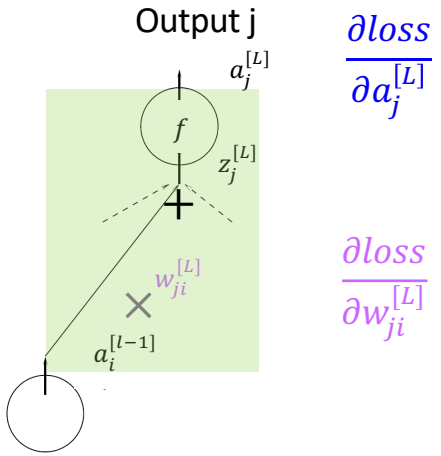
$$\frac{\partial loss}{\partial a_j^{[L]}} = (a_j^{[L]} - y_j)$$

$$a_j^{[L]} = f\left(z_j^{[L]}\right)$$

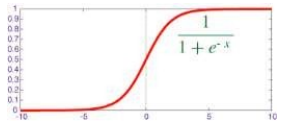
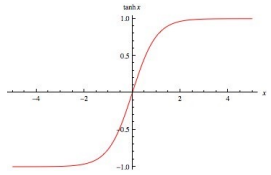
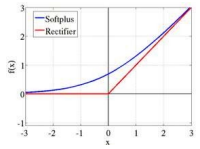
$$z_j^{[L]} = \sum_{i=0}^{M} w_{ji}^{[L]} a_i^{[L-1]}$$

$$\frac{\partial loss}{\partial w_{ji}^{[L]}} = \frac{\partial loss}{\partial a_j^{[L]}} f'\left(z_j^{[L]}\right) \frac{\partial z_j^{[L]}}{\partial w_{ji}^{[L]}}$$

$$= \frac{\partial loss}{\partial a_j^{[L]}} f'\left(z_j^{[L]}\right) a_i^{[L-1]}$$



Activations and their derivatives

	$f(z) = \frac{1}{1+\exp(-z)}$	$f'(z) = f(z)(1-f(z))$
	$f(z) = \tanh(z)$	$f'(z) = 1 - f^2(z)$
	$f(z) = \begin{cases} 0, & z < 0 \\ z, & z \geq 0 \end{cases}$	$f'(z) = \begin{cases} 1, z \geq 0 \\ 0, z < 0 \end{cases}$
	$f(z) = \log(1+\exp(z))$	$f'(z) = \frac{1}{1+\exp(-z)}$

- Some popular activation functions and their derivatives

Previous layers gradients

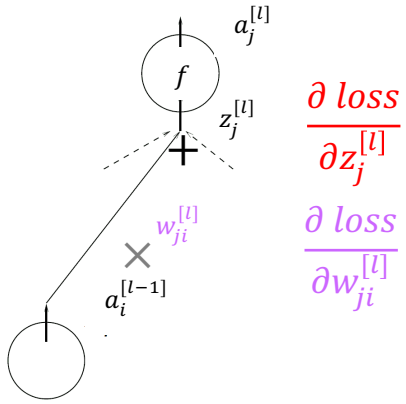
$$\frac{\partial\ loss}{\partial w_{ji}^{[l]}} = \frac{\partial\ loss}{\partial z_j^{[l]}} \frac{\partial z_j^{[l]}}{\partial w_{ji}^{[l]}} = \frac{\partial\ loss}{\partial z_j^{[l]}} a_i^{[l-1]}$$

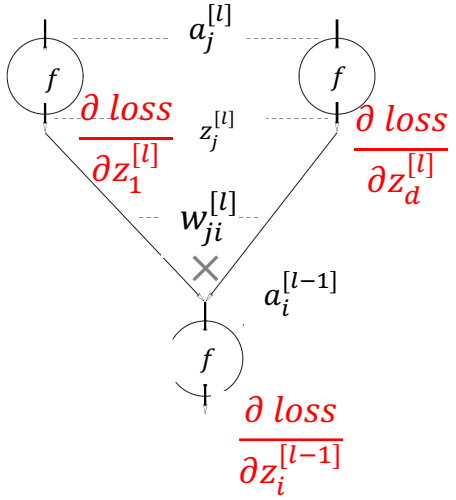
$$\frac{\partial\ loss}{\partial z_i^{[l-1]}} = \frac{\partial a_i^{[l-1]}}{\partial z_i^{[l-1]}} \sum_{j=1}^{d^{[l]}} \frac{\partial\ loss}{\partial z_j^{[l]}} \times \frac{\partial z_j^{[l]}}{\partial a_i^{[l-1]}}$$

$$= f'\left(z_i^{[l-1]}\right) \sum_{j=1}^{d^{[l]}} \frac{\partial\ loss}{\partial z_j^{[l]}} \times w_{ji}^{[l]}$$

$$a_j^{[l]} = f\left(z_j^{[l]}\right)$$

$$z_j^{[l]} = \sum_{i=0}^{M} w_{ji}^{[l]} a_i^{[l-1]}$$





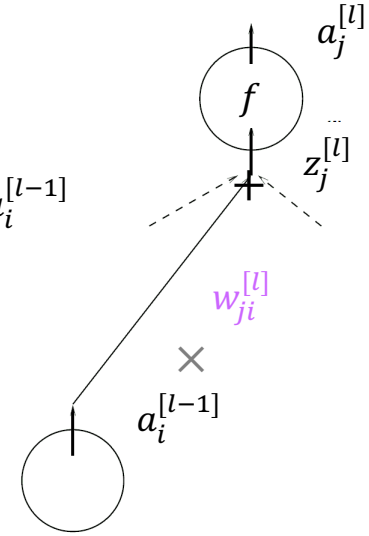
Backpropagation:

$$\frac{\partial\, loss}{\partial w_{ji}^{[l]}} = \frac{\partial\, loss}{\partial z_j^{[l]}} \times \frac{\partial z_j^{[l]}}{\partial w_{ji}^{[l]}}$$

$$= \delta_j^{[l]} \times a_i^{[l-1]}$$

$$a_j^{[l]} = f\left(z_j^{[l]}\right)$$

$$z_j^{[l]} = \sum_{i=0}^{M} w_{ji}^{[l]} a_i^{[l-1]}$$



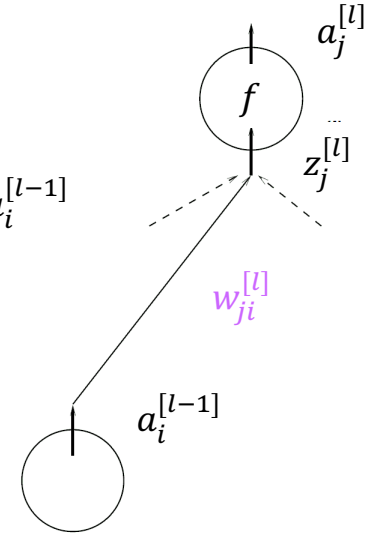
Backpropagation:

$$\frac{\partial\, loss}{\partial w_{ji}^{[l]}} = \frac{\partial\, loss}{\partial z_j^{[l]}} \times \frac{\partial z_j^{[l]}}{\partial w_{ji}^{[l]}}$$

$$= \delta_j^{[l]} \times a_i^{[l-1]}$$

$$a_j^{[l]} = f\left(z_j^{[l]}\right)$$

$$z_j^{[l]} = \sum_{i=0}^{M} w_{ji}^{[l]} a_i^{[l-1]}$$



- $\delta_j^{[l]} = \frac{\partial\, loss}{\partial z_j^{[l]}}$ is the sensitivity of the loss to $z_j^{[l]}$
- Sensitivity vectors can be obtained by running a backward process in the network architecture (hence the name backpropagation.)

We will compute $\boldsymbol{\delta}^{[l-1]}$ from $\boldsymbol{\delta}^{[l]}$:

$$\delta_i^{[l-1]} = f'\left(z_i^{[l-1]}\right) \sum_{j=1}^{d^{[l]}} \delta_j^{[l]} \times w_{ji}^{[l]}$$

Backward process on sensitivity vectors

- For the final layer $l = L$:

$$\delta_j^{[L]} = \frac{\partial\, loss}{\partial z_j^{[L]}}$$

- Compute $\boldsymbol{\delta}^{[l-1]}$ from $\boldsymbol{\delta}^{[l]}$: by running a backward process in the network architecture:

$$\delta_i^{[l-1]} = f'\left(z_i^{[l-1]}\right) \sum_{j=1}^{d^{[l]}} \delta_j^{[l]} \times w_{ji}^{[l]}$$

Backpropagation Algorithm

- Initialize all weights to small random numbers.
- **While not satisfied**
- **For** each training example **do**:
  1. Feed forward the training example to the network and compute the outputs of all units in forward step (z and a) and the loss
  2. For each unit find its δ in the backward step
  3. Update each network weight $w_{ji}^{[l]}$ as $w_{ji}^{[l]} \leftarrow w_{ji}^{[l]} - \eta \frac{\partial\, loss}{\partial w_{ji}^{[l]}}$ where $\frac{\partial\, loss}{\partial w_{ji}^{[l]}} = \delta_j^{[l]} \times a_i^{[l-1]}$

Vector formulation

- For layered networks it is generally simpler to think of the process in terms of vector operations
  - Simpler arithmetic
  - Fast matrix libraries make operations *much* faster

- We can restate the entire process in vector terms
  - This is what is *actually* used in any real system

The Jacobian

- The derivative of a vector function w.r.t. vector input is called a *Jacobian*
- It is the matrix of partial derivatives given below

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = f\left(\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}\right)$$

Using vector notation

$$\mathbf{y} = f(\mathbf{x})$$

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_2} \\ \cdots & \cdots & \ddots & \cdots \\ \frac{\partial y_!}{\partial x_d} & \frac{\partial y_2}{\partial x_d} & \cdots & \frac{\partial y_m}{\partial x_d} \end{bmatrix}$$

Matrix calculus

- Scalar-by-Vector

$$\frac{\partial y}{\partial \boldsymbol{x}} = \left[\frac{\partial y}{\partial x_1} \quad \cdots \quad \frac{\partial y}{\partial x_n}\right]^T$$

- Vector-by-Vector

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_n} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}$$

- Scalar-by-Matrix

$$\frac{\partial y}{\partial \boldsymbol{A}} = \begin{bmatrix} \frac{\partial y}{\partial A_{11}} & \cdots & \frac{\partial y}{\partial A_{1n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y}{\partial A_{m1}} & \cdots & \frac{\partial y}{\partial A_{mn}} \end{bmatrix}$$

- Vector-by-Matrix

$$\frac{\partial y}{\partial A_{ij}} = \frac{\partial y}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{z}}{\partial A_{ij}}$$

Vector derivatives

Scalar to Scalar

$$x \in \mathbb{R}, y \in \mathbb{R}$$

Regular derivative:

$$\frac{\partial y}{\partial x} \in \mathbb{R}$$

If x changes by a small amount, how much will y change?

Vector to Scalar

$$x \in \mathbb{R}^N, y \in \mathbb{R}$$

Derivative is **Gradient**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^N \quad \left(\frac{\partial y}{\partial x}\right)_n = \frac{\partial y}{\partial x_n}$$

For each element of x, if it changes by a small amount then how much will y change?

Vector to Vector

$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x}\right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

For each element of x, if it changes by a small amount then how much will each element of y change?

Examples of derivatives

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x}$$

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

$$z_i = \sum_j W_{ij} x_j$$

$$\frac{\partial z_i}{\partial x_j} = W_{ij}$$

Vector derivatives: Chain rule

- We can define a chain rule for Jacobians
- **For vector functions of vector inputs:**

$$\mathbf{y} = \boldsymbol{f}(\boldsymbol{g}(\mathbf{x}))$$

$$\mathbf{z} = \boldsymbol{g}(\mathbf{x})$$

$$\mathbf{y} = \boldsymbol{f}(\mathbf{z})$$

$$\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{z}}$$

Check

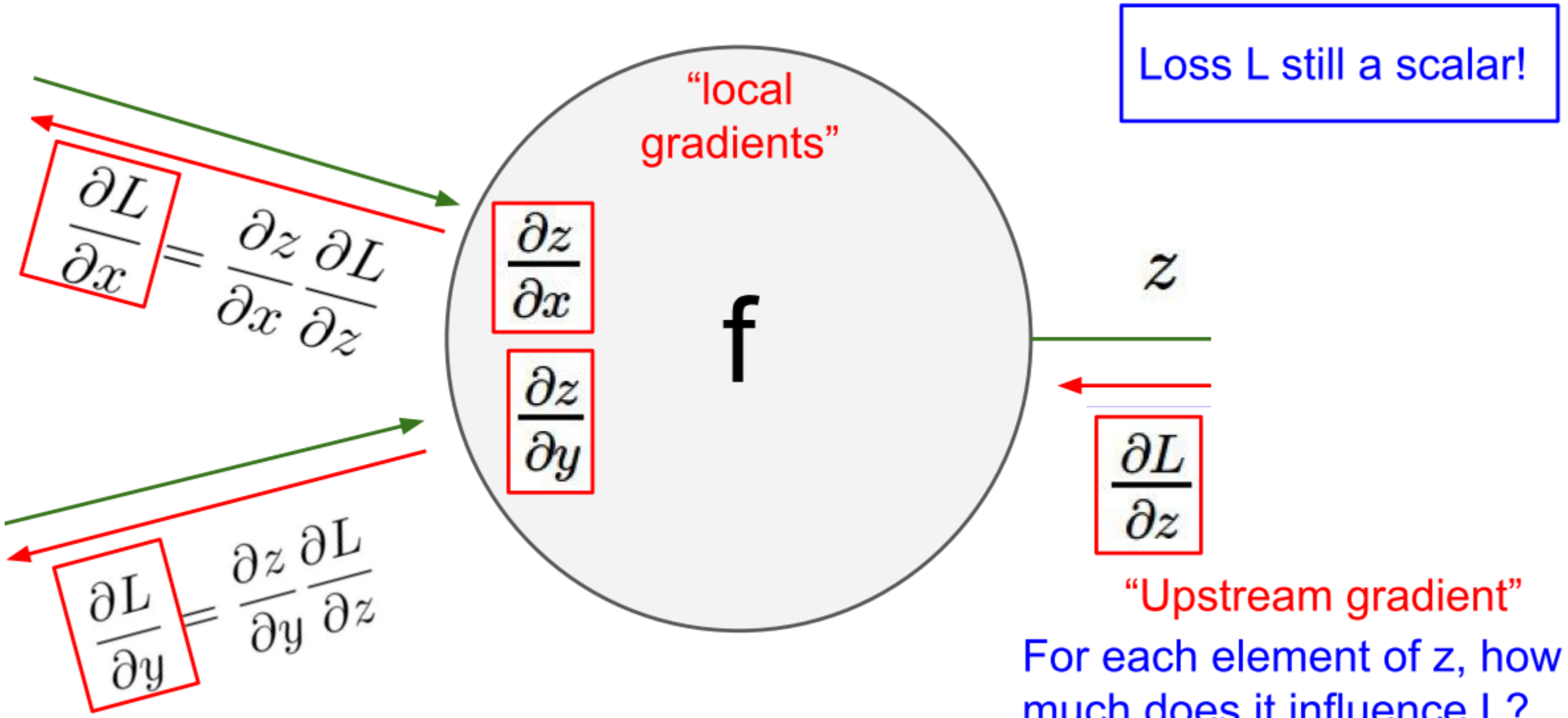
$$\Delta \mathbf{z} = \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}} \Delta \mathbf{x}$$

$$\Delta \mathbf{y} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{z}} \Delta \mathbf{z}$$

$$\Delta \mathbf{y} = \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{x}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{z}} \Delta \mathbf{x} = \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}} \Delta \mathbf{x}$$

Note the order: The derivative of the inner function comes first

Backprop with Vectors



Examples of derivatives

$$\boldsymbol{z} = \boldsymbol{W}\boldsymbol{x}$$

$$\frac{\partial L}{\partial \boldsymbol{z}} = \boldsymbol{\delta}$$

$$\frac{\partial L}{\partial \boldsymbol{W}} = \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{W}}\boldsymbol{\delta}$$

$$\frac{\partial L}{\partial \boldsymbol{W}} = \boldsymbol{\delta}\boldsymbol{x}^T$$

$$\frac{\partial \boldsymbol{z}}{\partial W_{ij}} = [0 \quad \cdots \quad 0 \quad x_j \quad 0 \quad \cdots \quad 0]$$

i-th element

$$\frac{\partial L}{\partial W_{ij}} = \delta_i x_j$$

Backpropagation shape rule

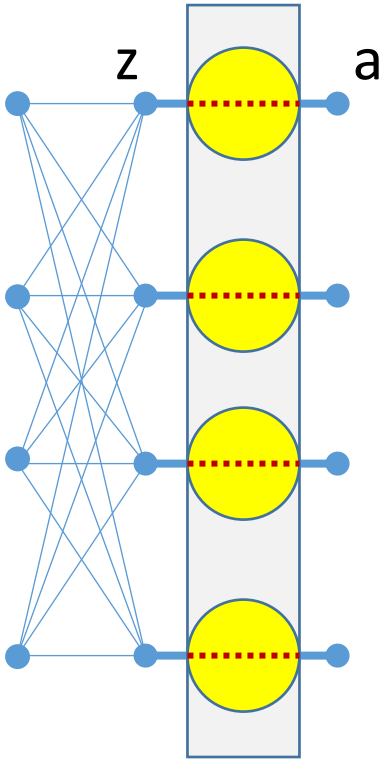
- When you take gradients against a **scalar,** the gradient at each intermediate step has **shape of denominator**

$$\boldsymbol{X} \in \mathbb{R}^{m \times n} \iff \frac{\partial L}{\partial \boldsymbol{W}} \in \mathbb{R}^{m \times n}$$

Dimension balancing

$Z = XW$	$[m \times w]$	$\frac{\partial Loss}{\partial Z} = \delta$
W	$[n \times w]$	$\frac{\partial Loss}{\partial W} = X^\top \delta$
X	$[m \times n]$	$\frac{\partial Loss}{\partial X} = \delta W^T$

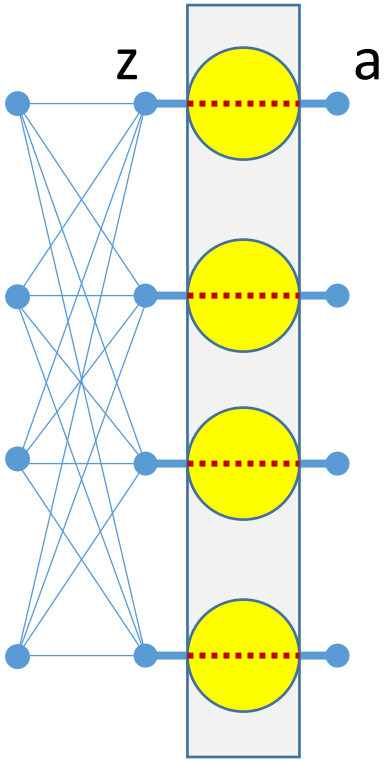
Jacobians can describe derivatives of activations w.r.t their input



$$\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{z}} = \begin{bmatrix} \frac{da_1}{dz_1} & 0 & \cdots & 0 \\ 0 & \frac{da_2}{dz_2} & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots \\ 0 & 0 & \cdots & \frac{da_m}{dz_m} \end{bmatrix}$$

- **For Scalar activations**
  - Number of outputs is identical to the number of inputs
- Jacobian is a diagonal matrix
  - Diagonal entries are individual derivatives of outputs w.r.t inputs
  - Not showing the superscript "[k]" in equations for brevity

Activation function: sigmoid

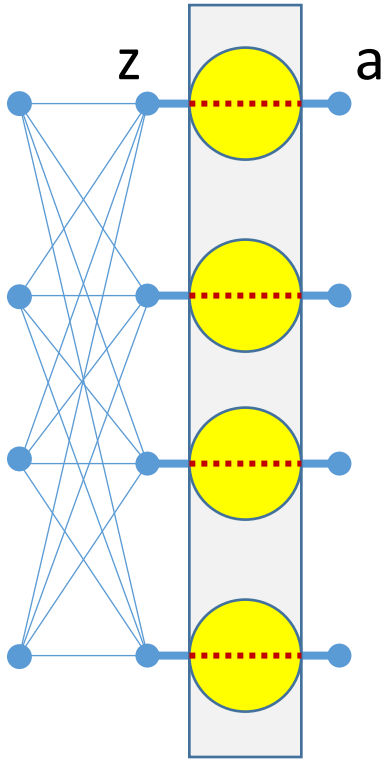


$$a_i = f(z_i)$$

$$\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{z}} = \begin{bmatrix} f'(z_1) & 0 & \cdots & 0 \\ 0 & f'(z_2) & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots \\ 0 & 0 & \cdots & f'(z_m) \end{bmatrix}$$

- **For scalar activations (shorthand notation):**
  - Jacobian is a diagonal matrix
  - Diagonal entries are individual derivatives of outputs w.r.t inputs

Activation function: sigmoid

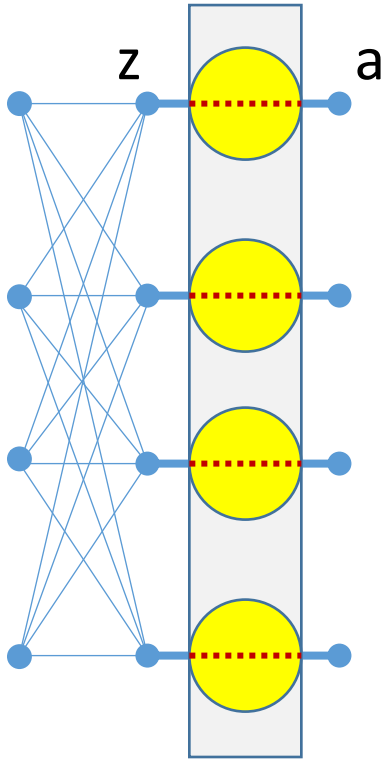


$$a_i = \sigma(z_i)$$

$$\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{z}} = \begin{bmatrix} \sigma(z_1)\big(1-\sigma(z_1)\big) & 0 & \cdots & 0 \\ 0 & \sigma(z_2)\big(1-\sigma(z_2)\big) & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots \\ 0 & 0 & \cdots & \sigma(z_m)\big(1-\sigma(z_m)\big) \end{bmatrix}$$

- **For scalar activations (shorthand notation):**
  - Jacobian is a diagonal matrix
  - Diagonal entries are individual derivatives of outputs w.r.t inputs

Activation function: ReLU

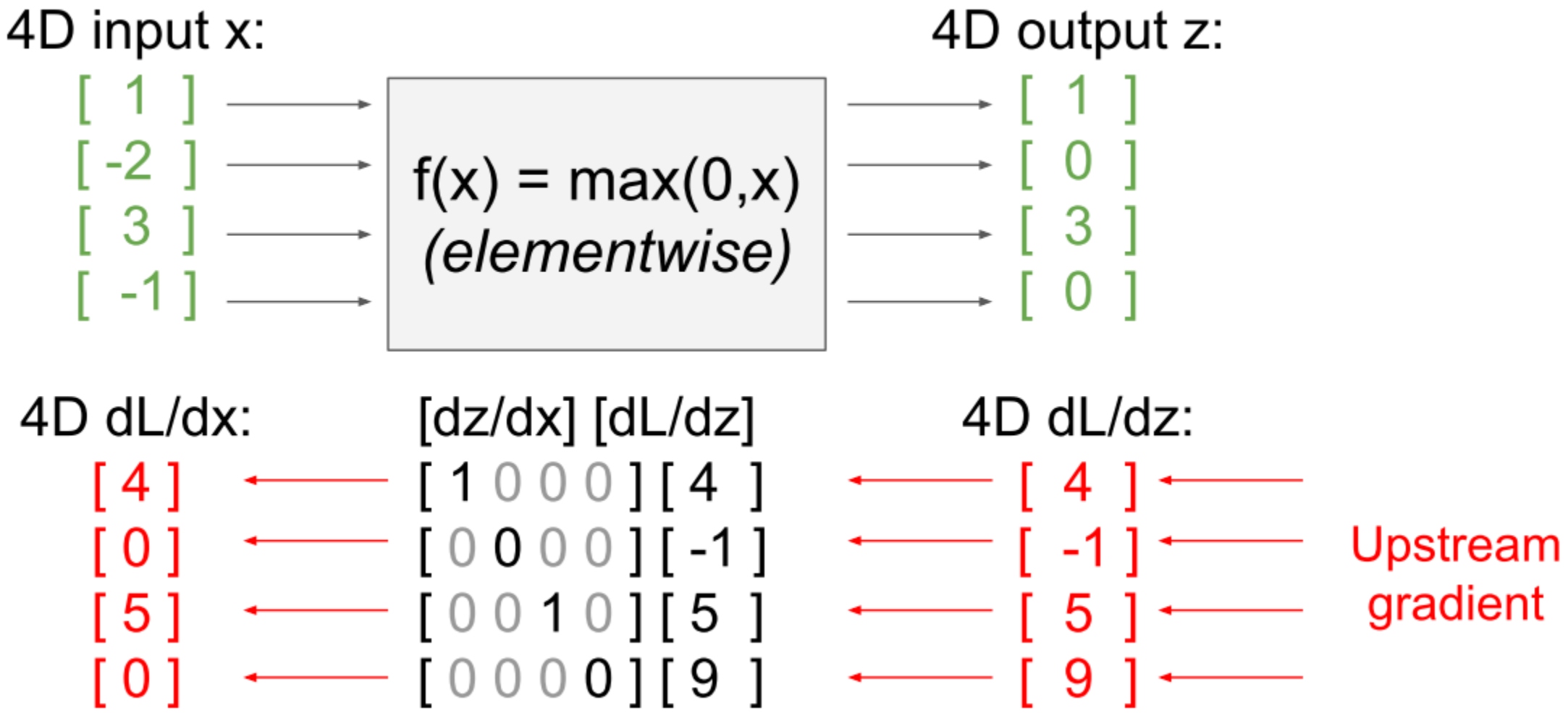


$$a_i = max(z_i, 0)$$

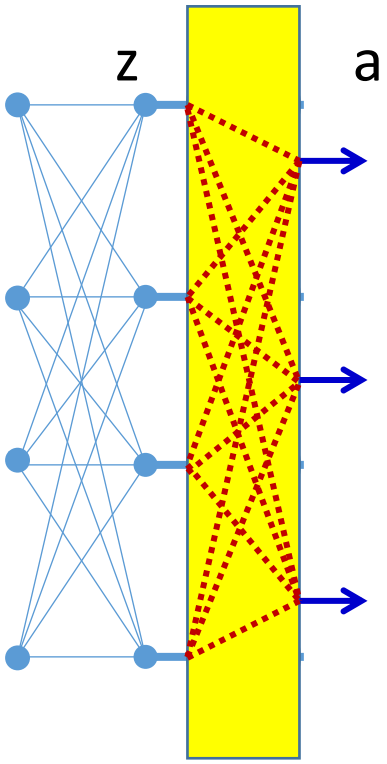
$$\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{z}} = \begin{bmatrix} I(z_1 > 0) & 0 & \cdots & 0 \\ 0 & I(z_2 > 0) & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots \\ 0 & 0 & \cdots & I(z_m > 0) \end{bmatrix}$$

- **For scalar activations (shorthand notation):**
  - Jacobian is a diagonal matrix
  - Diagonal entries are individual derivatives of outputs w.r.t inputs

Activation function: ReLU example



For *Vector* activations



$$\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{z}} = \begin{bmatrix} \frac{\partial a_1}{\partial z_1} & \frac{\partial a_2}{\partial z_1} & \cdots & \frac{\partial a_m}{\partial z_1} \\ \frac{\partial a_1}{\partial z_2} & \frac{\partial a_2}{\partial z_2} & \cdots & \frac{\partial a_m}{\partial z_2} \\ \cdots & \cdots & \ddots & \cdots \\ \frac{\partial a_1}{\partial z_n} & \frac{\partial a_2}{\partial z_n} & \cdots & \frac{\partial a_m}{\partial z_n} \end{bmatrix}$$

- Jacobian is a full matrix
  - Entries are partial derivatives of individual outputs w.r.t individual inputs

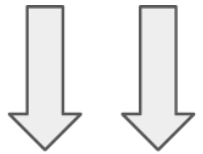
Special case: Affine functions

$$\mathbf{z}^{[l]} = \mathbf{W}^{[l]}\mathbf{a}^{[l-1]} + \mathbf{b}^{[l]}$$

$$\frac{\partial \mathbf{z}^{[l]}}{\partial \mathbf{a}^{[l-1]}} = \mathbf{W}^{[l]^T}$$

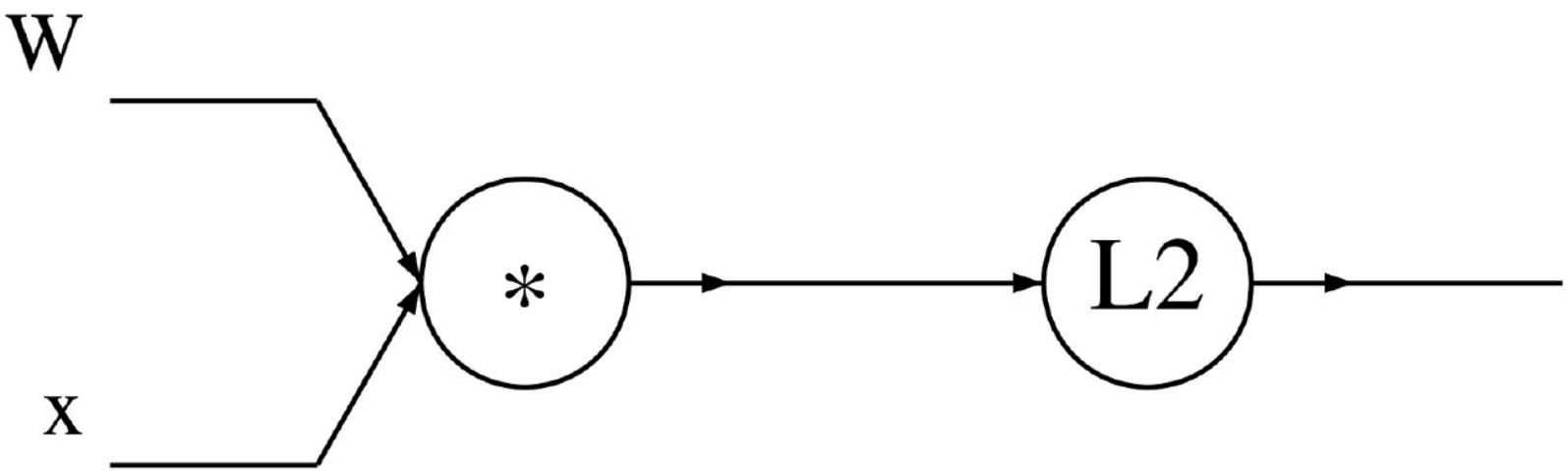
- Matrix $\mathbf{W}$ and bias $\mathbf{b}$ operating on vector $\mathbf{a}^{[l-1]}$ to produce vector $\mathbf{z}^{[l]}$

A vectorized example: $f(x, W) = ||W \cdot x||^2$

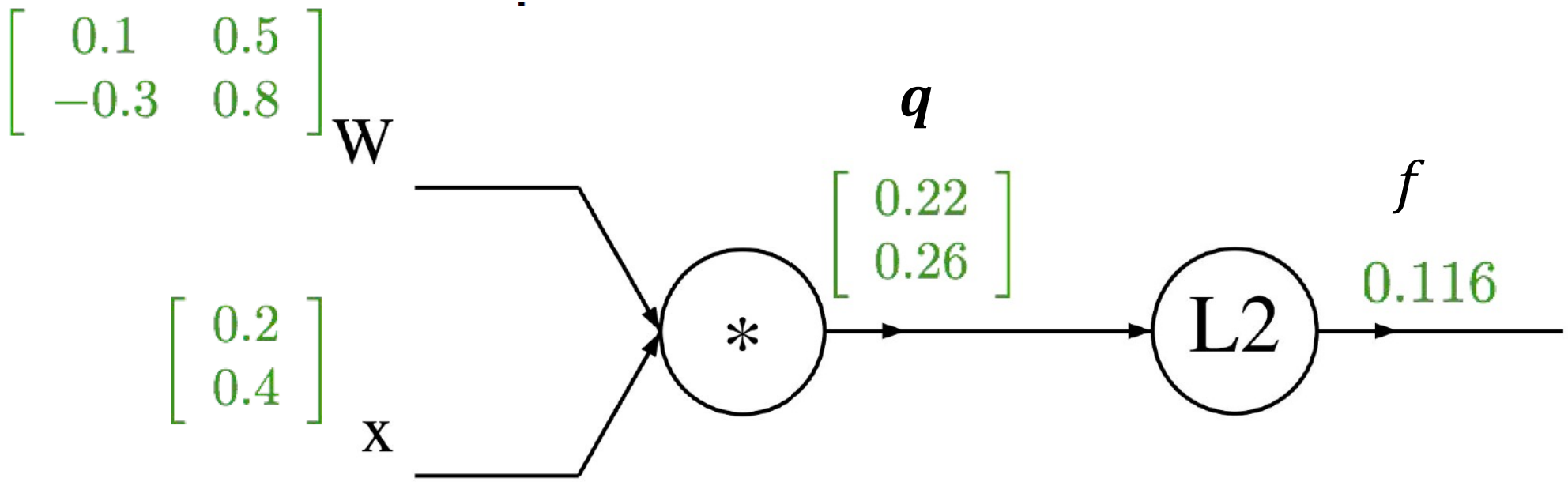


$\in \mathbb{R}^n \quad \in \mathbb{R}^{n \times n}$

A vectorized example: $f(x, W) = ||W \cdot x||^2$



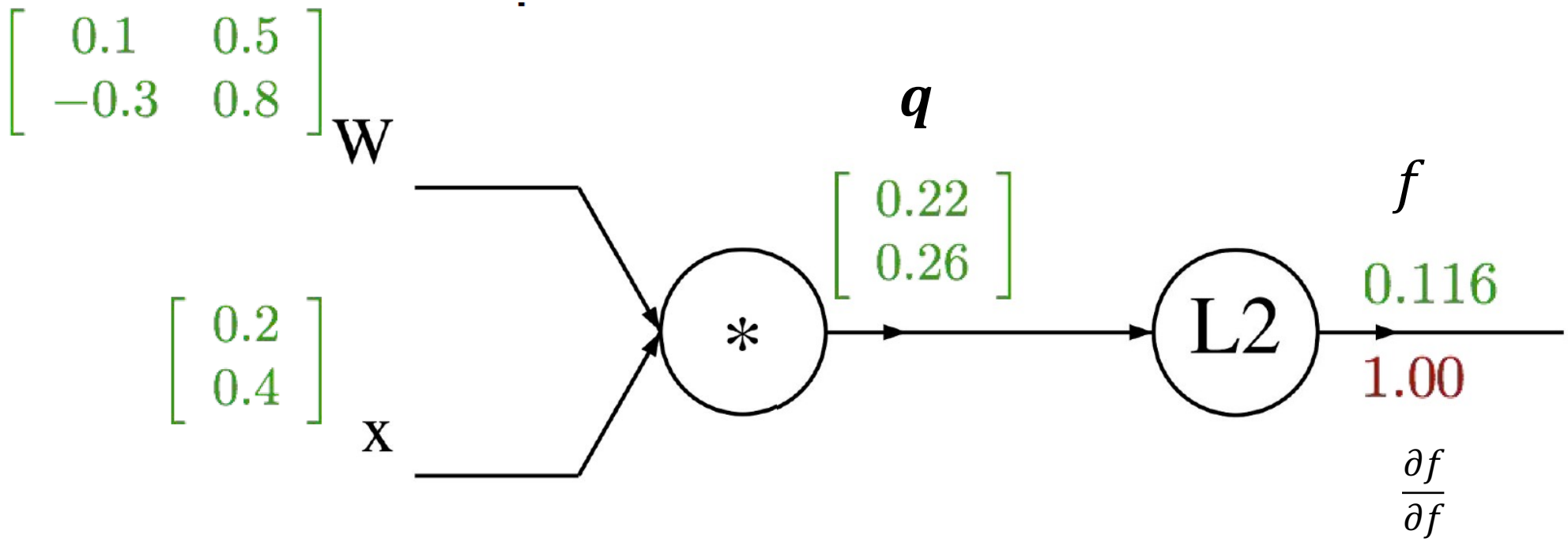
A vectorized example: $f(x, W) = ||W \cdot x||^2$



$\boldsymbol{q = Wx}$

$f(\boldsymbol{q}) = \|\boldsymbol{q}\|^2 = \boldsymbol{q}^T\boldsymbol{q}$

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



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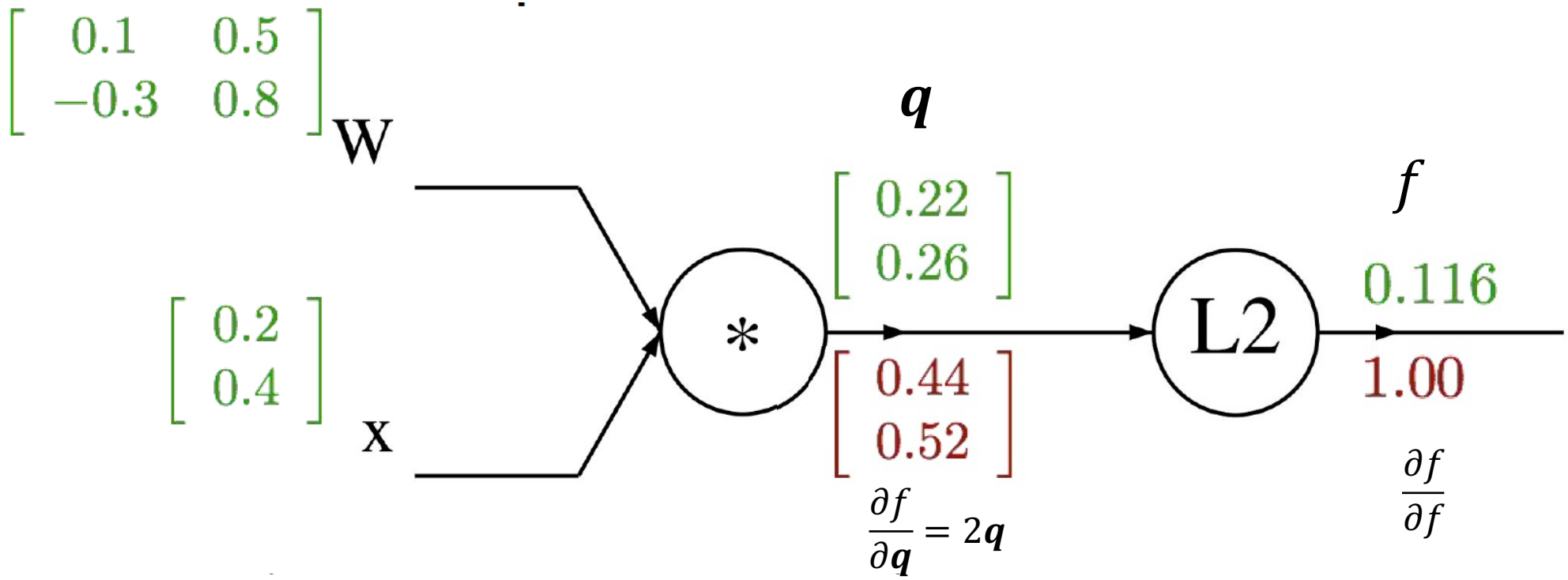


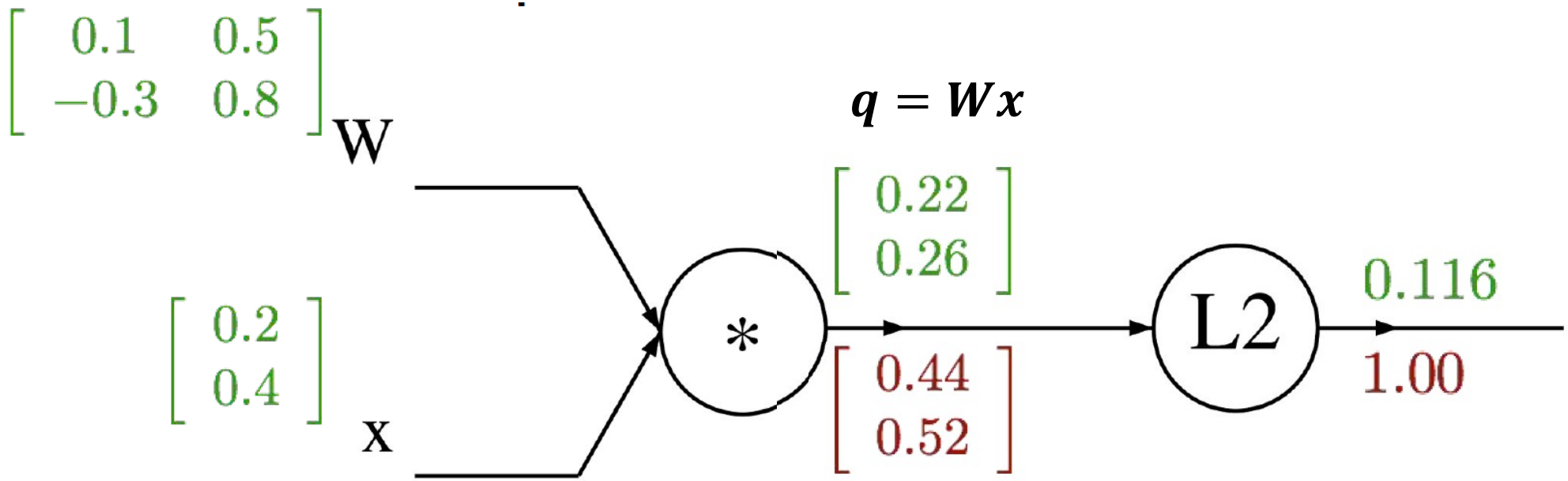
$\boldsymbol{q = Wx}$

$f(\boldsymbol{q}) = \|\boldsymbol{q}\|^2 = \boldsymbol{q}^T\boldsymbol{q} = q_1^2 + \cdots + q_m^2$

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

$$\frac{\partial f}{\partial \boldsymbol{q}} = 2\boldsymbol{q}$$

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



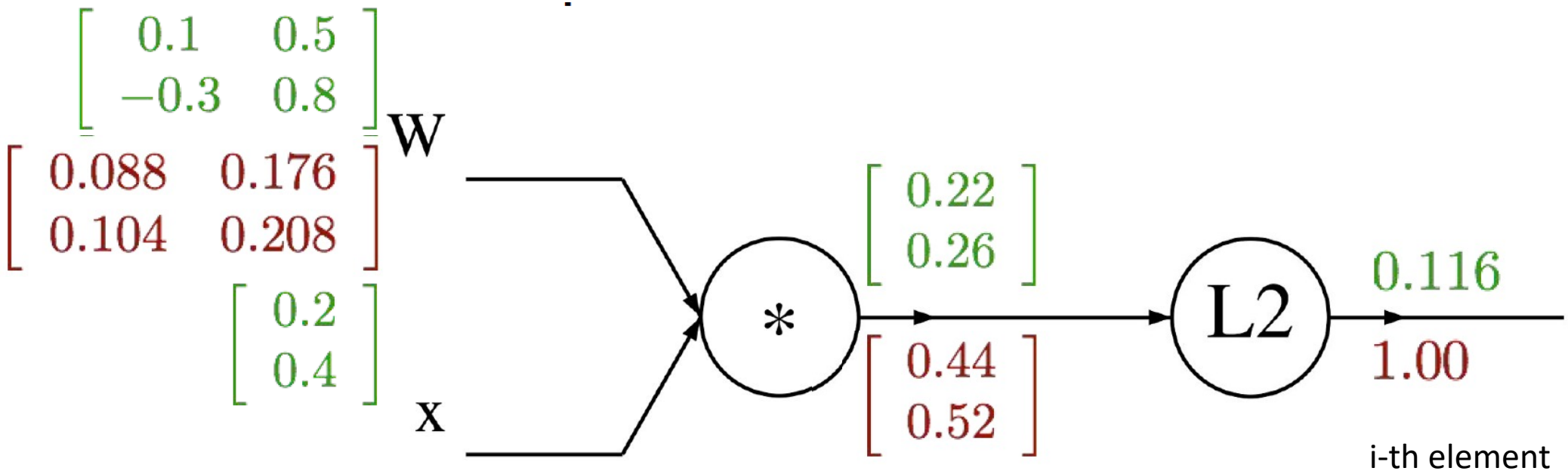
$\boldsymbol{q = Wx}$

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

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

$$\frac{\partial f}{\partial W} = \frac{\partial \boldsymbol{q}}{\partial W}\frac{\partial f}{\partial \boldsymbol{q}} = 2\frac{\partial \boldsymbol{q}}{\partial W}\boldsymbol{q}$$

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



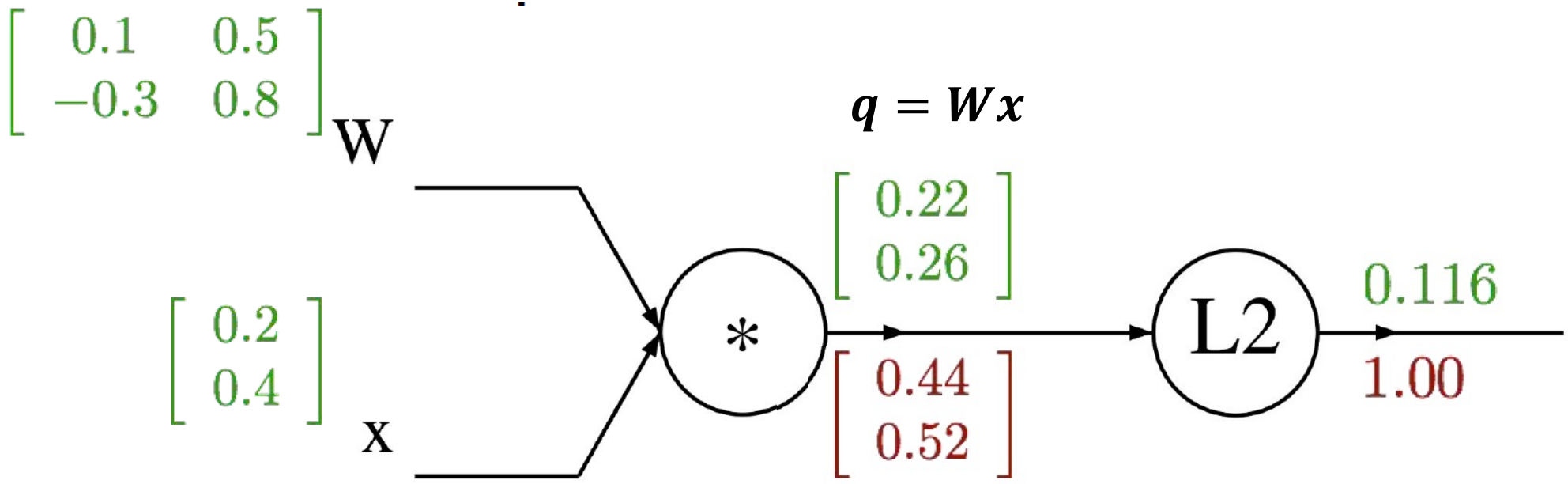
i-th element

$$\frac{\partial \boldsymbol{q}}{\partial W_{ij}} = [0 \quad \cdots \quad 0 \quad x_j \quad 0 \quad \cdots \quad 0]$$

$$\frac{\partial f}{\partial W_{ij}} = \frac{\partial \boldsymbol{q}}{\partial W_{ij}} \frac{\partial f}{\partial \boldsymbol{q}} = 2 q_i x_j$$

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

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



$\boldsymbol{q = Wx}$

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

$$\frac{\partial f}{\partial \boldsymbol{W}} = \frac{\partial f}{\partial \boldsymbol{q}} \frac{\partial \boldsymbol{q}}{\partial \boldsymbol{W}} = 2\boldsymbol{q}\boldsymbol{x}^T$$

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

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

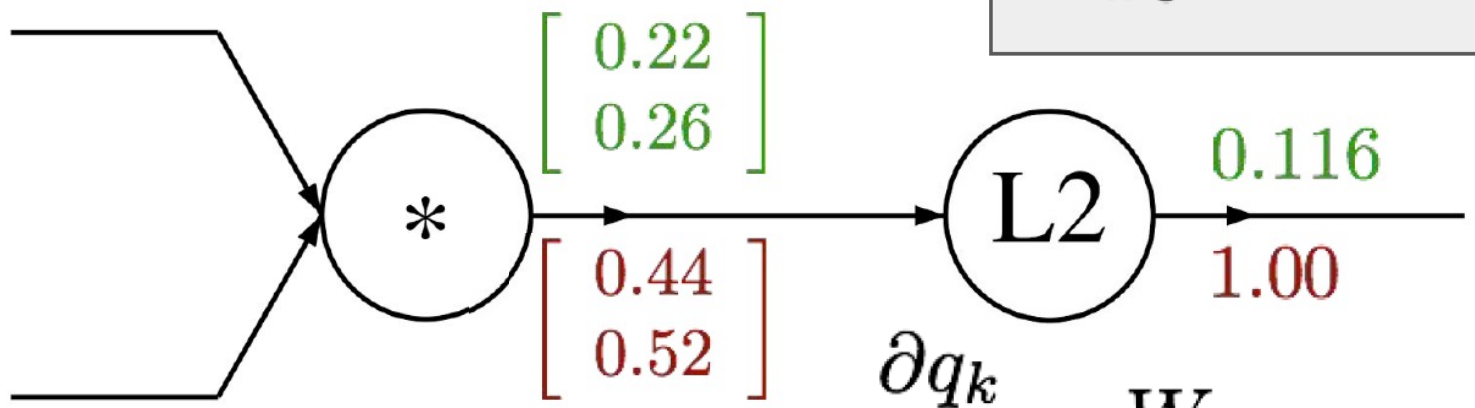
A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$

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

$$\begin{bmatrix} 0.088 & 0.176 \\ 0.104 & 0.208 \end{bmatrix}$$

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

$$\begin{bmatrix} -0.112 \\ 0.636 \end{bmatrix}$$



$$\begin{bmatrix} 0.22 \\ 0.26 \end{bmatrix}$$

$$\begin{bmatrix} 0.44 \\ 0.52 \end{bmatrix}$$

$$\nabla_x f = 2W^T \cdot q$$

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

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

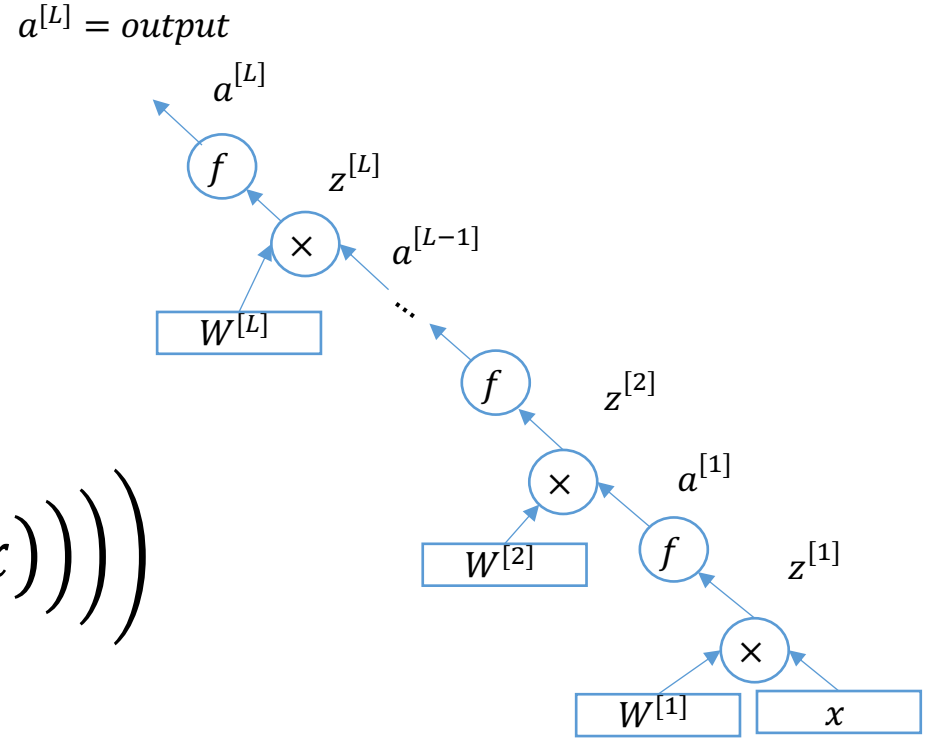
$$\frac{\partial f}{\partial x_i} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i}$$

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

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

Output as a composite function

$$Output = a^{[L]}$$
$$= f\left(z^{[L]}\right)$$
$$= f\left(W^{[L]}a^{[L-1]}\right)$$
$$= f\left(W^{[L]}f\left(W^{[L-1]}a^{[L-2]}\right)\right.$$
$$= f\left(W^{[L]}f\left(W^{[L-1]}\ldots f\left(W^{[2]}f\left(W^{[1]}x\right)\right)\right)\right)$$

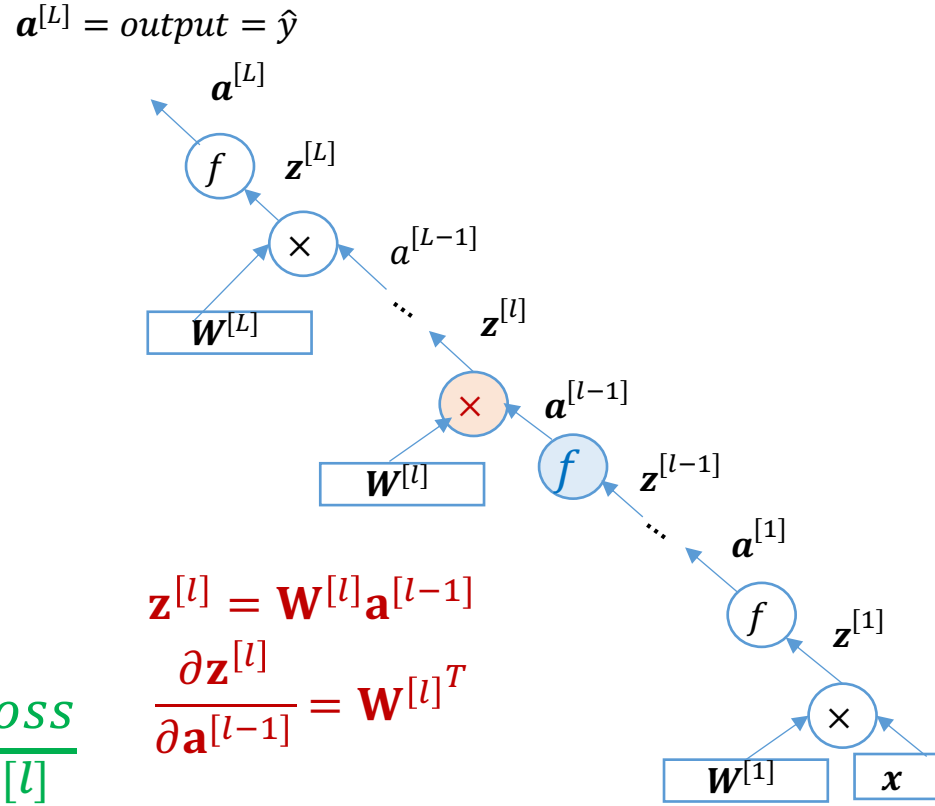


For convenience, we use the same activation functions for all layers.

However, output layer neurons most commonly do not need activation function (they show class scores or real-valued targets.)

Backward-pass vector

- Assume we have $\frac{\partial\, Loss}{\partial \boldsymbol{a}^{[L]}}$
- $\frac{\partial\, Loss}{\partial \boldsymbol{z}^{[L]}} = \frac{\partial \boldsymbol{a}^{[L]}}{\partial \boldsymbol{z}^{[L]}} \frac{\partial\, Loss}{\partial \boldsymbol{a}^{[L]}}$
- $\frac{\partial\, Loss}{\partial \boldsymbol{W}^{[l]}} = \frac{\partial \boldsymbol{z}^{[l]}}{\partial \boldsymbol{W}^{[l]}} \frac{\partial\, Loss}{\partial \boldsymbol{z}^{[l]}} = \frac{\partial\, Loss}{\partial \boldsymbol{z}^{[l]}} \boldsymbol{a}^{[l-1]^T}$
- $\frac{\partial\, Loss}{\partial \boldsymbol{z}^{[l-1]}} = \frac{\partial \boldsymbol{a}^{[l-1]}}{\partial \boldsymbol{z}^{[l-1]}} \frac{\partial \boldsymbol{z}^{[l]}}{\partial \boldsymbol{a}^{[l-1]}} \frac{\partial\, Loss}{\partial \boldsymbol{z}^{[l]}} = \frac{\partial \boldsymbol{a}^{[l-1]}}{\partial \boldsymbol{z}^{[l-1]}} W^{[l]^T} \frac{\partial\, Loss}{\partial \boldsymbol{z}^{[l]}}$



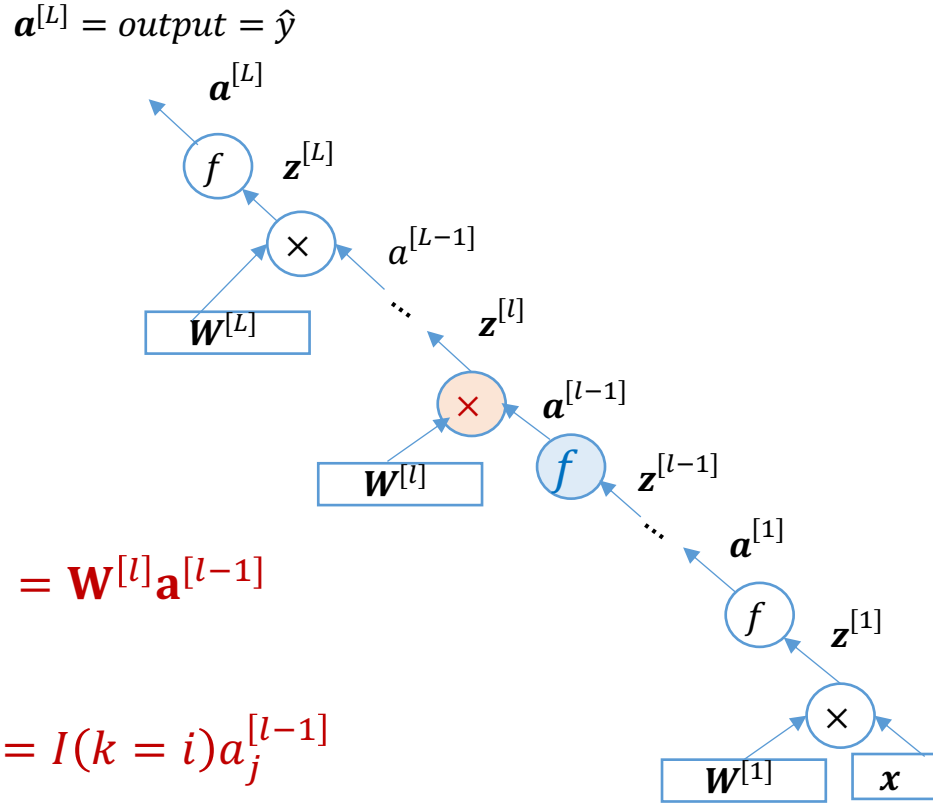
$$\mathbf{z}^{[l]} = \mathbf{W}^{[l]}\mathbf{a}^{[l-1]}$$

$$\frac{\partial \mathbf{z}^{[l]}}{\partial \mathbf{a}^{[l-1]}} = \mathbf{W}^{[l]^T}$$

$$\frac{\partial \boldsymbol{a}^{[l]}}{\partial \boldsymbol{z}^{[l]}} = \begin{bmatrix} f'\left(z_1^{[l]}\right) & 0 & \cdots & 0 \\ 0 & f'\left(z_2^{[l]}\right) & \cdots & 0 \\ \cdots & \cdots & \ddots & \cdots \\ 0 & 0 & \cdots & f'\left(z_m^{[l]}\right) \end{bmatrix}$$

Backward-pass vector

- Assume we have $\frac{\partial\ Loss}{\partial \boldsymbol{a}^{[L]}}$
- $\frac{\partial\ Loss}{\partial \boldsymbol{z}^{[L]}} = \frac{\partial \boldsymbol{a}^{[L]}}{\partial \boldsymbol{z}^{[L]}} \frac{\partial\ Loss}{\partial \boldsymbol{a}^{[L]}}$
- $\frac{\partial\ Loss}{\partial W_{ij}^{[l]}} = \frac{\partial \boldsymbol{z}^{[l]}}{\partial W_{ij}^{[l]}} \frac{\partial\ Loss}{\partial \boldsymbol{z}^{[l]}} = \frac{\partial\ Loss}{\partial z_i^{[l]}} \frac{\partial z_i^{[l]}}{\partial W_{ij}^{[l]}}$ $a_j^{[l-1]}$



$\mathbf{z}^{[l]} = \mathbf{W}^{[l]}\mathbf{a}^{[l-1]}$

$\frac{\partial \mathrm{z}_k^{[l]}}{\partial \mathrm{W}_{ij}^{[l]}} = I(k=i)a_j^{[l-1]}$

Find and save $\boldsymbol{\delta}^{[L]}$

- Called error, computed recursively in backward manner

- For the final layer $l = L$:

$$\boldsymbol{\delta}^{[L]} = \frac{\partial\ Loss}{\partial \boldsymbol{z}^{[L]}}$$

Compute $\boldsymbol{\delta}^{[l-1]}$ from $\boldsymbol{\delta}^{[l]}$

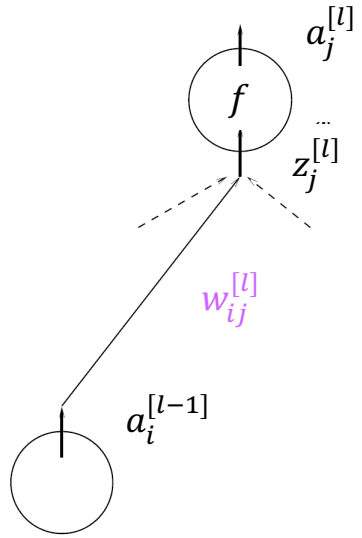
- $\boldsymbol{\delta}^{[l]} = \frac{\partial\, loss}{\partial \boldsymbol{z}^{[l]}}$ is the sensitivity of the output to $\boldsymbol{z}^{[l]}$

- Sensitivity vectors can be obtained by running a backward process in the network architecture (hence the name backpropagation.)

$$\boldsymbol{\delta}^{[l-1]} = W^{[l]^T} f'(\boldsymbol{a}^{[l-1]})\boldsymbol{\delta}^{[l]}$$

$$a_i^{[l]} = f\left(z_i^{[l]}\right)$$

$$z_j^{[l]} = \sum_{i=0}^{M} w_{ij}^{[l]} a_i^{[l-1]}$$



Mini-batch SGD

- Loop:
  1. **Sample** a batch of data
  2. **Forward** prop it through the graph (network), get loss
  3. **Backprop** to calculate the gradients
  4. **Update** the parameters using the gradient

Summary

- Neural nets may be very large: impractical to write down gradient formula by hand for all parameters

- **Backpropagation** = recursive application of the chain rule along a computational graph to compute the gradients of all inputs/parameters/intermediates + Dynamic Programming

- Implementations maintain a graph structure, where the nodes implement the **forward**() / **backward**() API
  - **forward**: compute result of an operation and save any intermediates needed for gradient computation in memory
  - **backward**: apply the chain rule to compute the gradient of the loss function with respect to the inputs

Converting error derivatives into a learning procedure

- The backpropagation algorithm is an efficient way of computing the gradient of the error function w.r.t. weights and biases.

- There are many other decisions to be made to have a learning procedure from these derivatives:
  - Convergence or optimization issues: How do we use the error derivatives?
  - Generalization issues: How can we improve its decisions on unseen data?