

# Lecture 4:

# Neural Networks and Backpropagation

# Administrative: Assignment 1

**Assignment 1** due **Wednesday April 17**, 11:59pm

If using Google Cloud, **you don't need GPUs** for this assignment!

We will distribute Google Cloud coupons by this weekend

# Administrative: Alternate Midterm Time

If you need to request an alternate midterm time:

See Piazza for form, fill it out by 4/25 (two weeks from today)

# Administrative: Project Proposal

Project proposal due 4/24

# Administrative: Discussion Section

Discussion section tomorrow (1:20pm in Gates B03):

How to pick a project / How to read a paper

# Where we are...

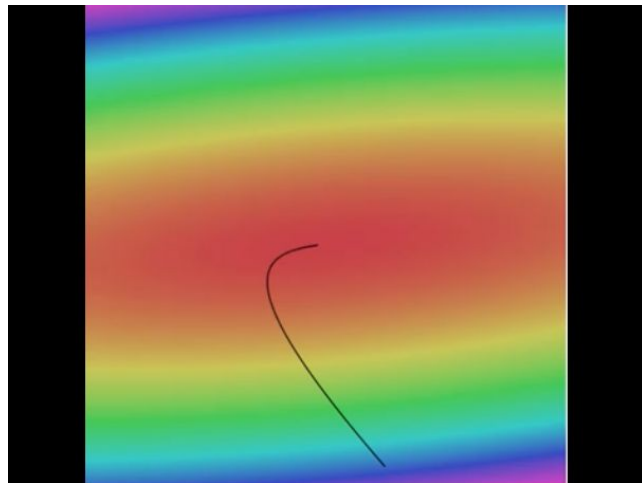
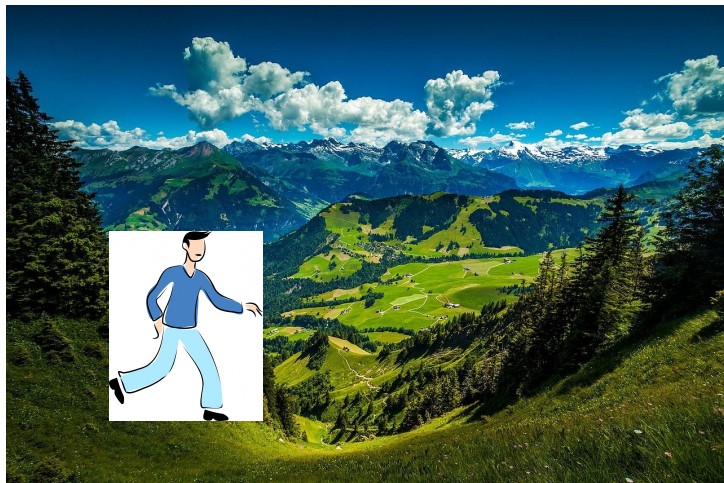
$$s = f(x; W) = Wx \quad \text{Linear score function}$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1) \quad \text{SVM loss (or softmax)}$$

$$L = \frac{1}{N} \sum_{i=1}^N L_i + \lambda \sum_k W_k^2 \quad \text{data loss + regularization}$$

How to find the best  $W$ ?

# Finding the best $W$ : Optimize with Gradient Descent



```
# Vanilla Gradient Descent
```

```
while True:
```

```
    weights_grad = evaluate_gradient(loss_fun, data, weights)
```

```
    weights += - step_size * weights_grad # perform parameter update
```

[Landscape image](#) is [CC0 1.0](#) public domain

[Walking man image](#) is [CC0 1.0](#) public domain

# Gradient descent

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

**Numerical gradient:** slow :(), approximate :(), easy to write :)

**Analytic gradient:** fast :), exact :), error-prone :(

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



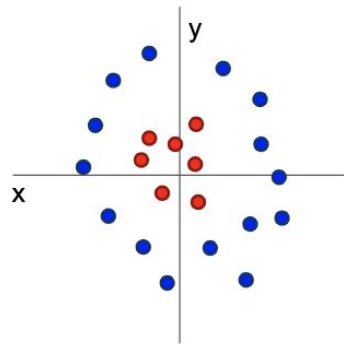
# Problem: Linear Classifiers are not very powerful

## Visual Viewpoint



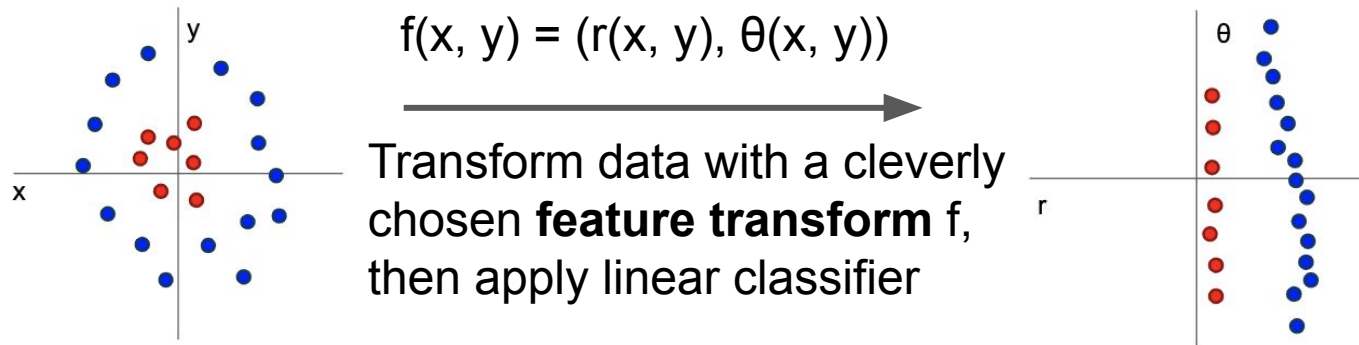
Linear classifiers learn  
one template per class

## Geometric Viewpoint

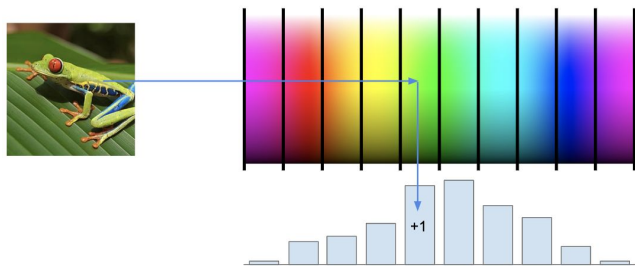


Linear classifiers  
can only draw linear  
decision boundaries

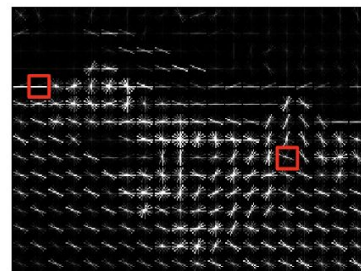
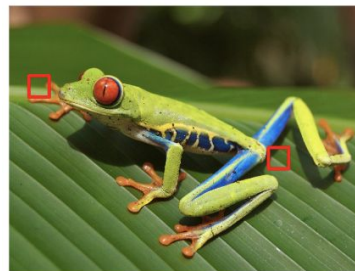
# One Solution: Feature Transformation



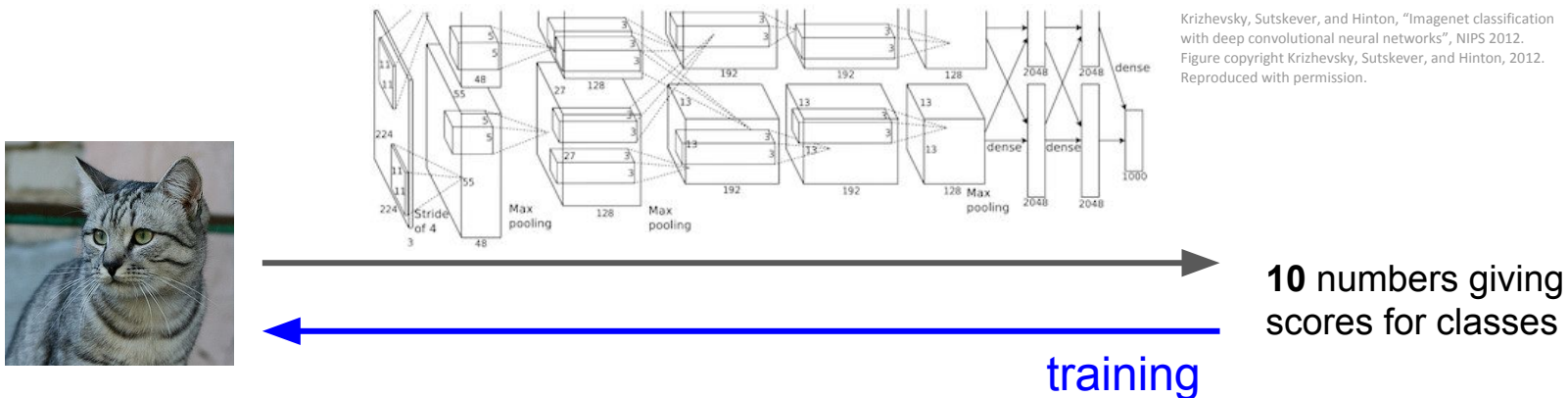
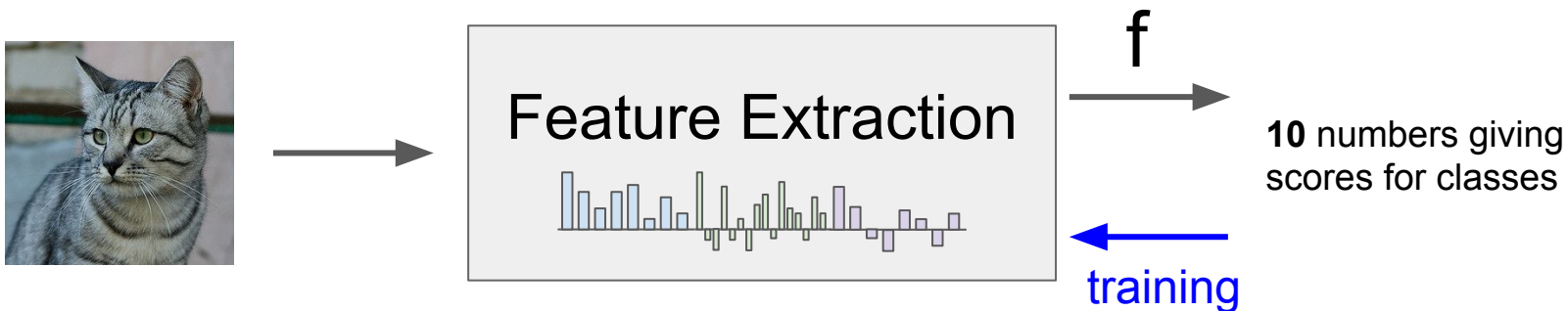
Color Histogram



Histogram of Oriented Gradients (HoG)



# Image features vs ConvNets



# Today: Neural Networks

# Neural networks: without the brain stuff

(**Before**) Linear score function:  $f = Wx$

$$x \in \mathbb{R}^D, W \in \mathbb{R}^{C \times D}$$

# Neural networks: without the brain stuff

(**Before**) Linear score function:  $f = Wx$

(**Now**) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

(In practice we will usually add a learnable bias at each layer as well)

# Neural networks: without the brain stuff

(**Before**) Linear score function:  $f = Wx$

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$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

“Neural Network” is a very broad term; these are more accurately called “fully-connected networks” or sometimes “multi-layer perceptrons” (MLP)

(In practice we will usually add a learnable bias at each layer as well)

# Neural networks: without the brain stuff

(**Before**) Linear score function:  $f = Wx$

(**Now**) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$   
or 3-layer Neural Network

$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

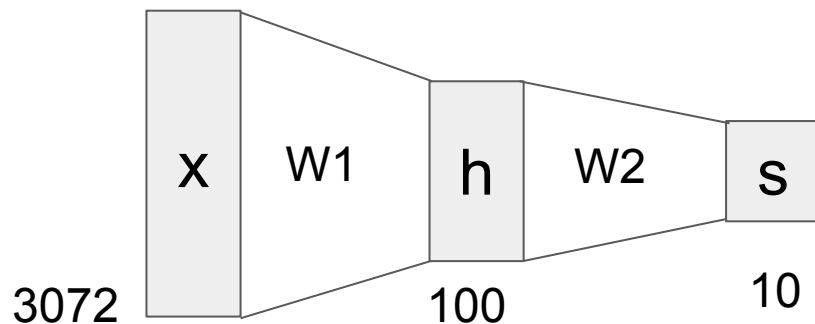
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# Neural networks: without the brain stuff

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(**Now**) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$

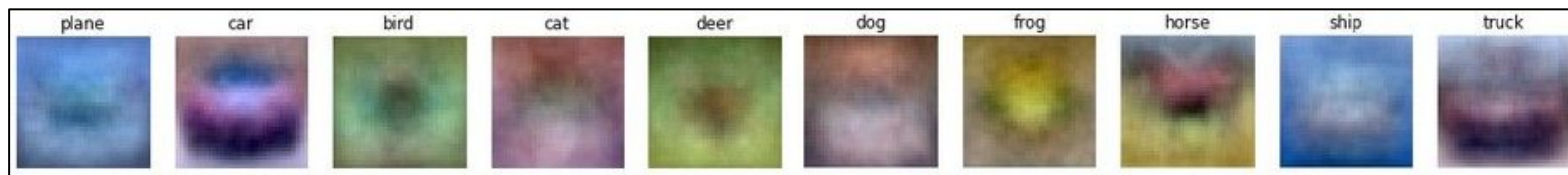
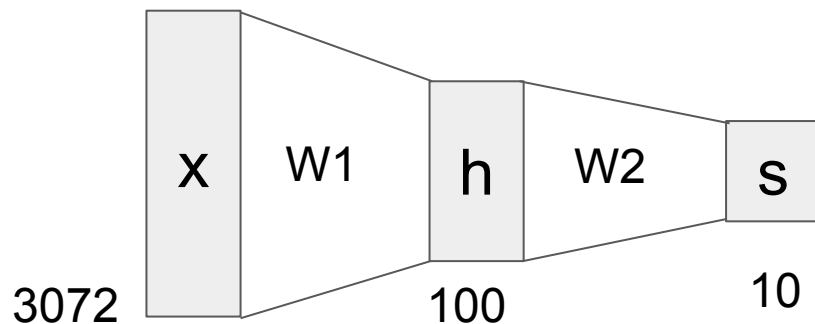


$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

# Neural networks: without the brain stuff

(**Before**) Linear score function:  $f = Wx$

(**Now**) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$



# Neural networks: without the brain stuff

(**Before**) Linear score function:  $f = Wx$

(**Now**) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$

The function  $\max(0, z)$  is called the **activation function**.

**Q:** What if we try to build a neural network without one?

$$f = W_2 W_1 x$$

# Neural networks: without the brain stuff

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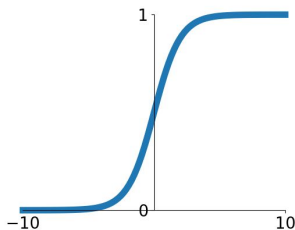
$$f = W_2 W_1 x \quad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

**A:** We end up with a linear classifier again!

# Activation functions

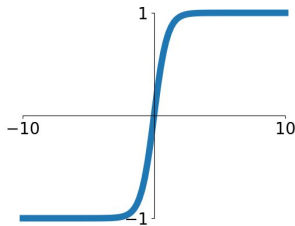
## Sigmoid

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



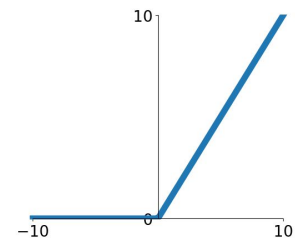
## tanh

$$\tanh(x)$$



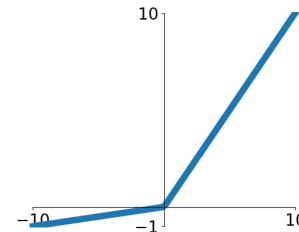
## ReLU

$$\max(0, x)$$



## Leaky ReLU

$$\max(0.1x, x)$$

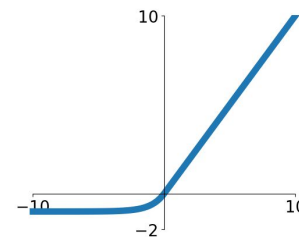


## Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

## ELU

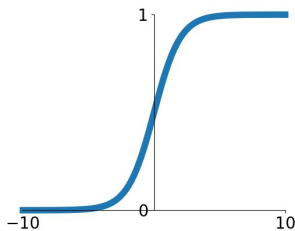
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



# Activation functions

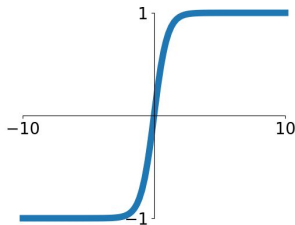
## Sigmoid

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



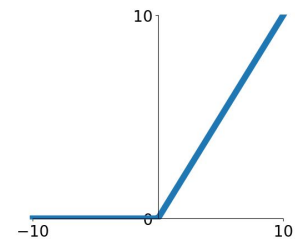
## tanh

$$\tanh(x)$$



## ReLU

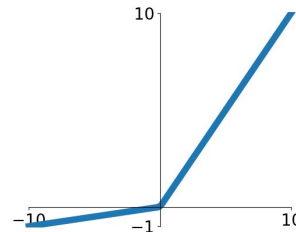
$$\max(0, x)$$



ReLU is a good default  
choice for most problems

## Leaky ReLU

$$\max(0.1x, x)$$

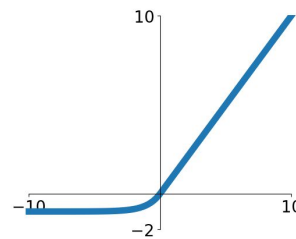


## Maxout

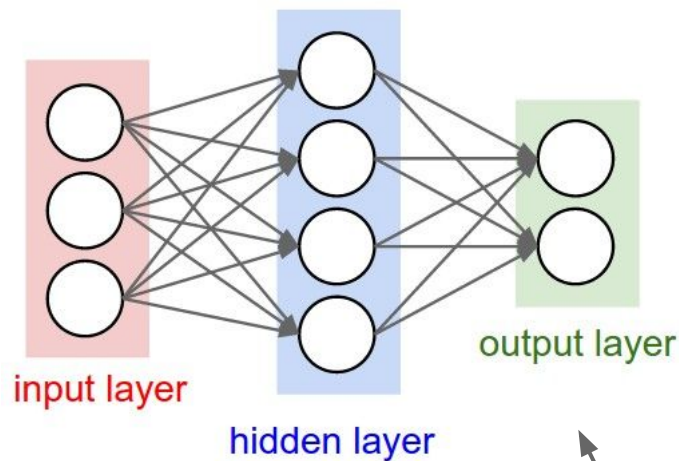
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

## ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$

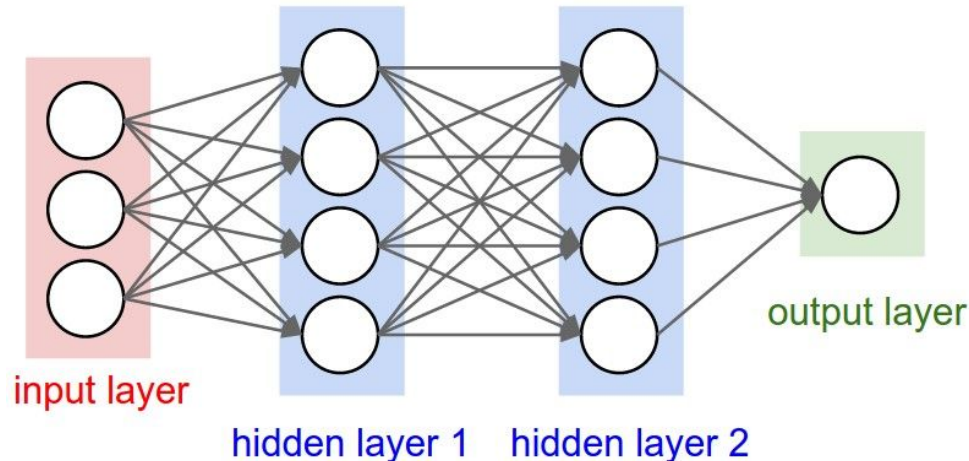


# Neural networks: Architectures



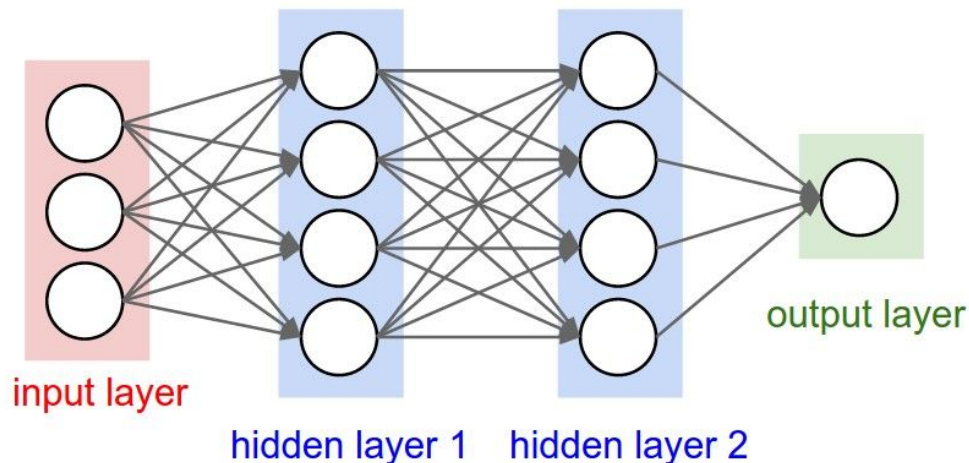
“2-layer Neural Net”, or  
“1-hidden-layer Neural Net”

“Fully-connected” layers



“3-layer Neural Net”, or  
“2-hidden-layer Neural Net”

# Example feed-forward computation of a neural network



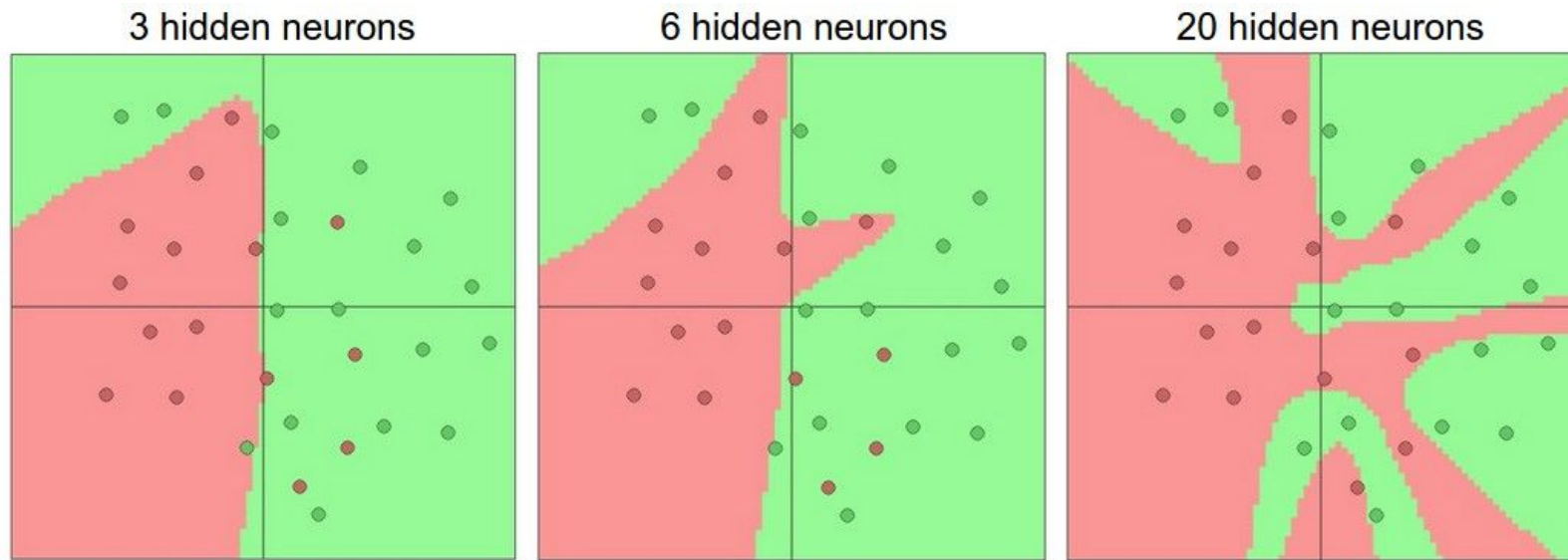
```
# forward-pass of a 3-layer neural network:  
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)  
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)  
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)  
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)  
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```



Full implementation of training a 2-layer Neural Network needs ~20 lines:

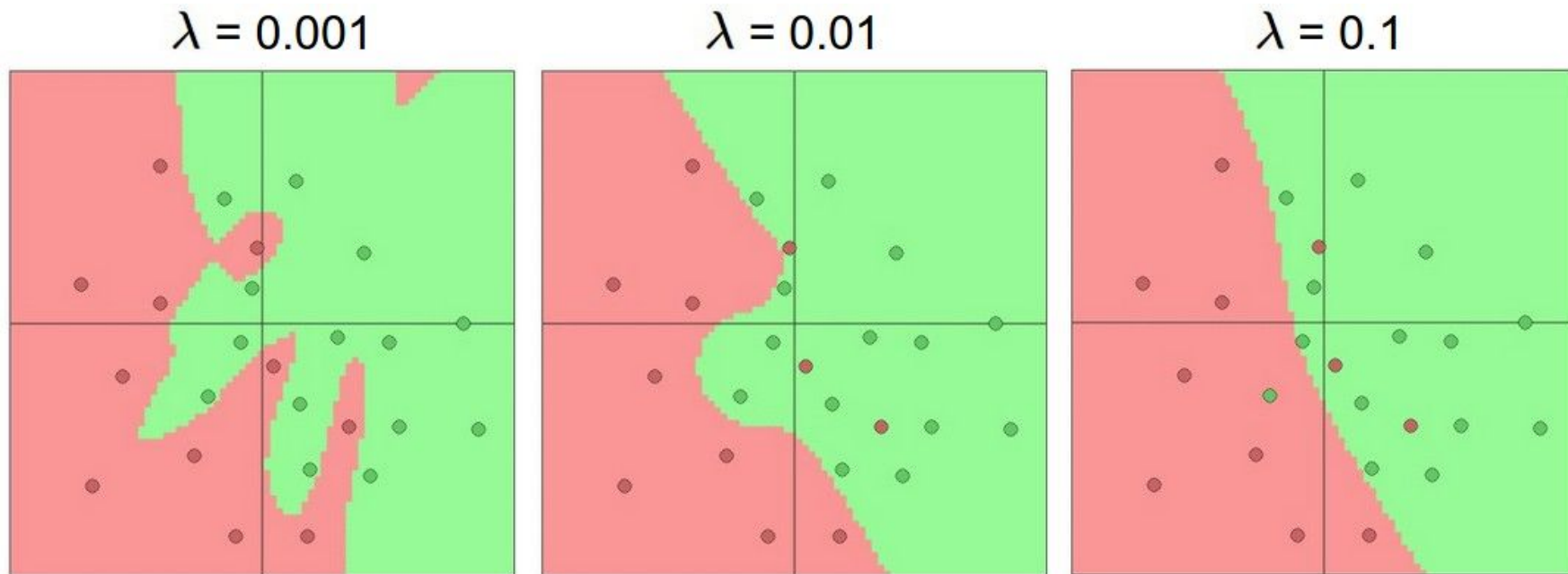
```
1  import numpy as np
2  from numpy.random import randn
3
4  N, D_in, H, D_out = 64, 1000, 100, 10
5  x, y = randn(N, D_in), randn(N, D_out)
6  w1, w2 = randn(D_in, H), randn(H, D_out)
7
8  for t in range(2000):
9      h = 1 / (1 + np.exp(-x.dot(w1)))
10     y_pred = h.dot(w2)
11     loss = np.square(y_pred - y).sum()
12     print(t, loss)
13
14     grad_y_pred = 2.0 * (y_pred - y)
15     grad_w2 = h.T.dot(grad_y_pred)
16     grad_h = grad_y_pred.dot(w2.T)
17     grad_w1 = x.T.dot(grad_h * h * (1 - h))
18
19     w1 -= 1e-4 * grad_w1
20     w2 -= 1e-4 * grad_w2
```

# Setting the number of layers and their sizes



↑  
more neurons = more capacity

Do not use size of neural network as a regularizer. Use stronger regularization instead:



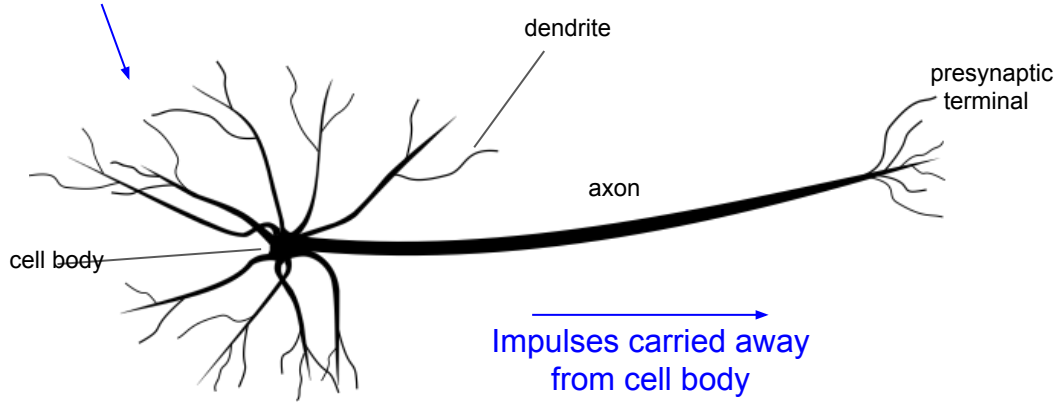
(Web demo with ConvNetJS:

<http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html>)



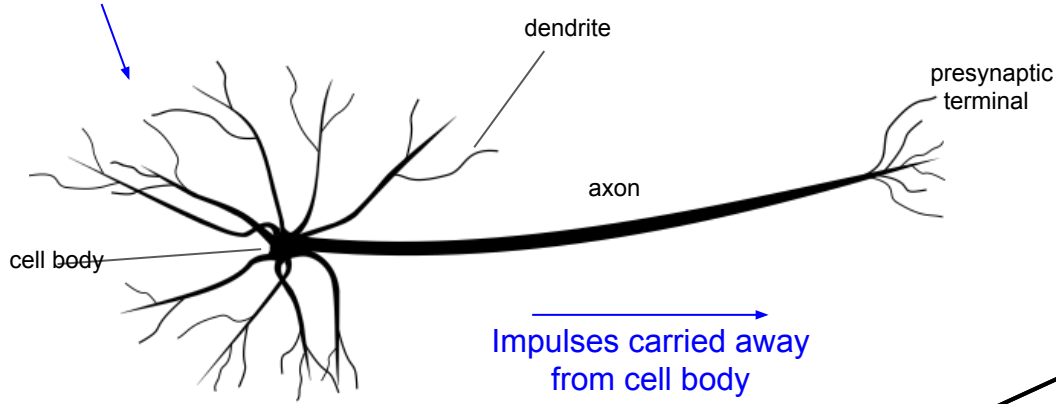
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Impulses carried toward cell body

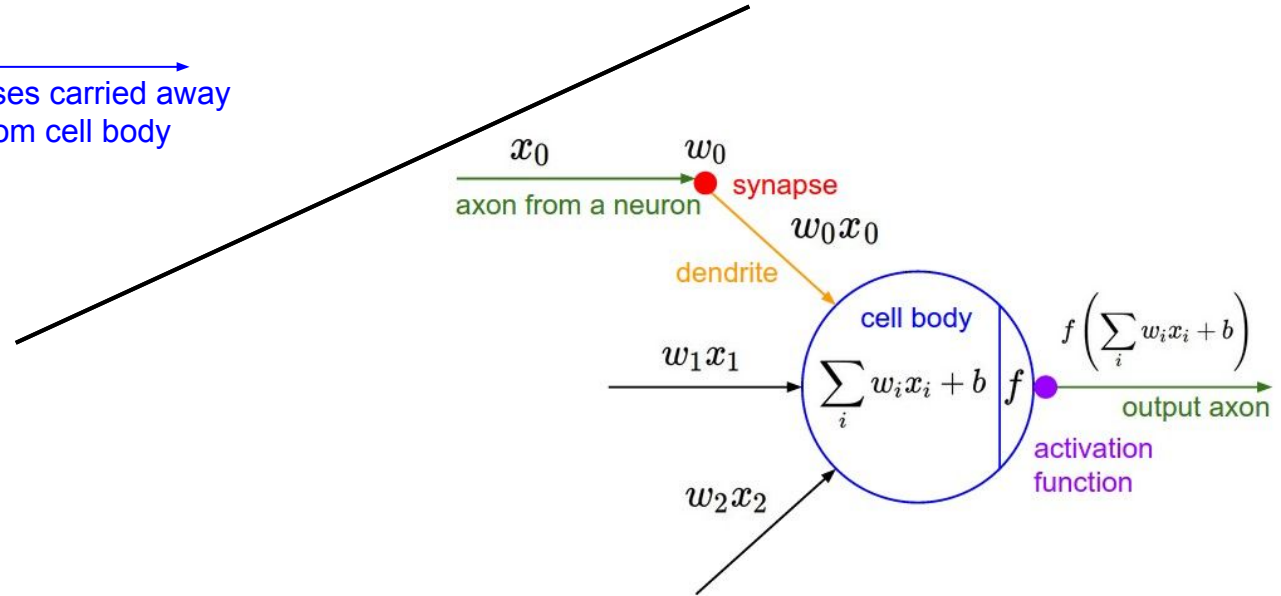


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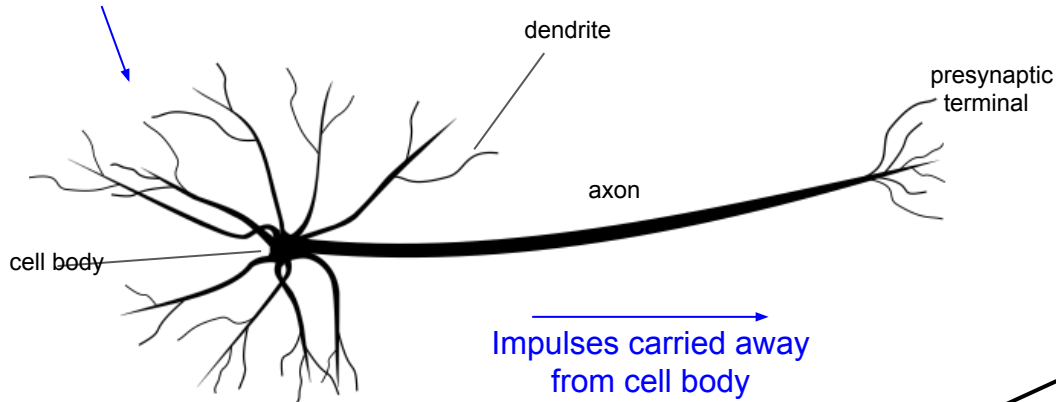
Impulses carried toward cell body



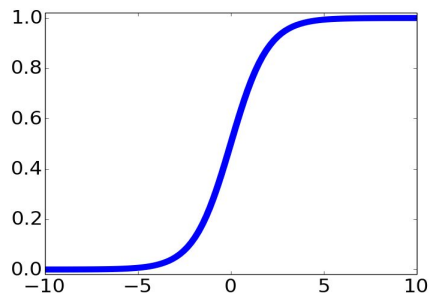
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Impulses carried toward cell body

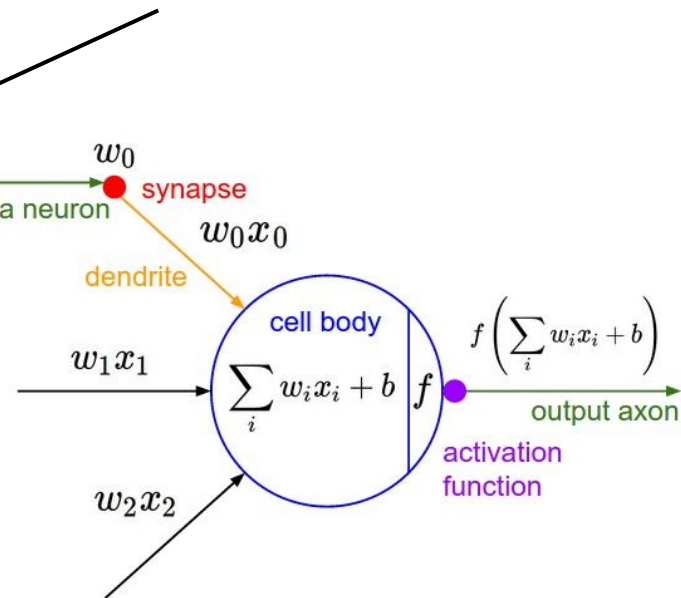


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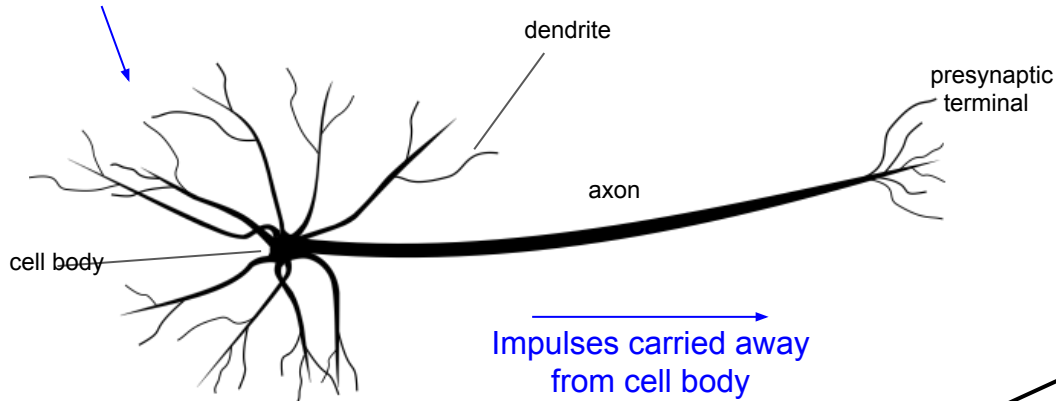


sigmoid activation function

$$\frac{1}{1 + e^{-x}}$$

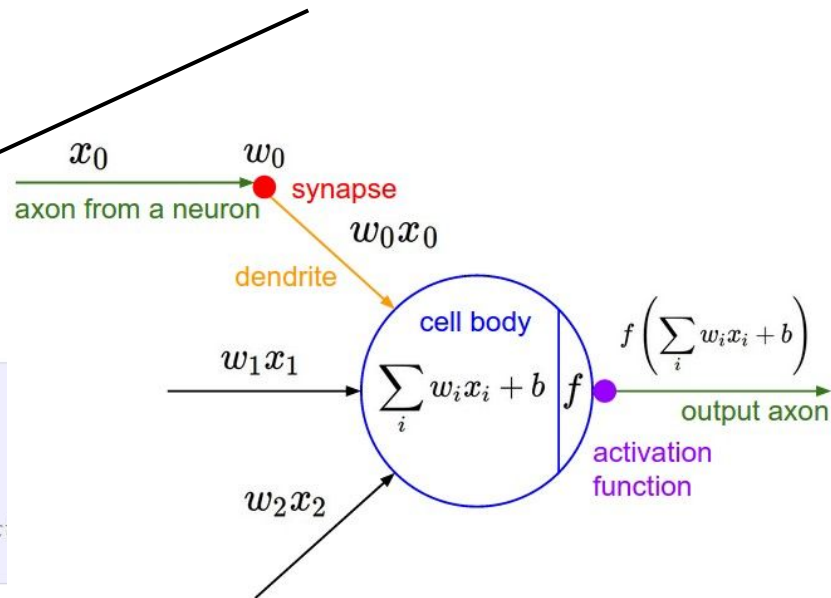


Impulses carried toward cell body



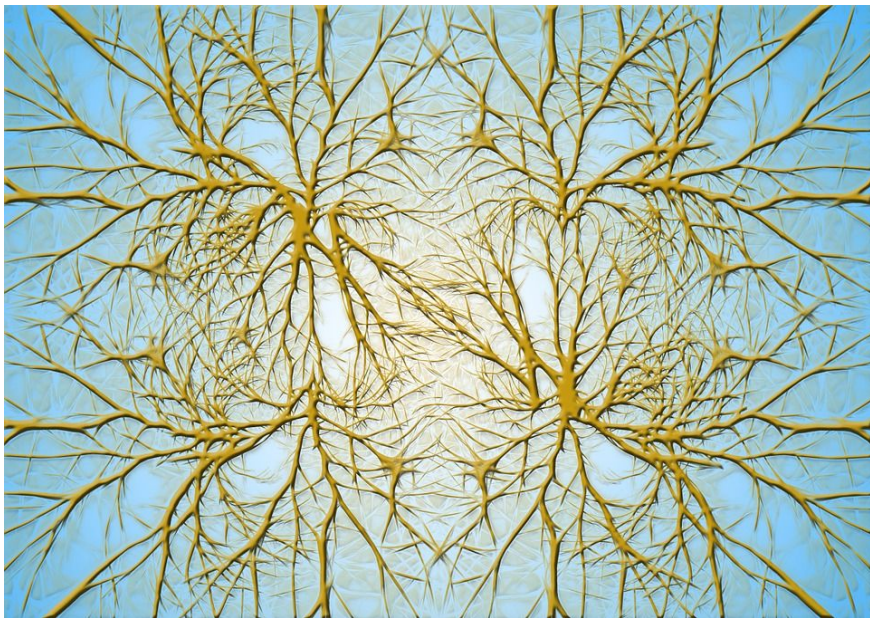
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```
class Neuron:
    # ...
    def neuron_tick(inputs):
        """ assume inputs and weights are 1-D numpy arrays and bias is a number """
        cell_body_sum = np.sum(inputs * self.weights) + self.bias
        firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation func
        return firing_rate
```



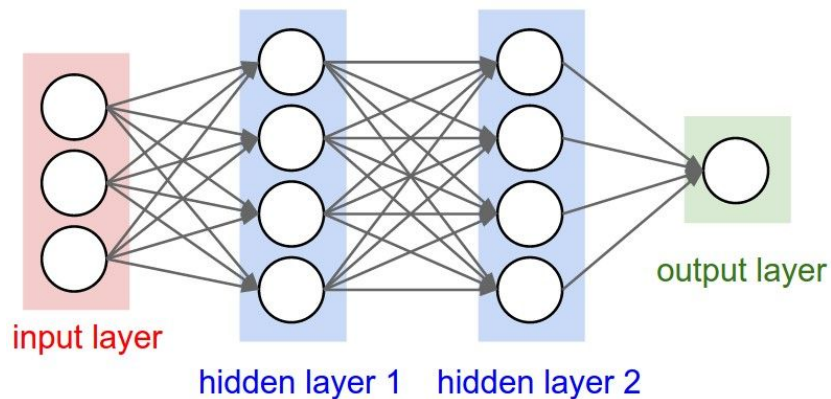


## Biological Neurons: Complex connectivity patterns

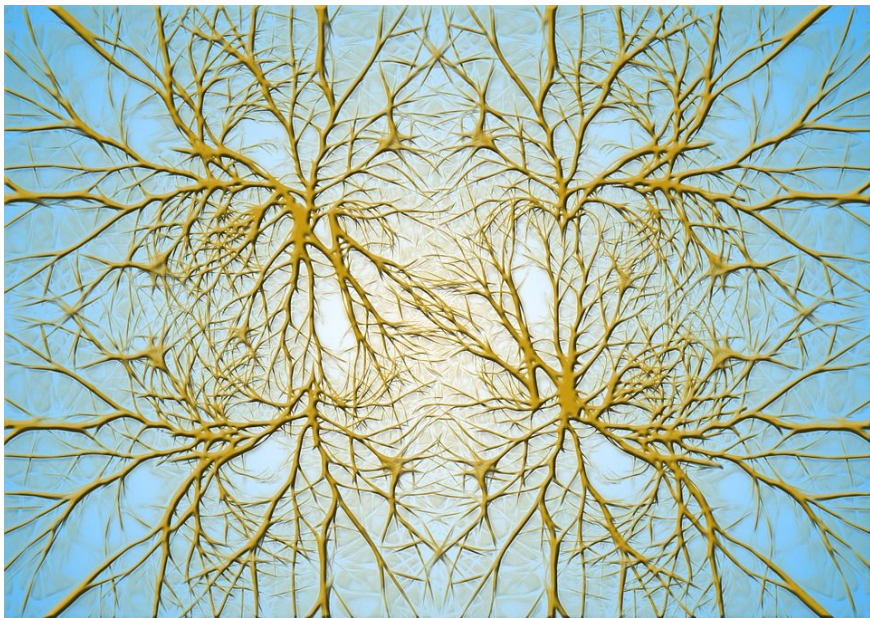


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## Neurons in a neural network: Organized into regular layers for computational efficiency

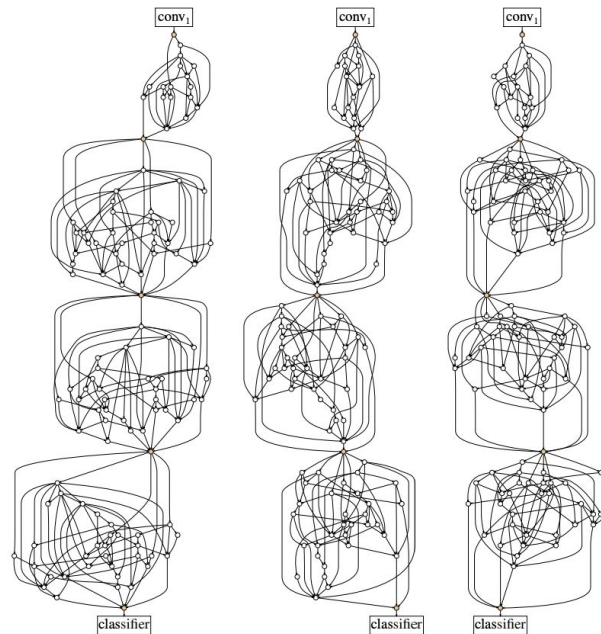


## Biological Neurons: Complex connectivity patterns



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But neural networks with random connections can work too!



Xie et al, "Exploring Randomly Wired Neural Networks for Image Recognition", arXiv 2019

# Be very careful with your brain analogies!

## **Biological Neurons:**

- Many different types
- Dendrites can perform complex non-linear computations
- Synapses are not a single weight but a complex non-linear dynamical system
- Rate code may not be adequate

[Dendritic Computation. London and Hausser]

# Problem: How to compute gradients?

$$s = f(x; W_1, W_2) = W_2 \max(0, W_1 x) \quad \text{Nonlinear score function}$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1) \quad \text{SVM Loss on predictions}$$

$$R(W) = \sum_k W_k^2 \quad \text{Regularization}$$

$$L = \frac{1}{N} \sum_{i=1}^N L_i + \lambda R(W_1) + \lambda R(W_2) \quad \text{Total loss: data loss + regularization}$$

If we can compute  $\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial W_2}$  then we can learn  $W_1$  and  $W_2$

# (Bad) Idea: Derive $\nabla_W L$ on paper

$$s = f(x; W) = Wx$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

$$= \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1)$$

$$L = \frac{1}{N} \sum_{i=1}^N L_i + \lambda \sum_k W_k^2$$

$$= \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2$$

$$\nabla_W L = \nabla_W \left( \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

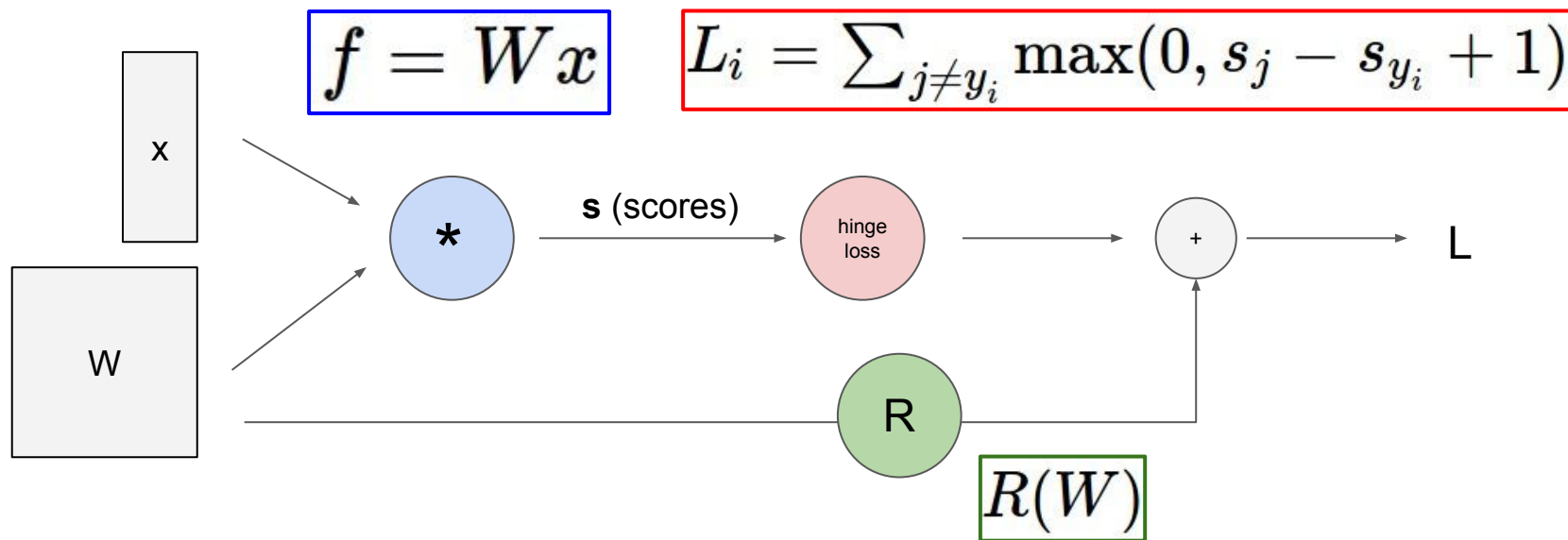
**Problem:** Very tedious: Lots of matrix calculus, need lots of paper

**Problem:** What if we want to change loss? E.g. use softmax instead of SVM? Need to re-derive from scratch =

**Problem:** Not feasible for very complex models!



# Better Idea: Computational graphs + Backpropagation



# Convolutional network (AlexNet)

input image

weights

loss

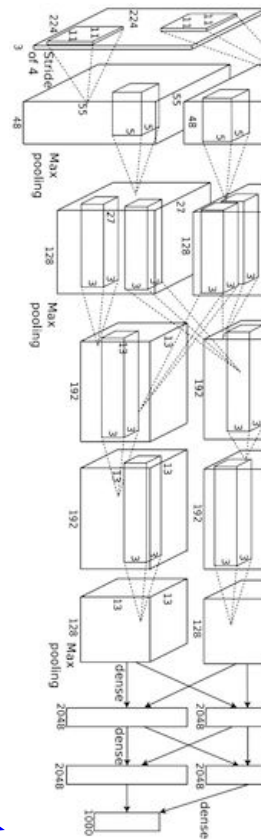


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

# Neural Turing Machine

input image

loss

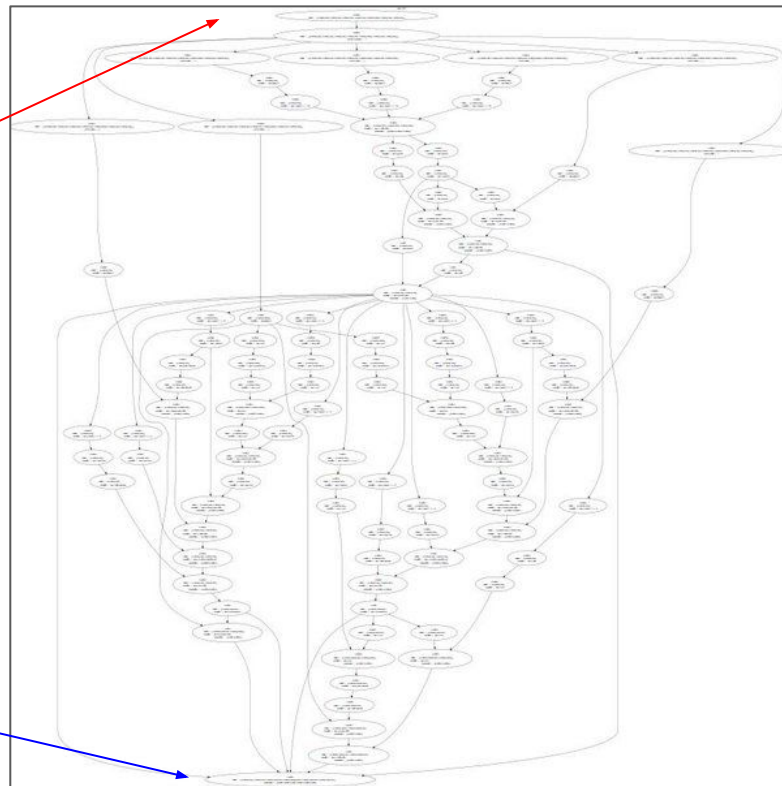


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.



# Neural Turing Machine

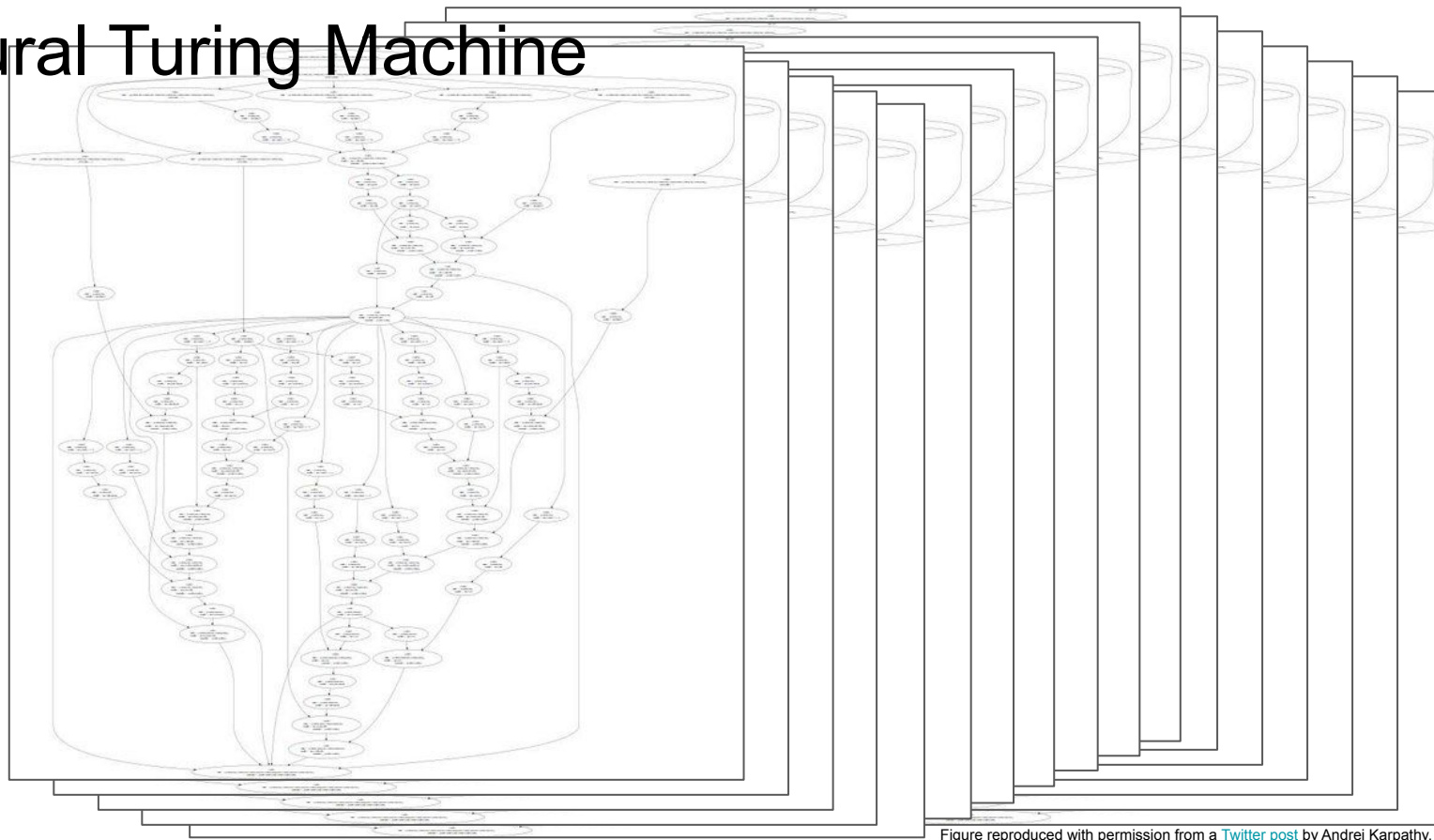


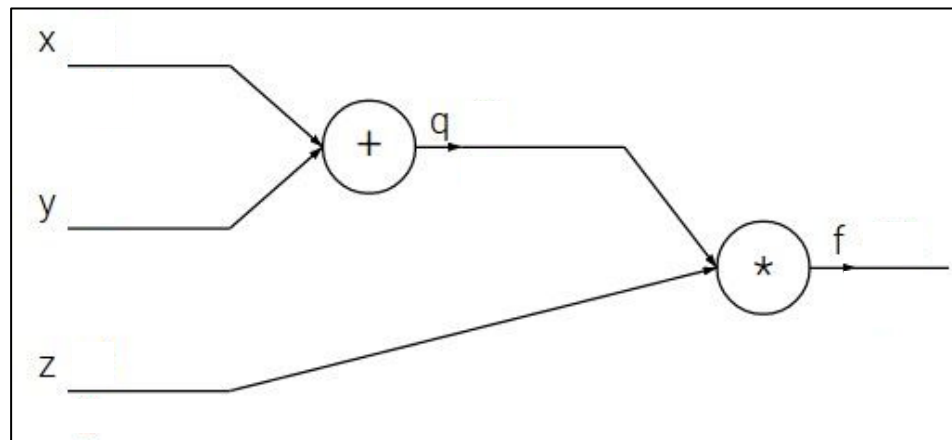
Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

## Backpropagation: a simple example

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

## Backpropagation: a simple example

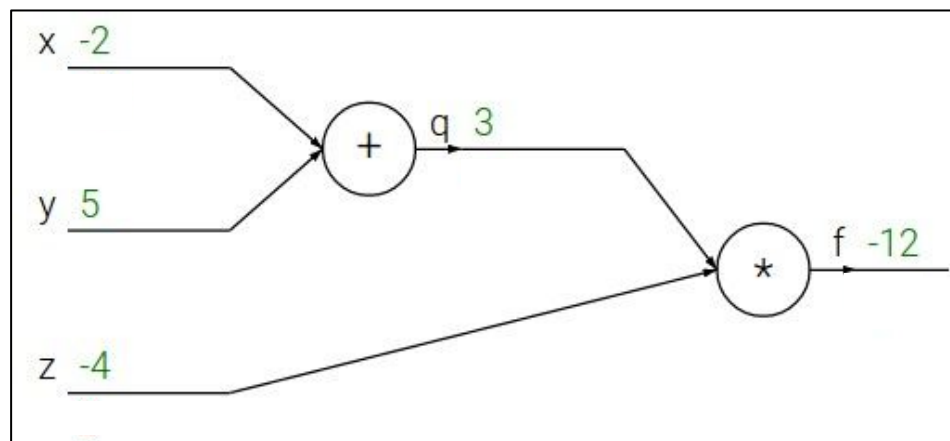
$$f(x, y, z) = (x + y)z$$



## Backpropagation: a simple example

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

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



## Backpropagation: a simple example

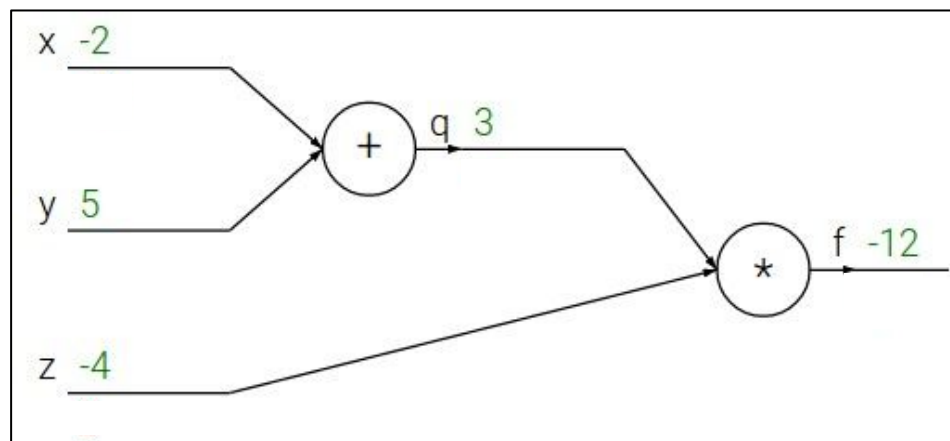
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



## Backpropagation: a simple example

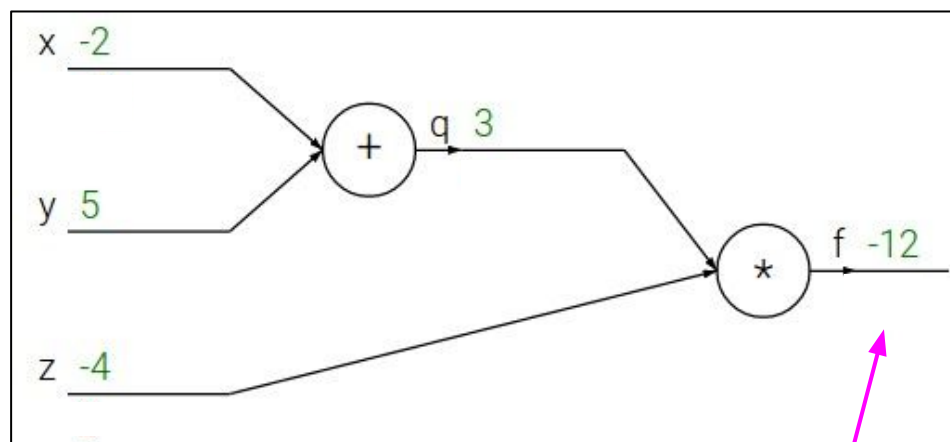
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$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

## Backpropagation: a simple example

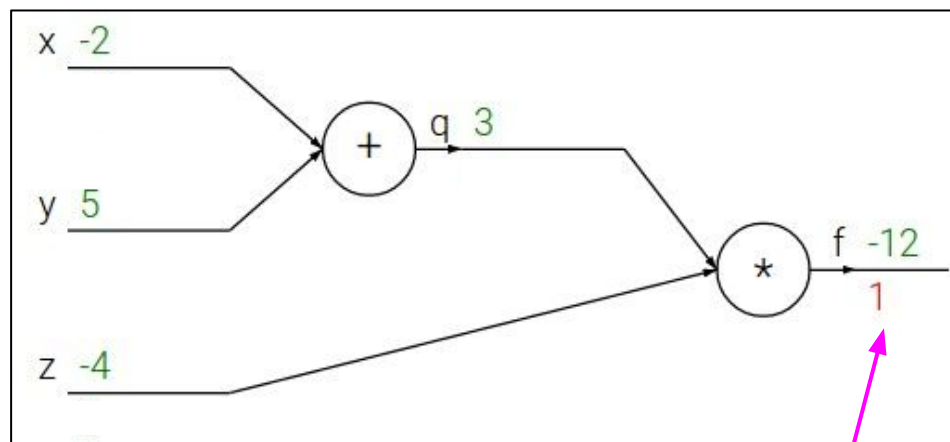
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

## Backpropagation: a simple example

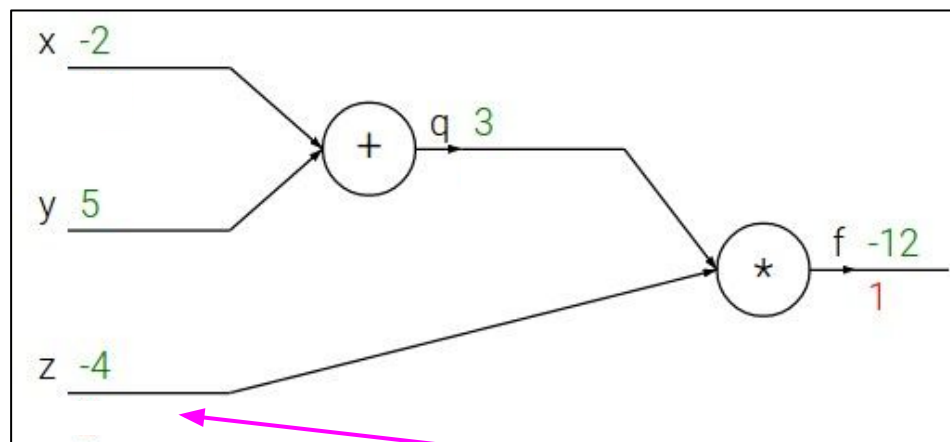
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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



## Backpropagation: a simple example

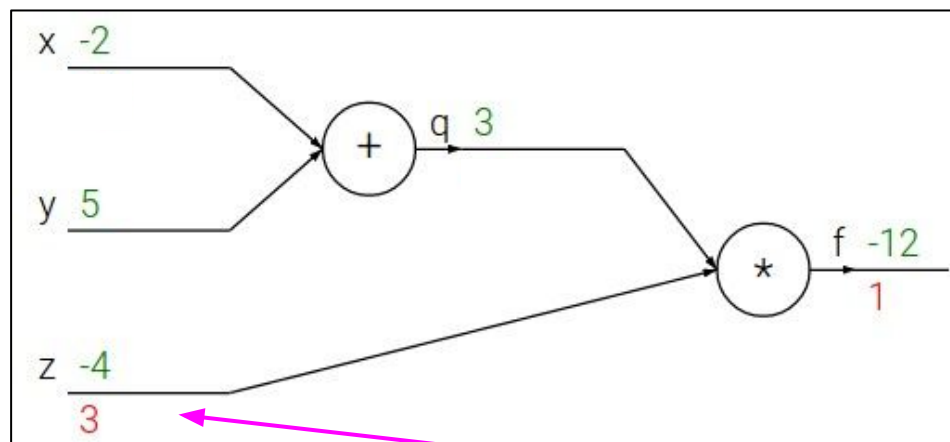
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

## Backpropagation: a simple example

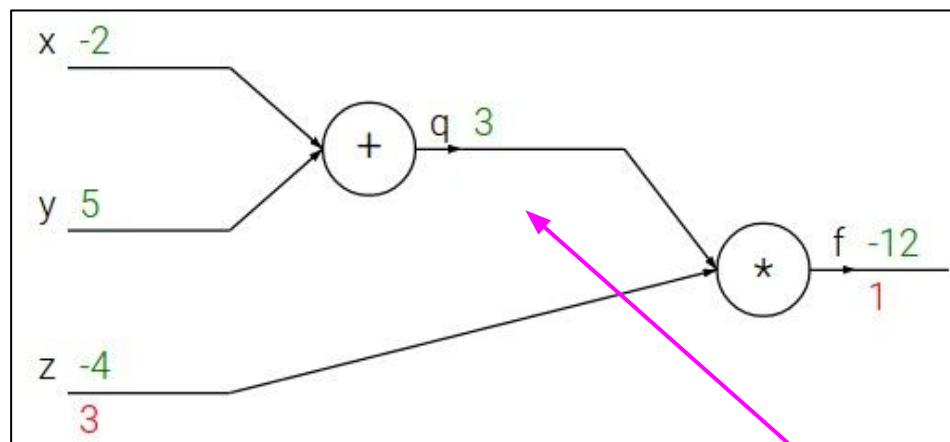
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

## Backpropagation: a simple example

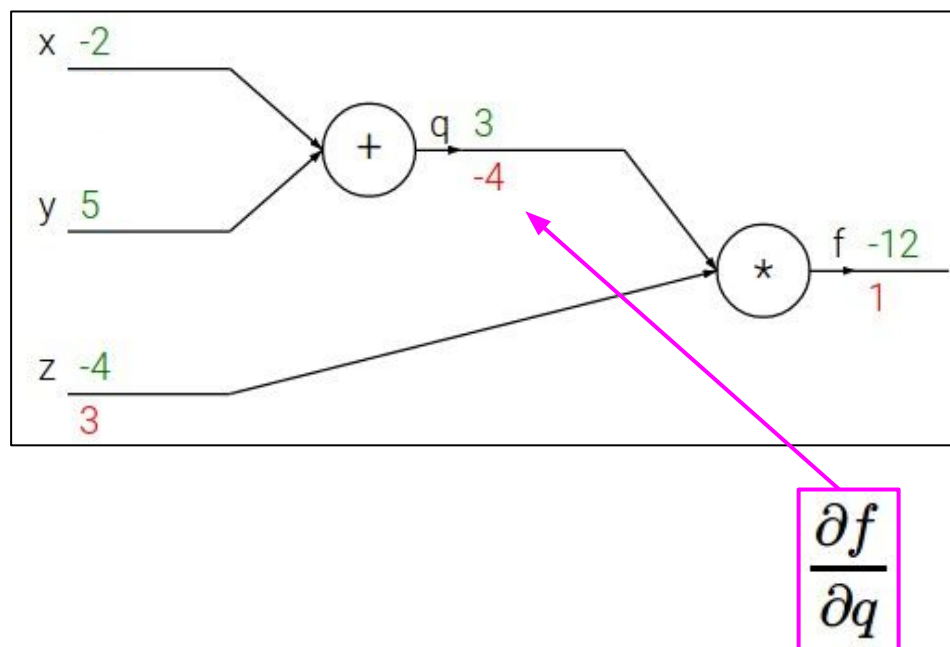
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



## Backpropagation: a simple example

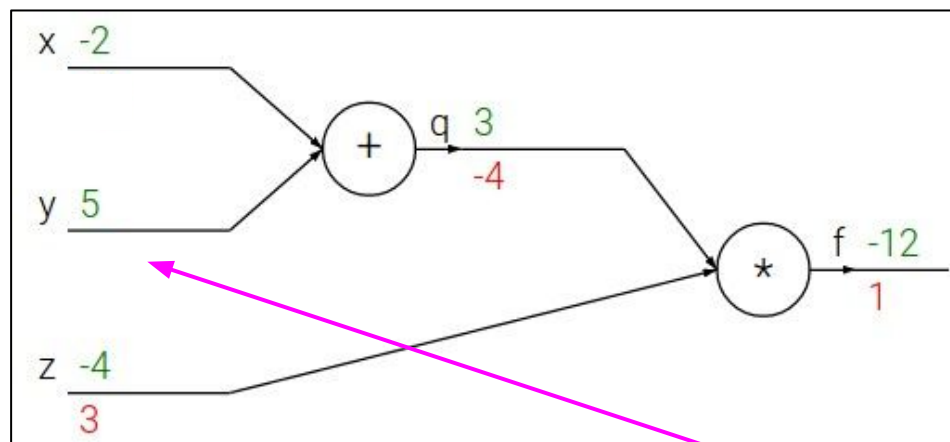
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

Chain rule:

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

Upstream  
gradient

Local  
gradient

## Backpropagation: a simple example

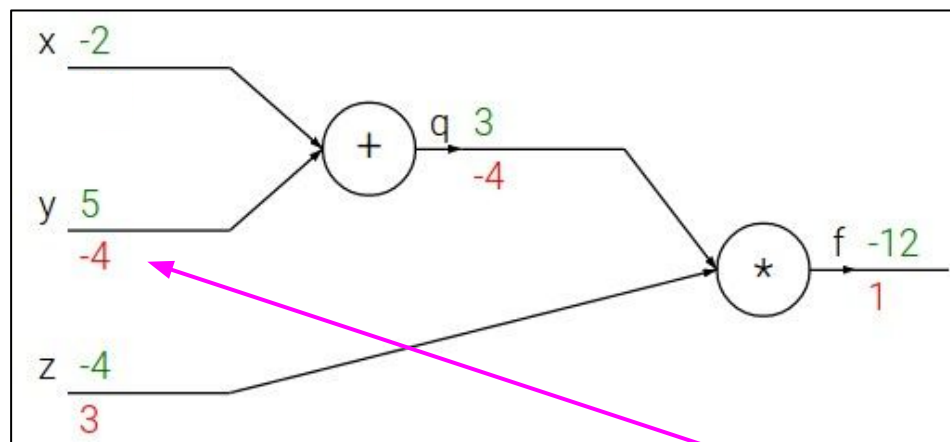
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

Chain rule:

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

Upstream  
gradient

Local  
gradient

## Backpropagation: a simple example

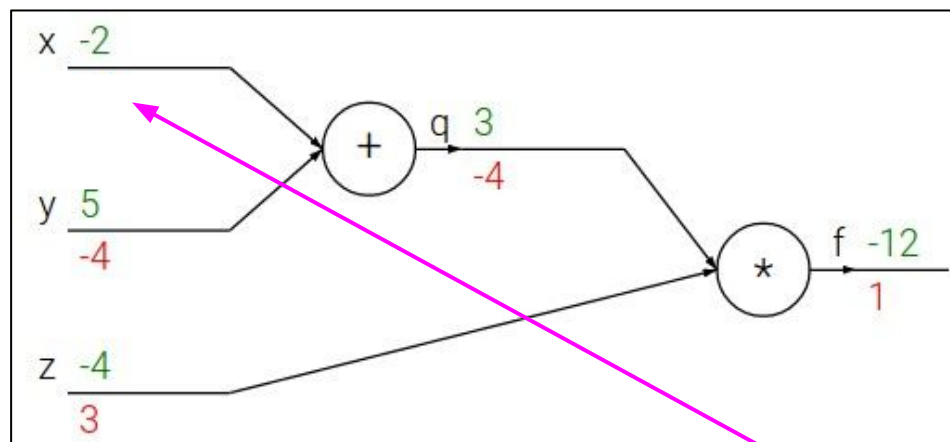
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

Chain rule:

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

Upstream  
gradient

Local  
gradient

# Backpropagation: a simple example

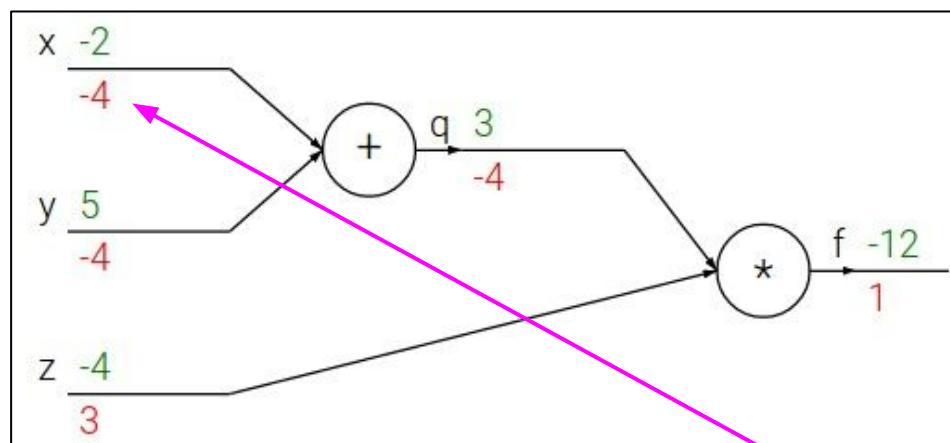
$$f(x, y, z) = (x + y)z$$

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

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

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



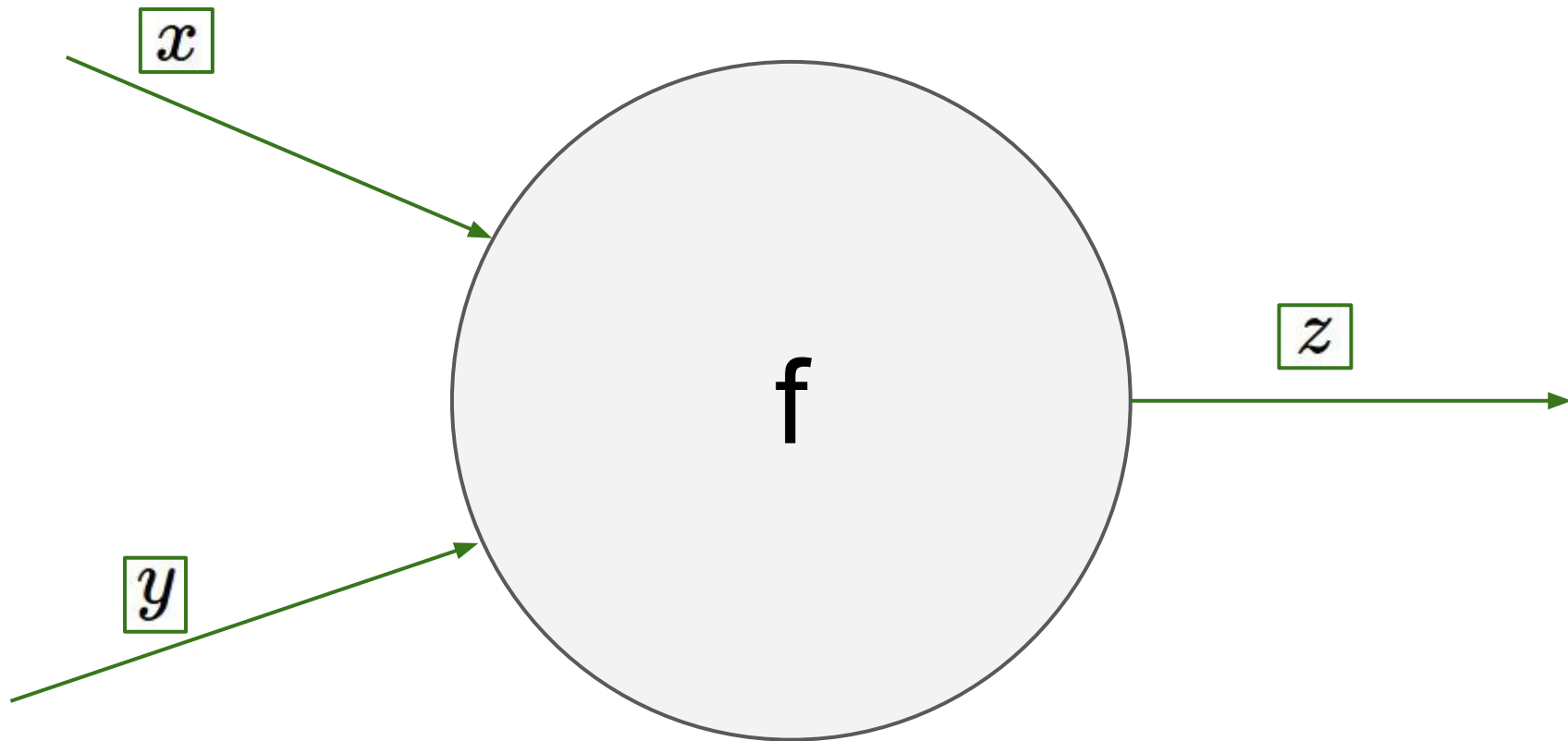
$$\frac{\partial f}{\partial x}$$

Chain rule:

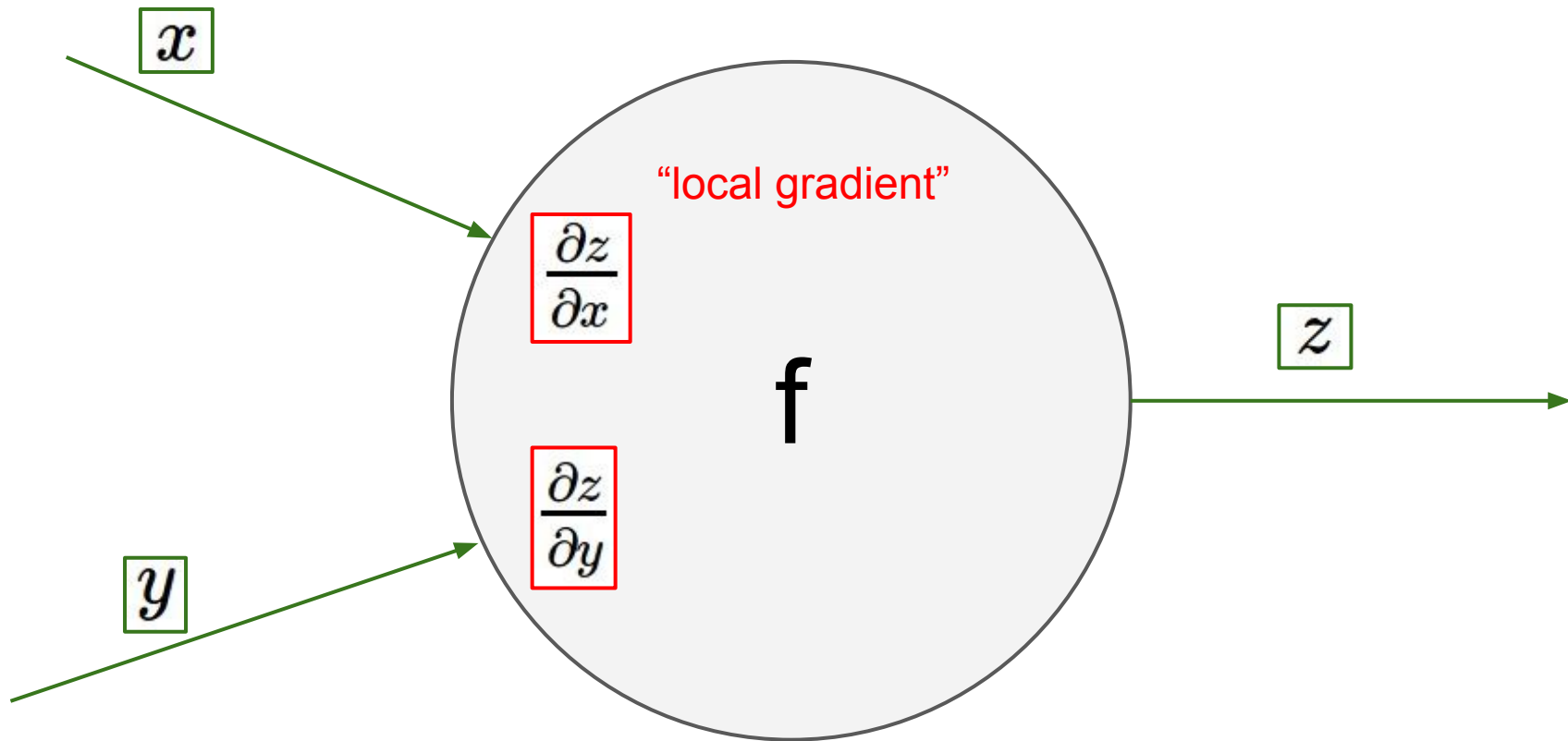
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

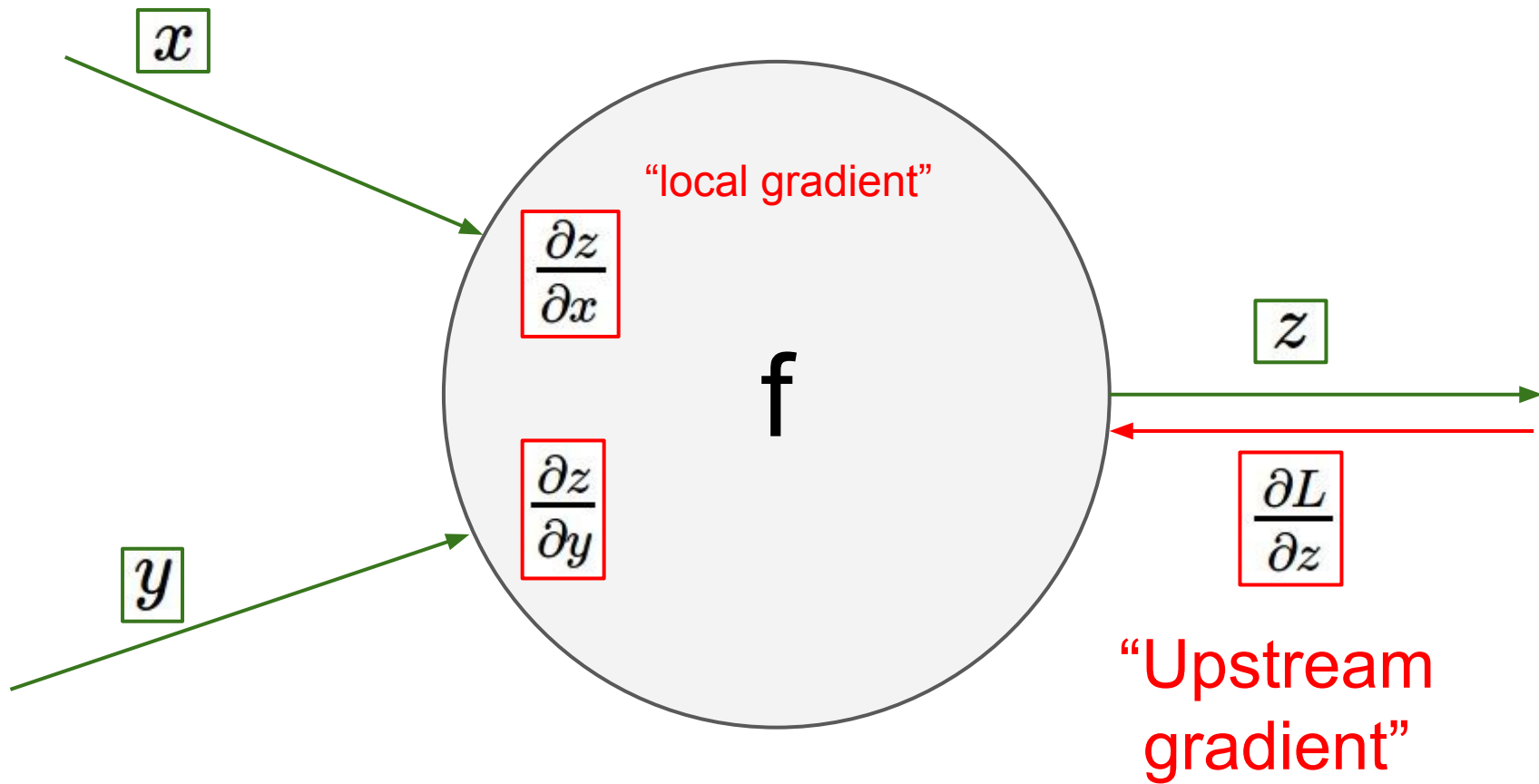
Upstream  
gradient

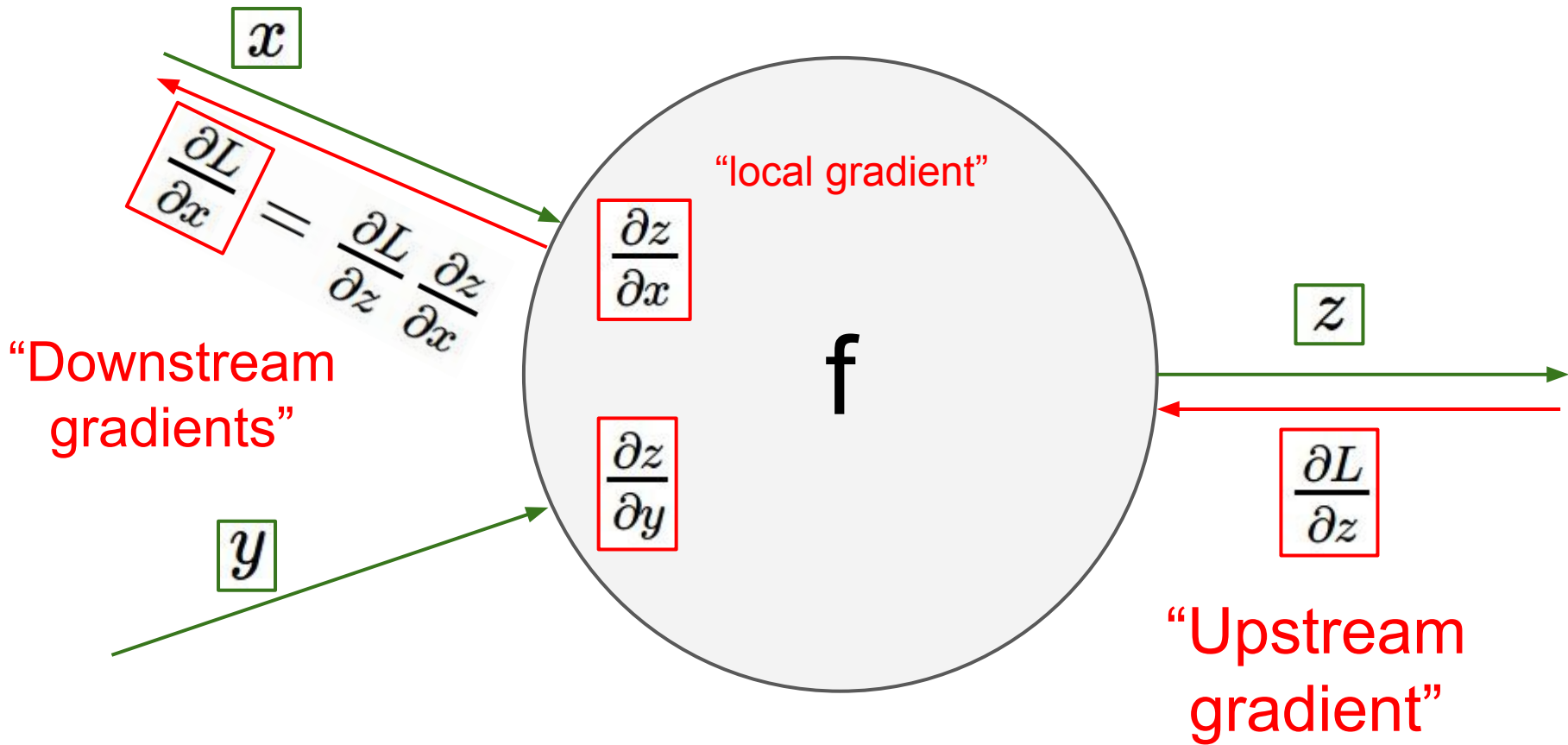
Local  
gradient

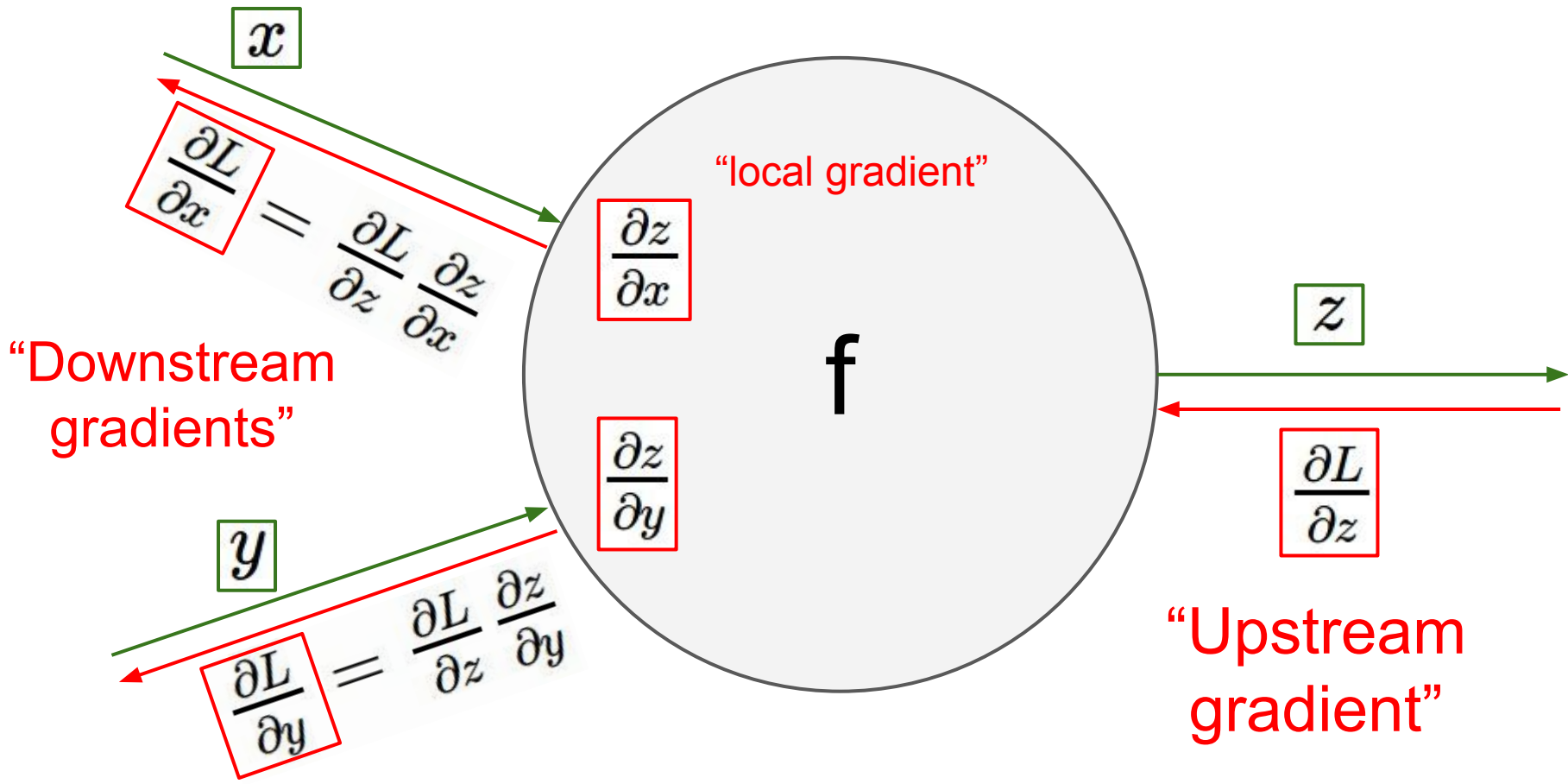


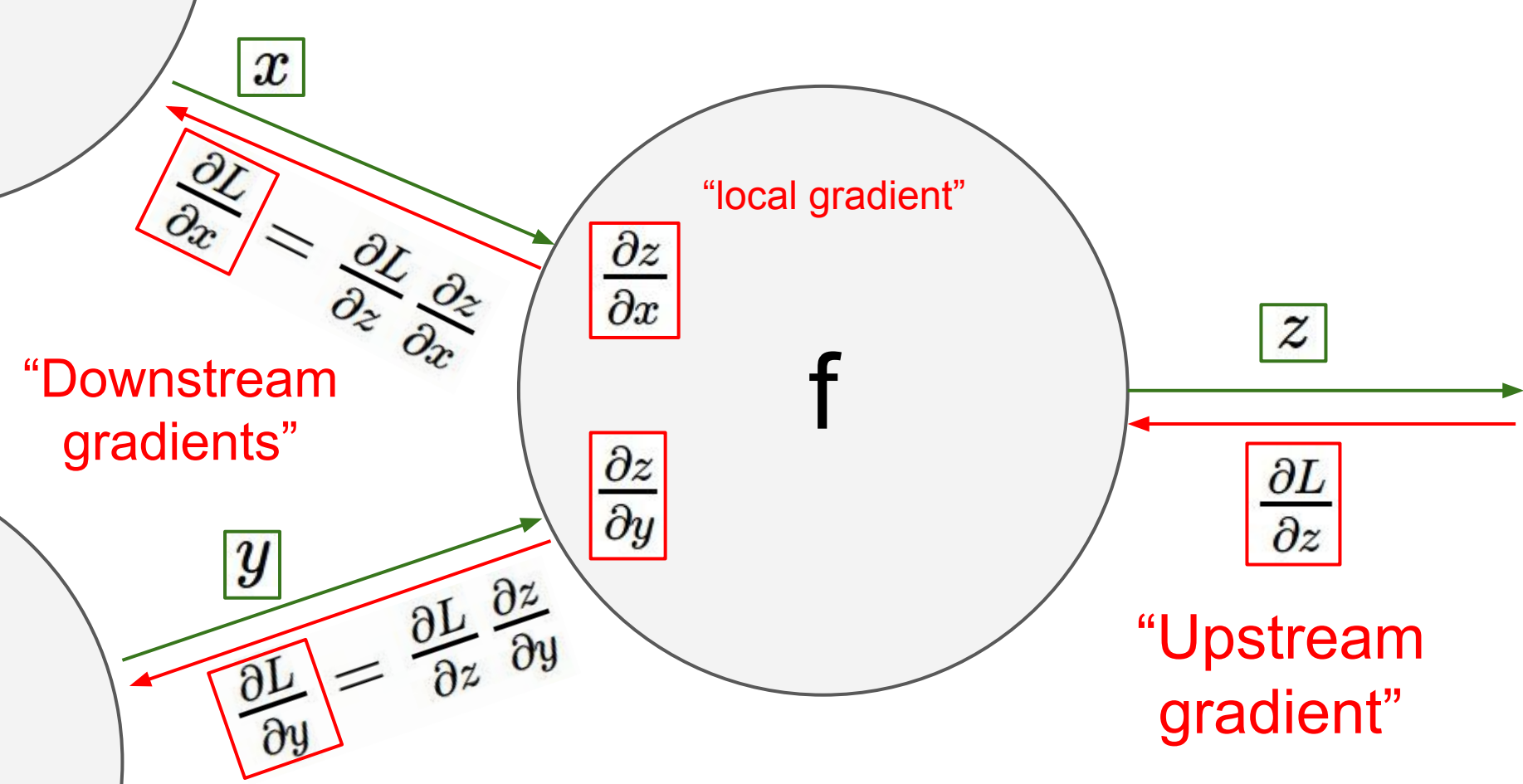




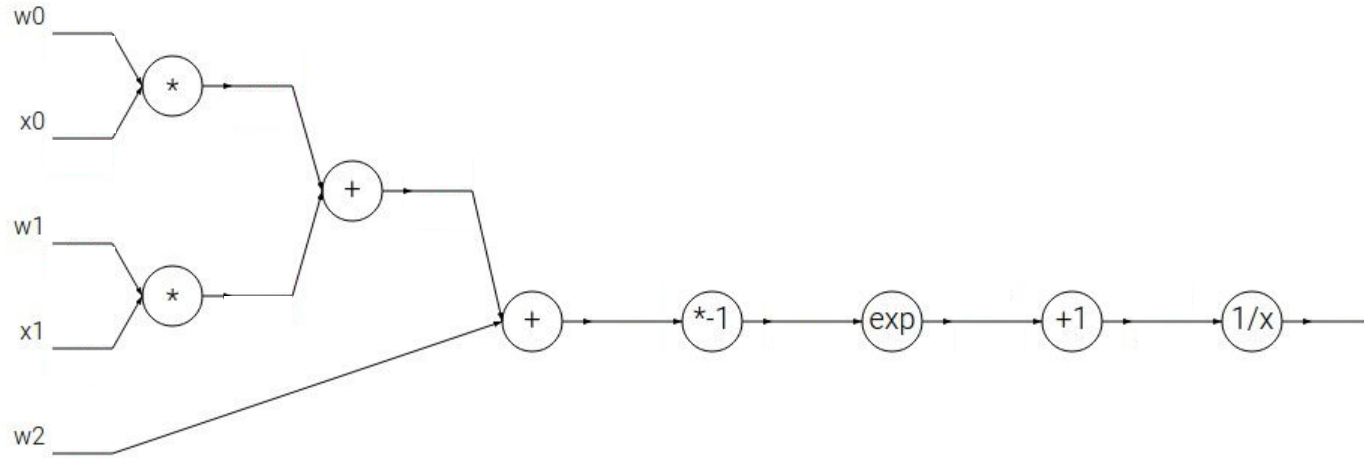






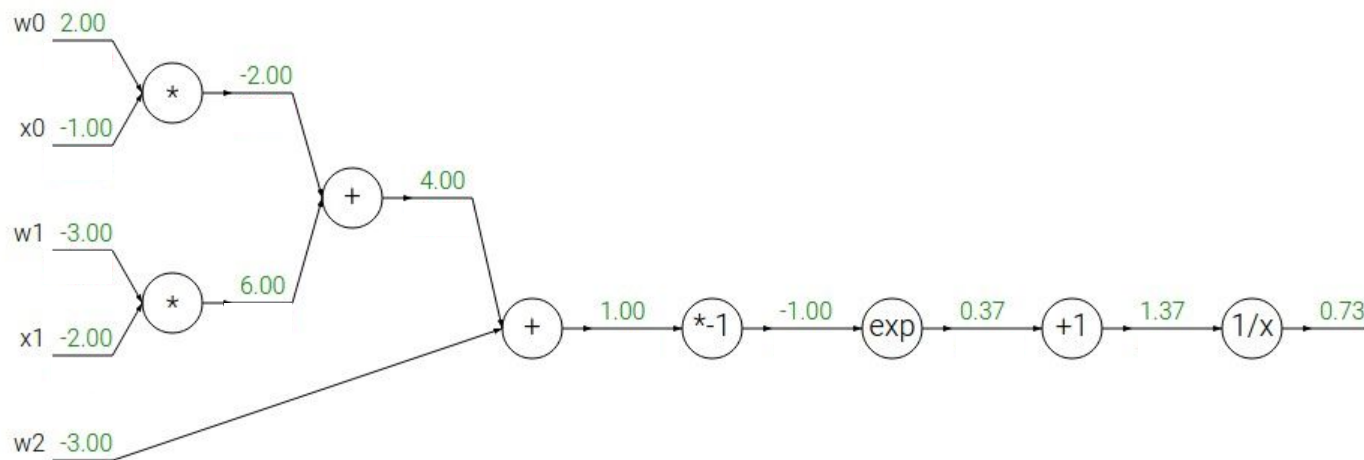


Another example: 
$$f(w, x) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$



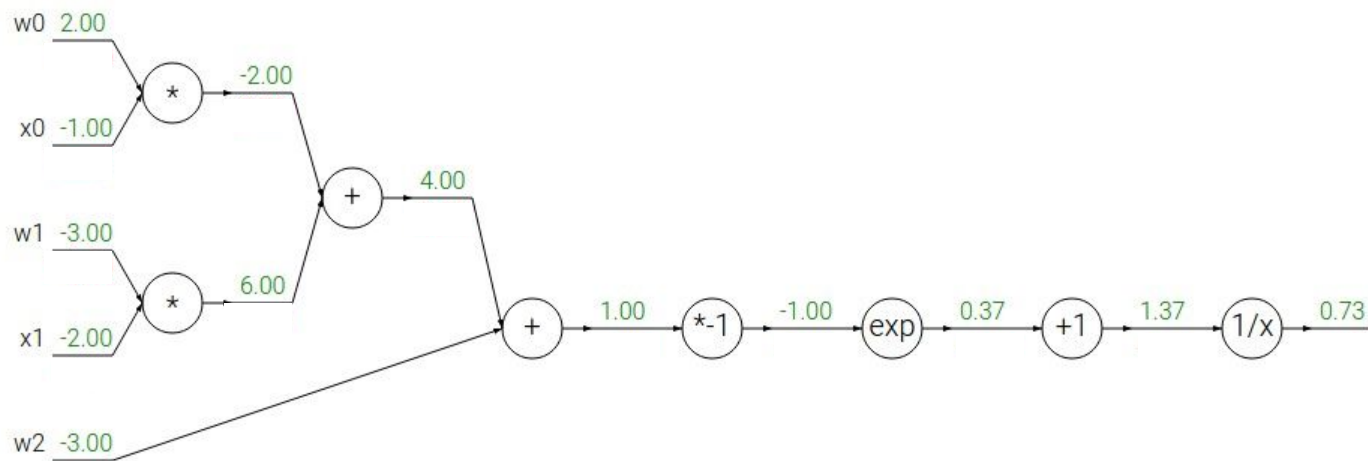
Another example:

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



Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x$$

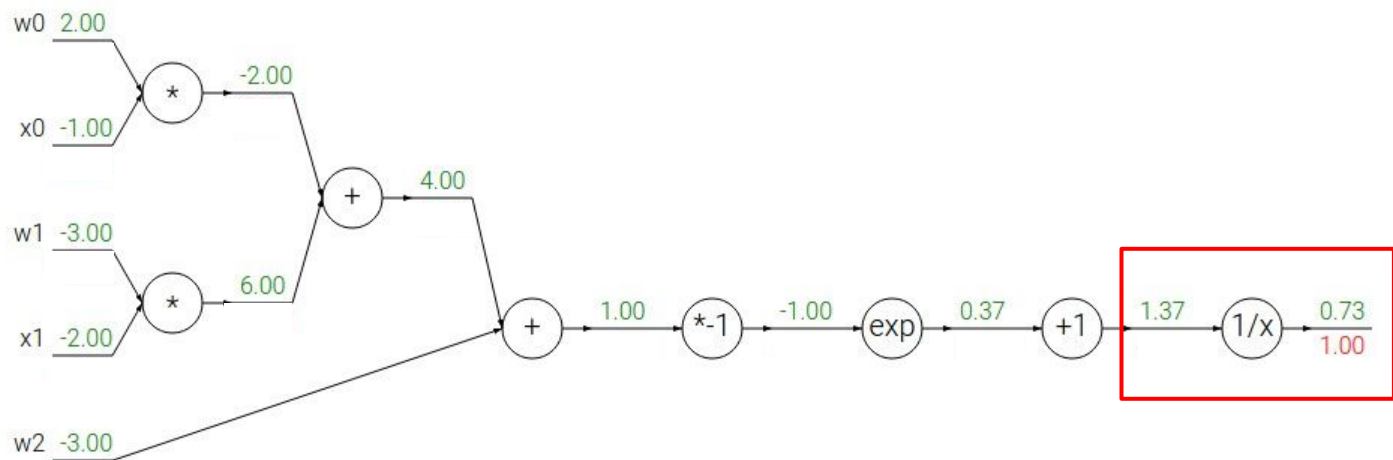
→

$$\frac{df}{dx} = 1$$



Another example:

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



$$f(x) = e^x$$

$\rightarrow$

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

$\rightarrow$

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

$\rightarrow$

$$\frac{df}{dx} = -1/x^2$$

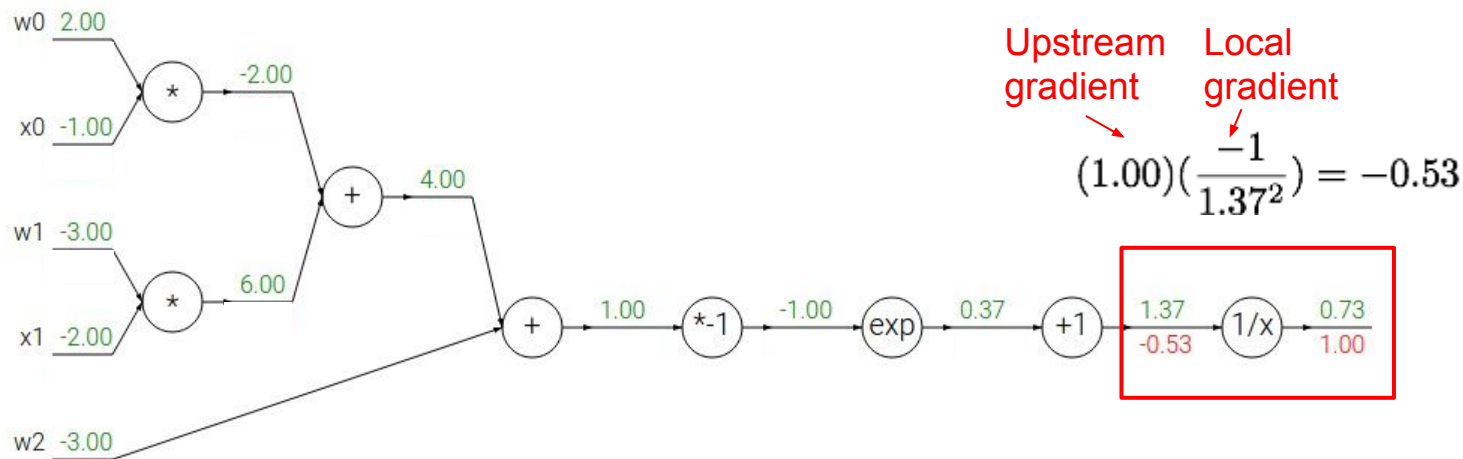
$$f_c(x) = c + x$$

$\rightarrow$

$$\frac{df}{dx} = 1$$

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

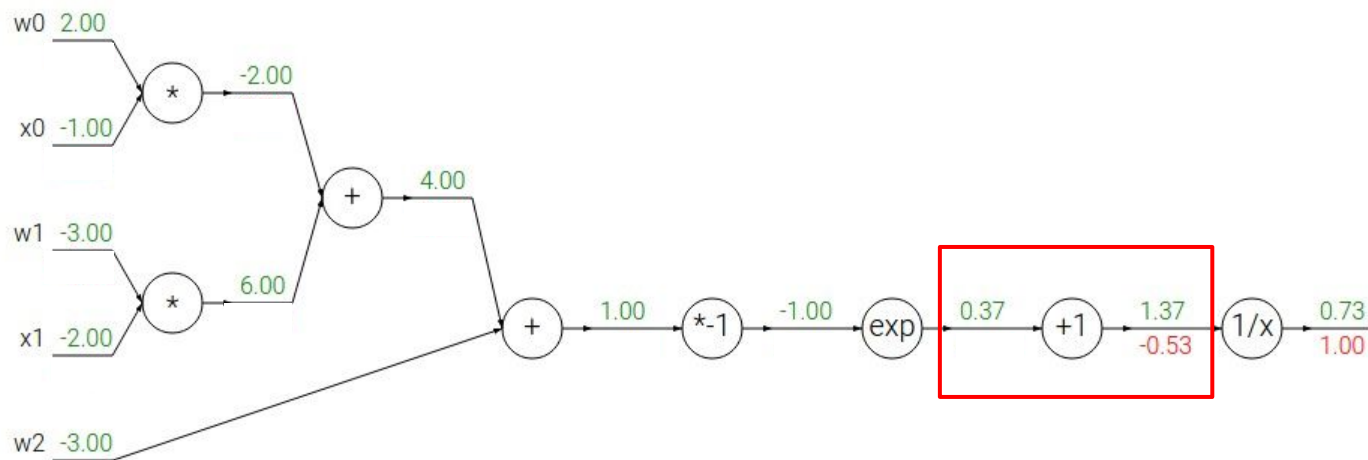
$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

Another example:

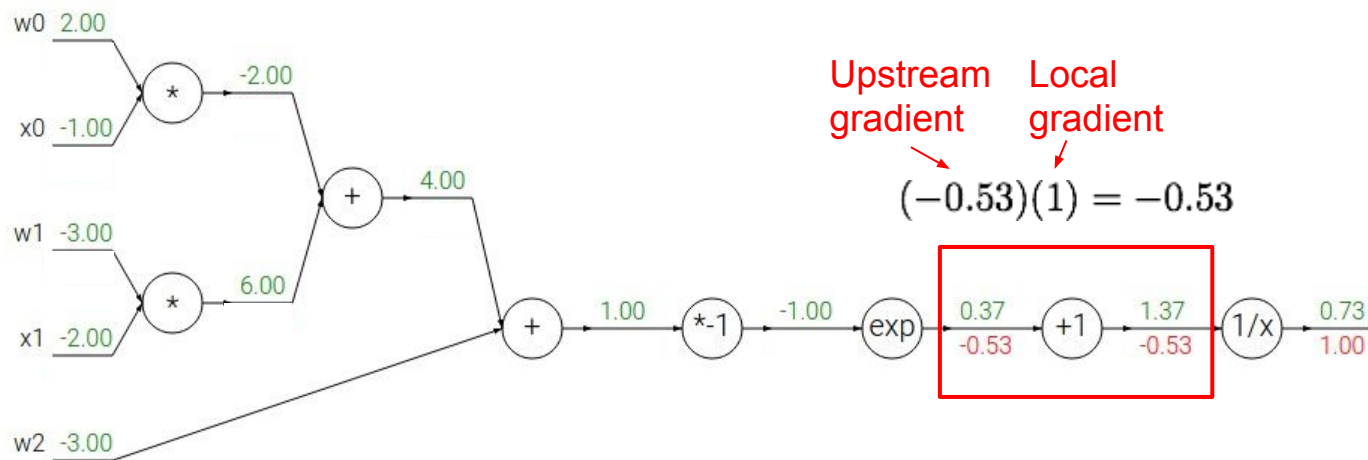
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

Another example:

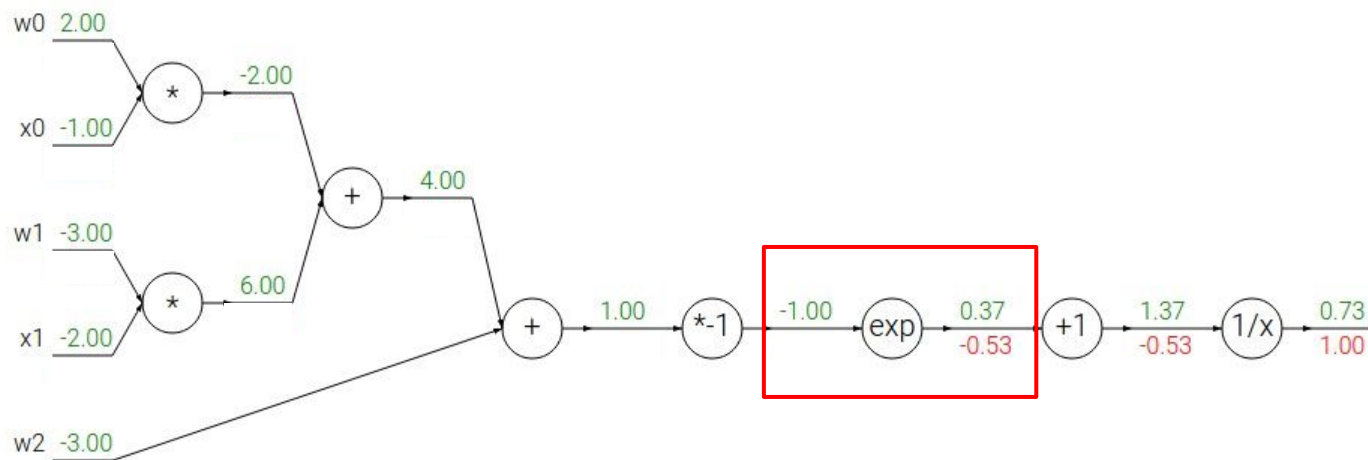
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



$f(x) = e^x$	$\rightarrow$	$\frac{df}{dx} = e^x$		$f(x) = \frac{1}{x}$	$\rightarrow$	$\frac{df}{dx} = -1/x^2$
$f_a(x) = ax$	$\rightarrow$	$\frac{df}{dx} = a$		<div style="border: 1px solid red; padding: 5px;"><math>f_c(x) = c + x</math></div>	$\rightarrow$	<div style="border: 1px solid red; padding: 5px;"><math>\frac{df}{dx} = 1</math></div>

Another example:

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



$$f(x) = e^x$$

$\rightarrow$

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

$\rightarrow$

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

$\rightarrow$

$$\frac{df}{dx} = -1/x^2$$

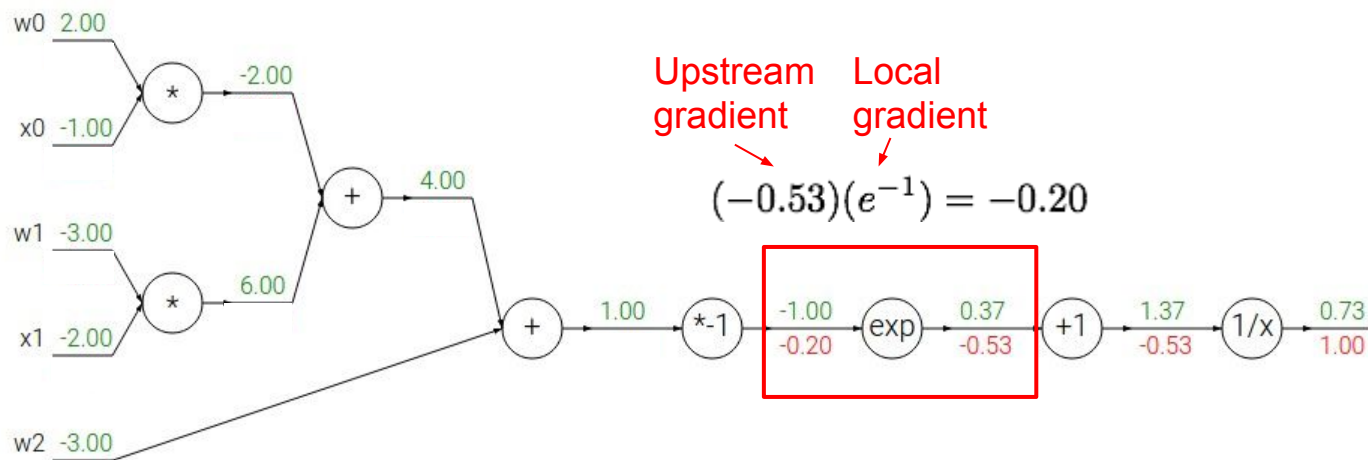
$$f_c(x) = c + x$$

$\rightarrow$

$$\frac{df}{dx} = 1$$

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

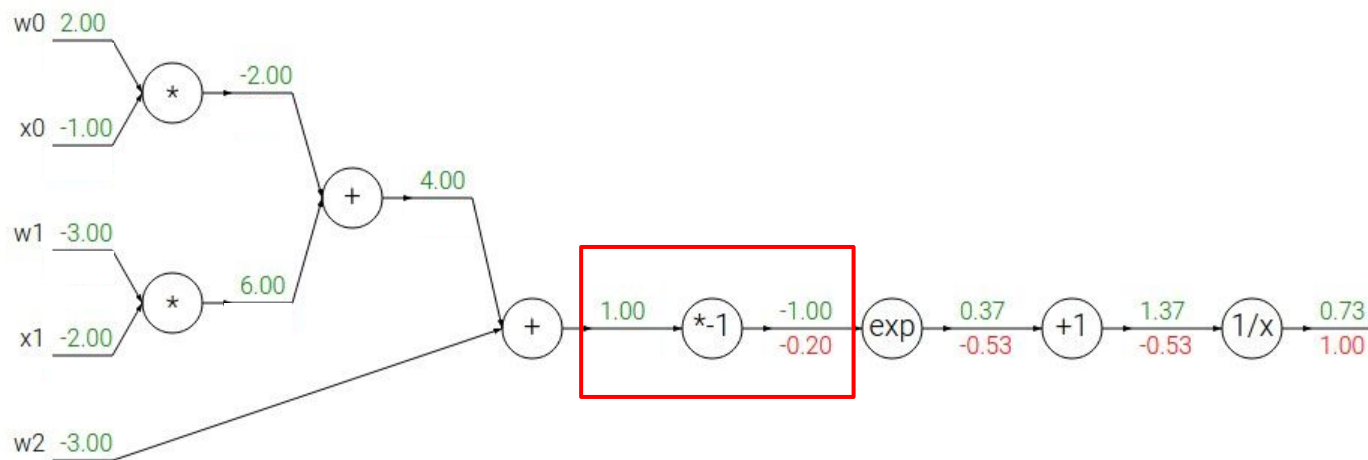
$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

Another example:

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



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

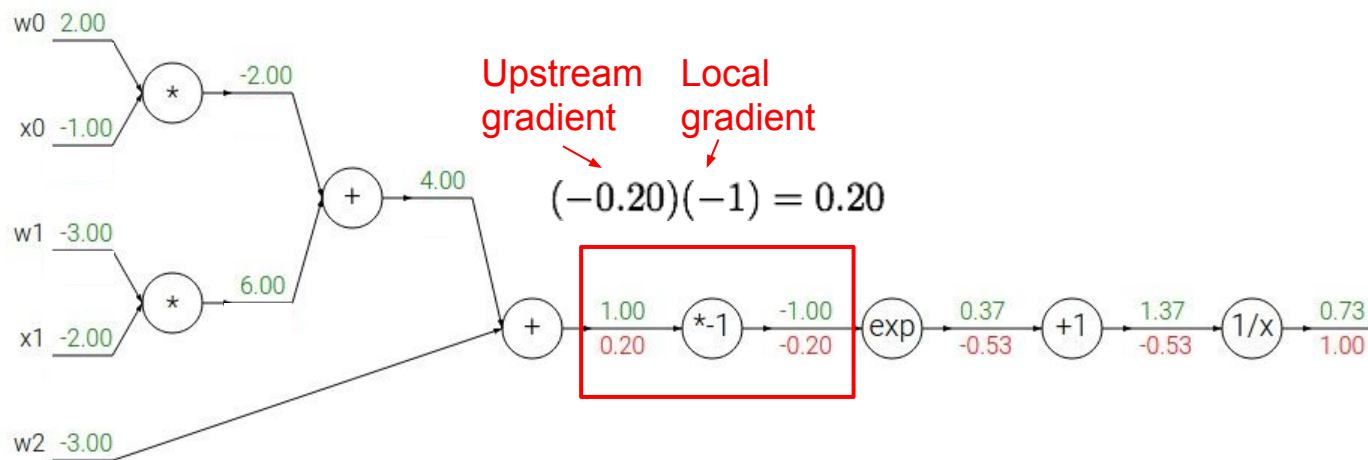
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



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

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

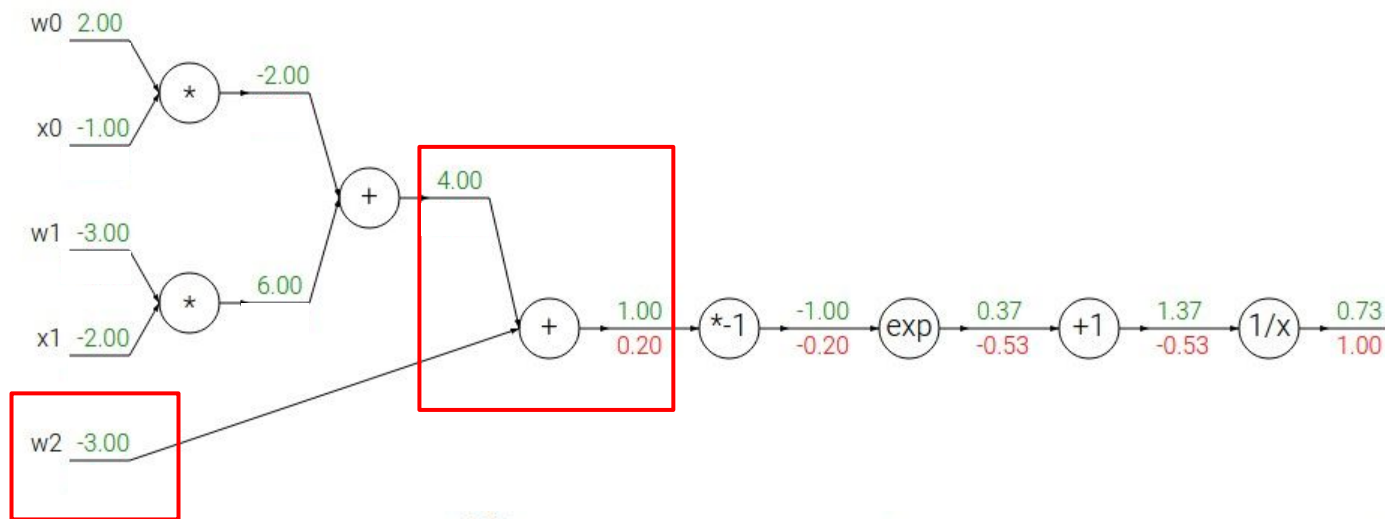
$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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



Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

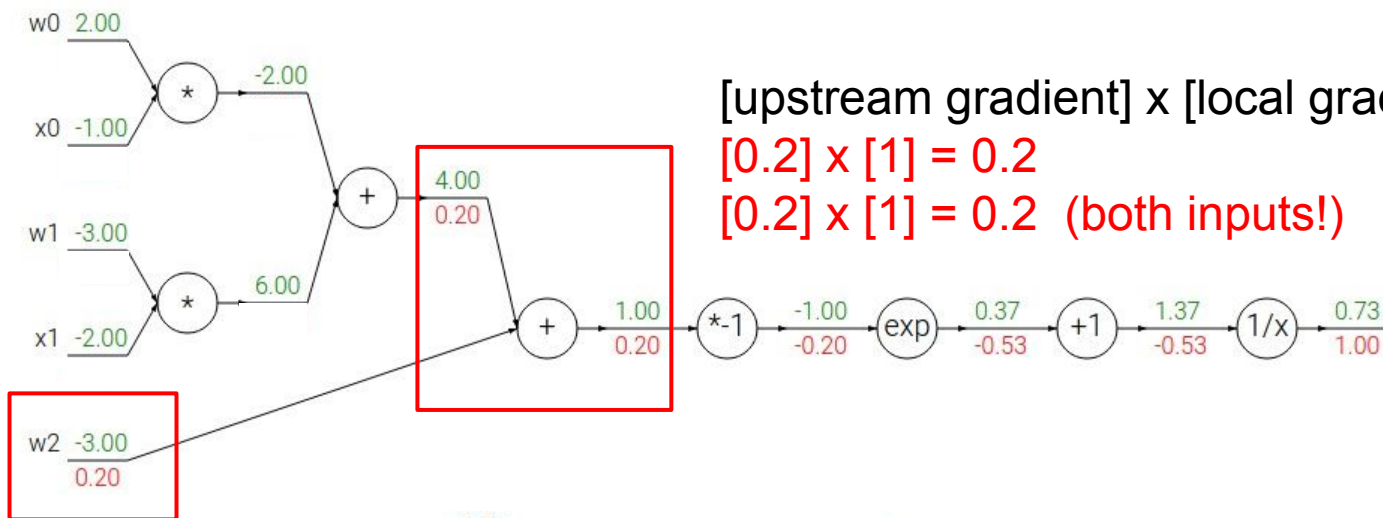
$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

Another example:

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



[upstream gradient] x [local gradient]

$$[0.2] \times [1] = 0.2$$

$$[0.2] \times [1] = 0.2 \text{ (both inputs!)}$$

$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

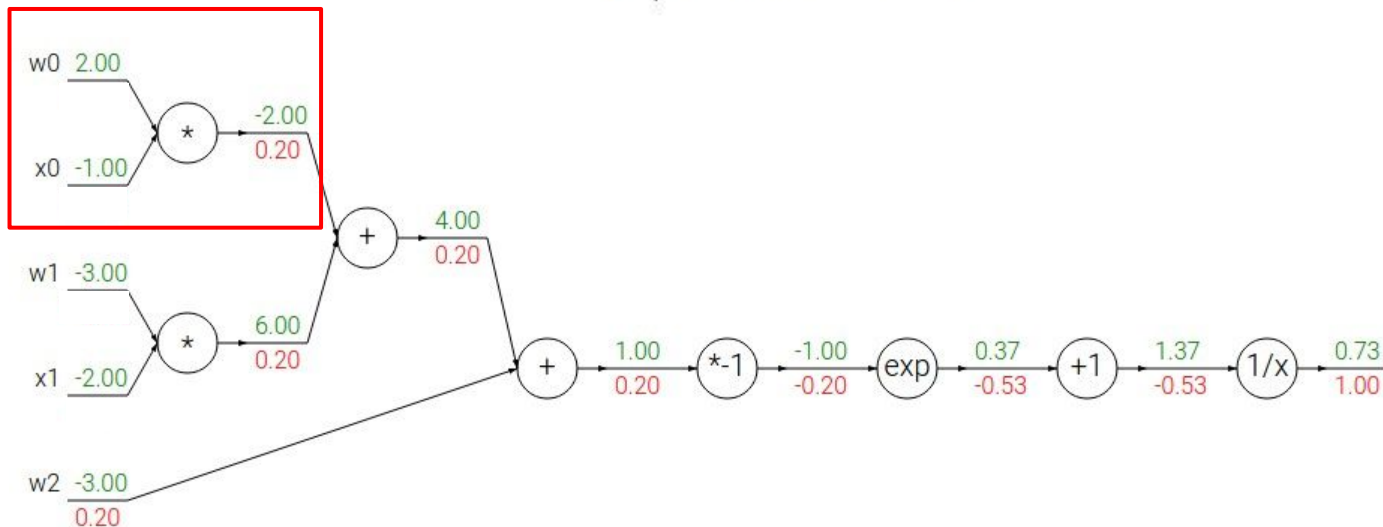
$$f_c(x) = c + x$$

→

$$\frac{df}{dx} = 1$$

Another example:

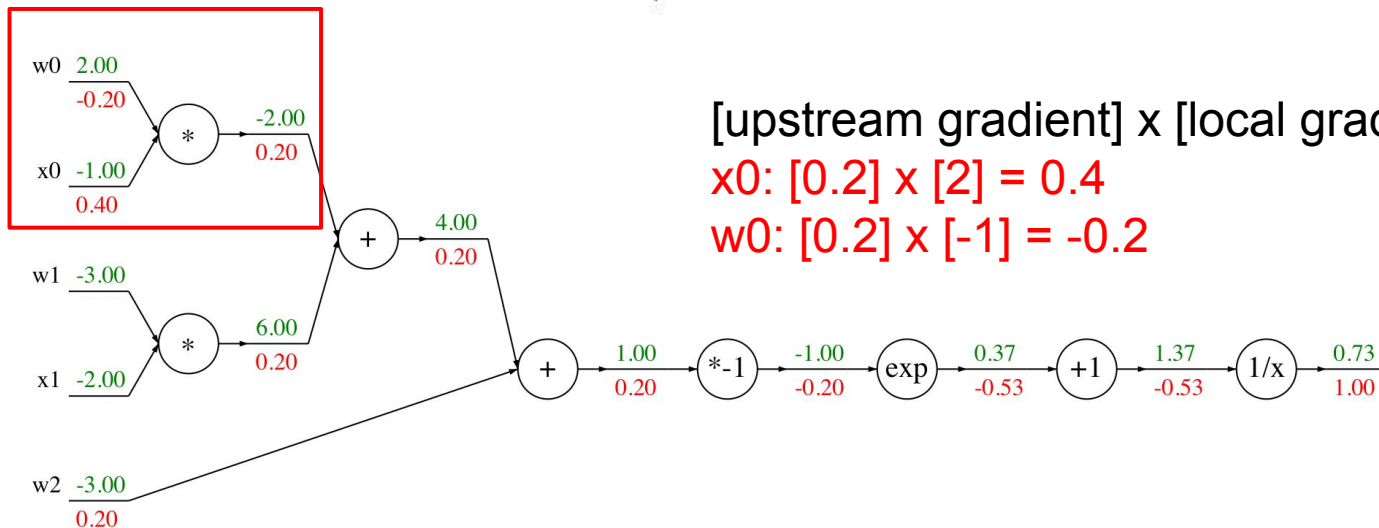
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

Another example:

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



[upstream gradient] x [local gradient]

$$x_0: [0.2] \times [2] = 0.4$$

$$w_0: [0.2] \times [-1] = -0.2$$

$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

$$\frac{df}{dx} = a$$

$$f(x) = \frac{1}{x}$$

→

$$\frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x$$

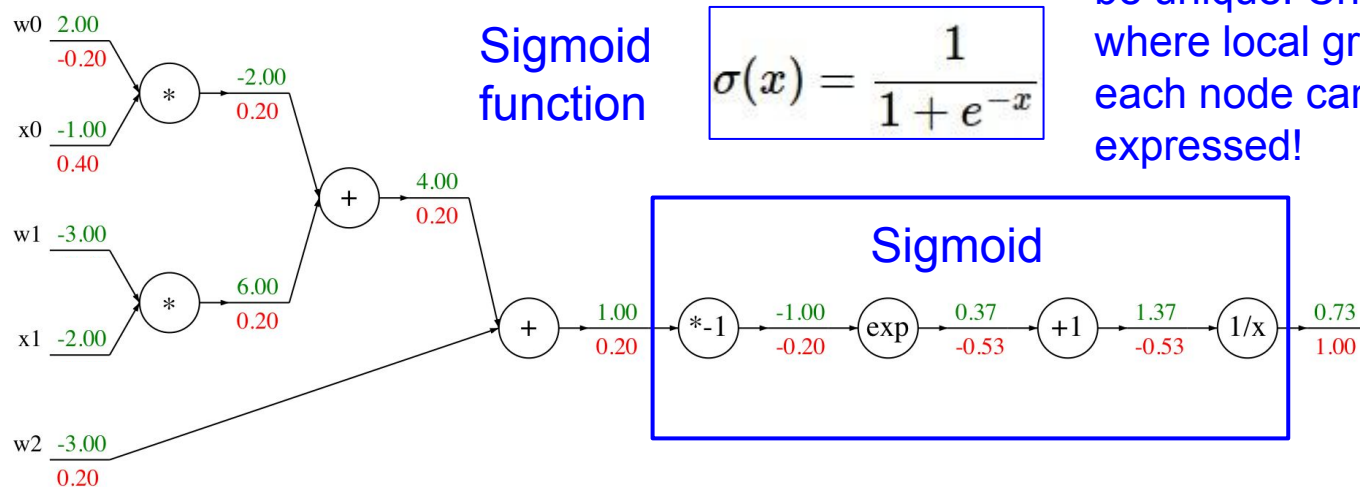
→

$$\frac{df}{dx} = 1$$

Another example:

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

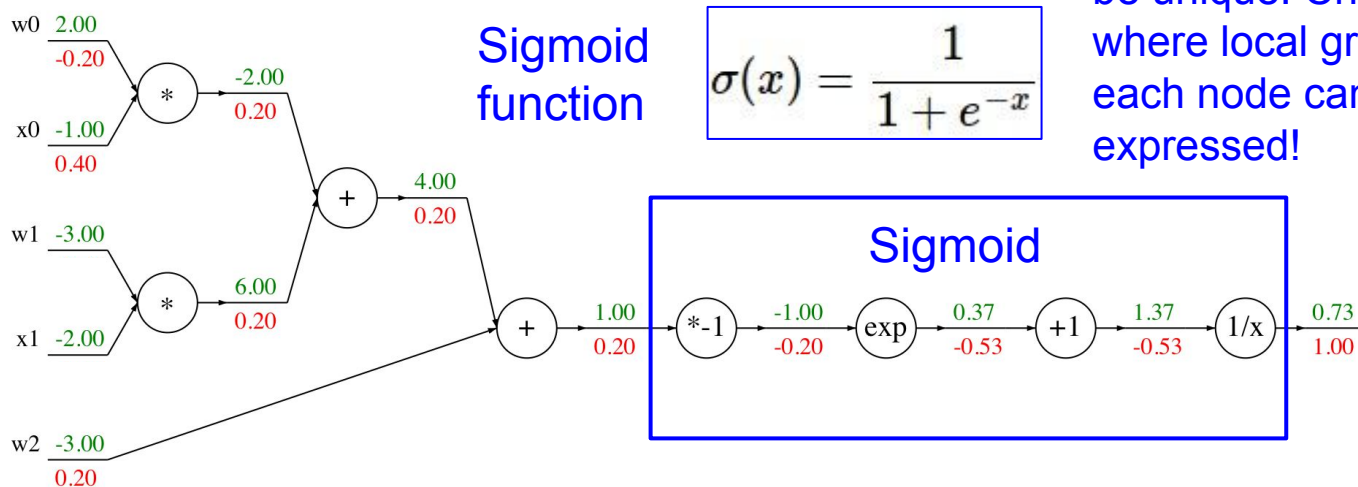
Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!



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!



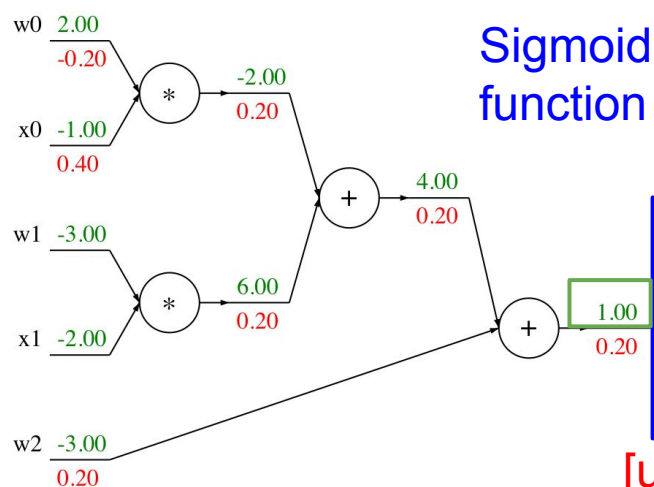
Sigmoid local gradient:

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

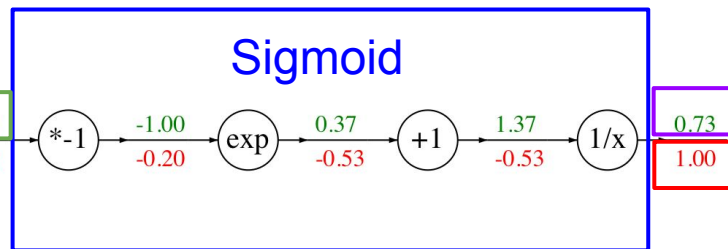
Another example:

$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2x_2)}}$$

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



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



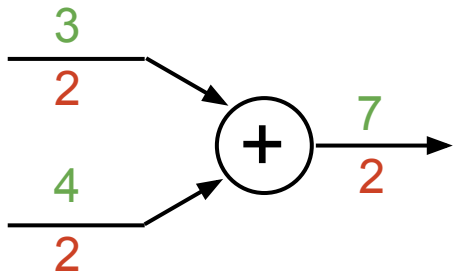
[upstream gradient] x [local gradient]  
 $[1.00] \times [(1 - 0.73) (0.73)] = 0.2$

Sigmoid local gradient:

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

# Patterns in gradient flow

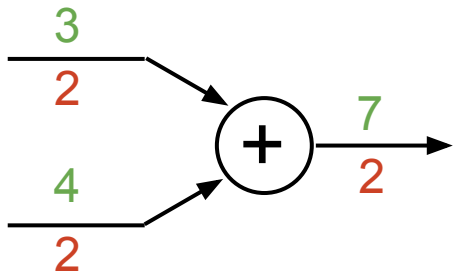
**add** gate: gradient distributor



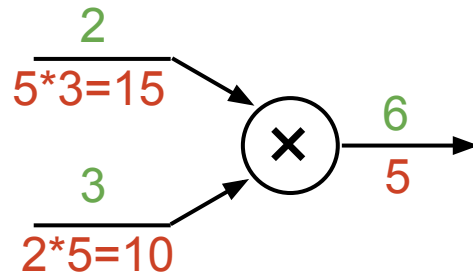


# Patterns in gradient flow

**add** gate: gradient distributor

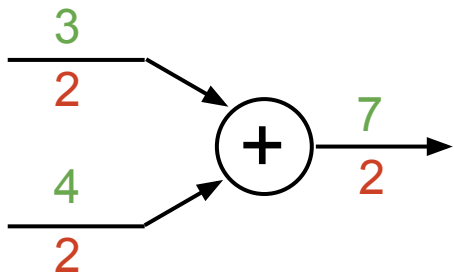


**mul** gate: “swap multiplier”

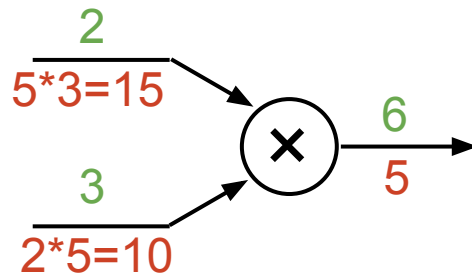


# Patterns in gradient flow

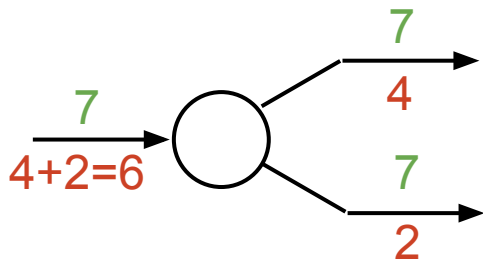
**add** gate: gradient distributor



**mul** gate: “swap multiplier”

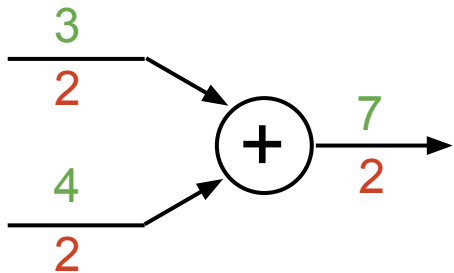


**copy** gate: gradient adder

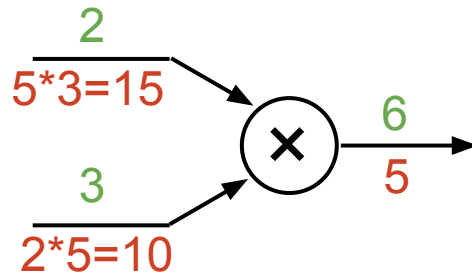


# Patterns in gradient flow

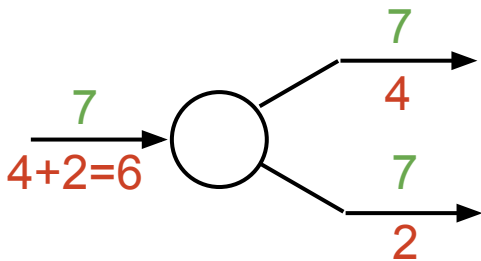
**add** gate: gradient distributor



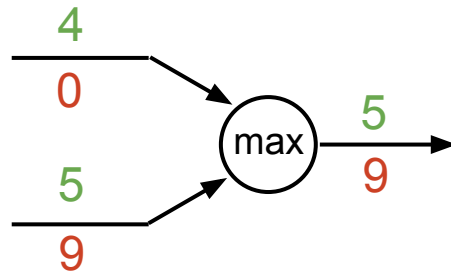
**mul** gate: “swap multiplier”



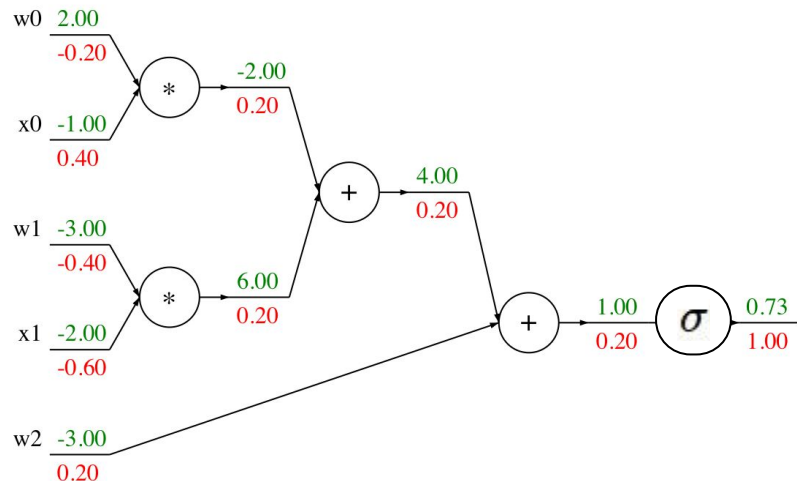
**copy** gate: gradient adder



**max** gate: gradient router



# Backprop Implementation: “Flat” code



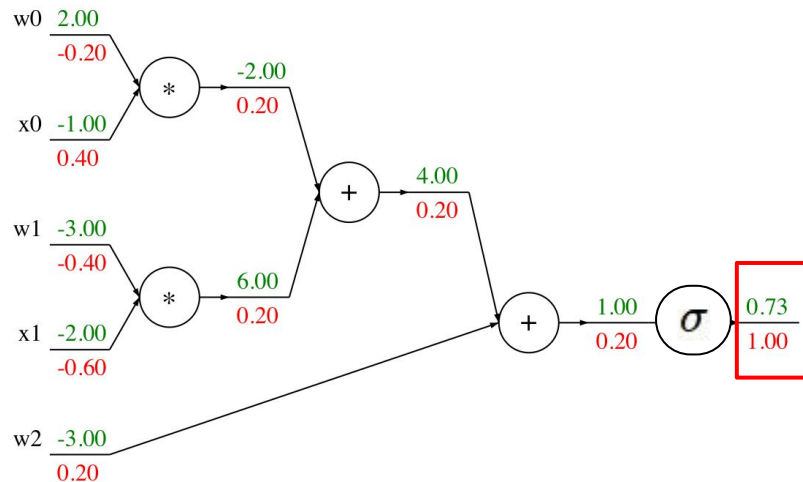
Forward pass:  
Compute output

```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

Backward pass:  
Compute grads

```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

```
def f(w0, x0, w1, x1, w2):
```

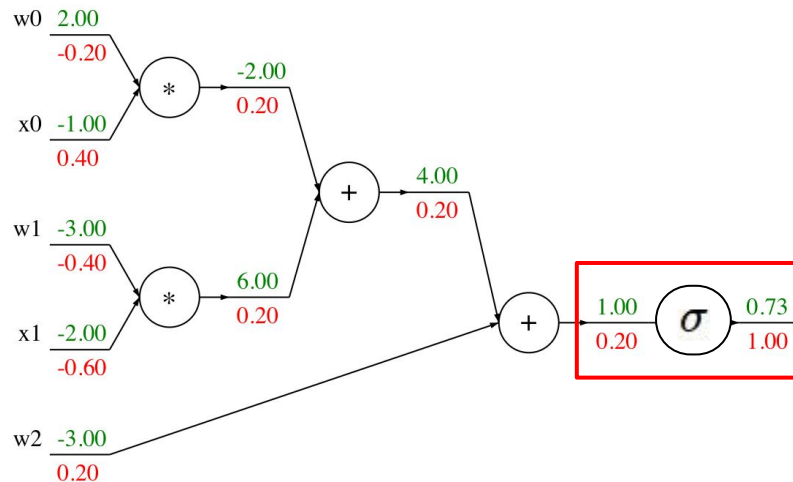
```
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

Base case

```
    grad_L = 1.0
```

```
    grad_s3 = grad_L * (1 - L) * L  
    grad_w2 = grad_s3  
    grad_s2 = grad_s3  
    grad_s0 = grad_s2  
    grad_s1 = grad_s2  
    grad_w1 = grad_s1 * x1  
    grad_x1 = grad_s1 * w1  
    grad_w0 = grad_s0 * x0  
    grad_x0 = grad_s0 * w0
```

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

```
def f(w0, x0, w1, x1, w2):
```

```
    s0 = w0 * x0
```

```
    s1 = w1 * x1
```

```
    s2 = s0 + s1
```

```
    s3 = s2 + w2
```

```
    L = sigmoid(s3)
```

Sigmoid

```
    grad_L = 1.0
```

```
    grad_s3 = grad_L * (1 - L) * L
```

```
    grad_w2 = grad_s3
```

```
    grad_s2 = grad_s3
```

```
    grad_s0 = grad_s2
```

```
    grad_s1 = grad_s2
```

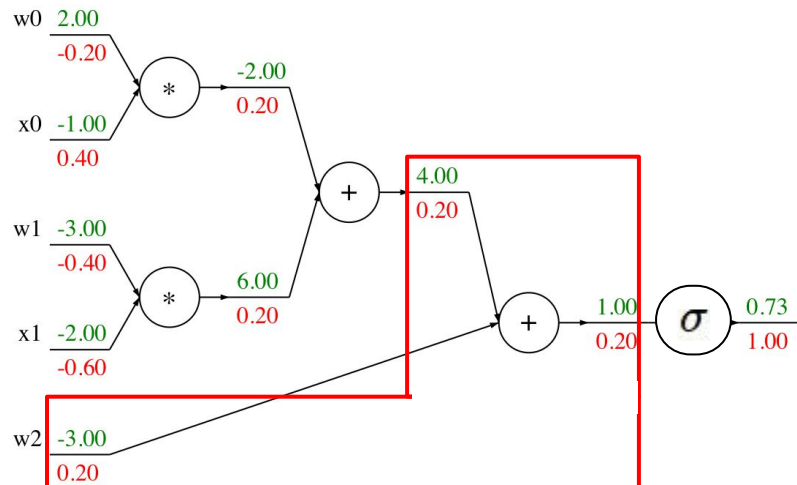
```
    grad_w1 = grad_s1 * x1
```

```
    grad_x1 = grad_s1 * w1
```

```
    grad_w0 = grad_s0 * x0
```

```
    grad_x0 = grad_s0 * w0
```

# Backprop Implementation: “Flat” code



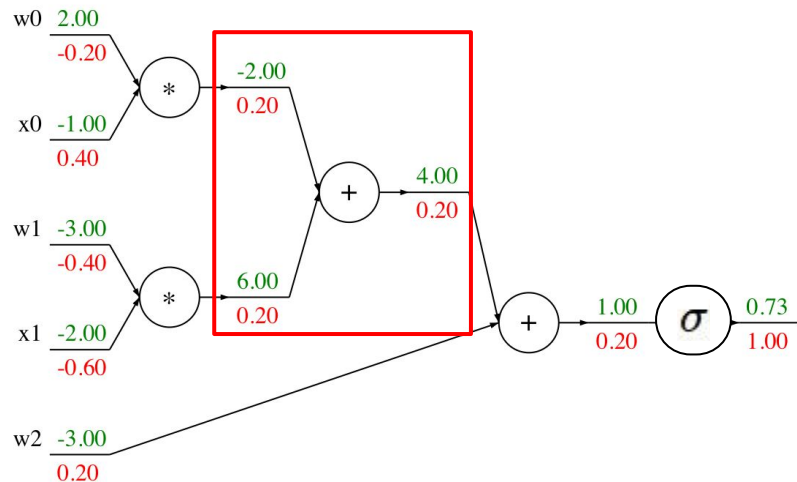
Forward pass:  
Compute output

```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

Add gate

```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

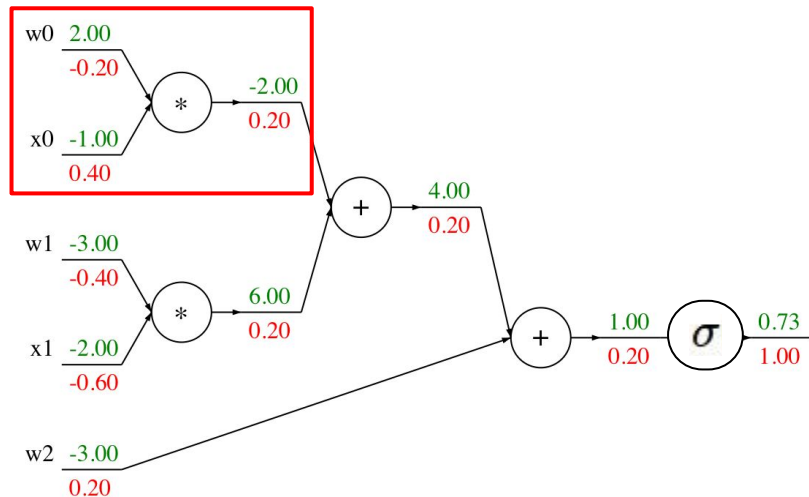
```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

Add gate

```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```



# Backprop Implementation: “Flat” code



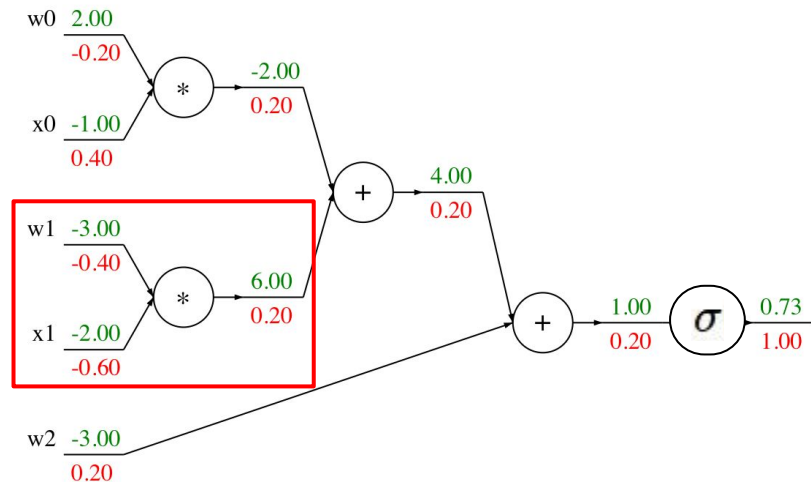
Forward pass:  
Compute output

```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

Multiply gate

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

```
def f(w0, x0, w1, x1, w2):
```

```
    s0 = w0 * x0
```

```
    s1 = w1 * x1
```

```
    s2 = s0 + s1
```

```
    s3 = s2 + w2
```

```
    L = sigmoid(s3)
```

```
grad_L = 1.0
```

```
grad_s3 = grad_L * (1 - L) * L
```

```
grad_w2 = grad_s3
```

```
grad_s2 = grad_s3
```

```
grad_s0 = grad_s2
```

```
grad_s1 = grad_s2
```

```
grad_w1 = grad_s1 * x1
```

```
grad_x1 = grad_s1 * w1
```

```
grad_w0 = grad_s0 * x0
```

```
grad_x0 = grad_s0 * w0
```

Multiply gate

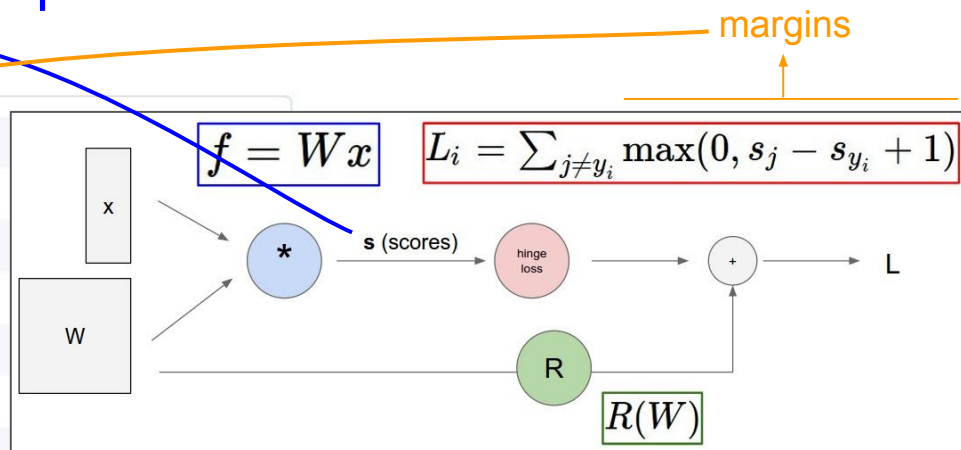
# “Flat” Backprop: Do this for assignment 1!

Stage your forward/backward computation!

E.g. for the SVM:

```
# receive W (weights), X (data)
# forward pass (we have 8 lines)
scores = #...
margins = #...
data_loss = #...
reg_loss = #...
loss = data_loss + reg_loss

# backward pass (we have 5 lines)
dmargins = # ... (optionally, we go direct to dscores)
dscores = #...
dW = #...
```



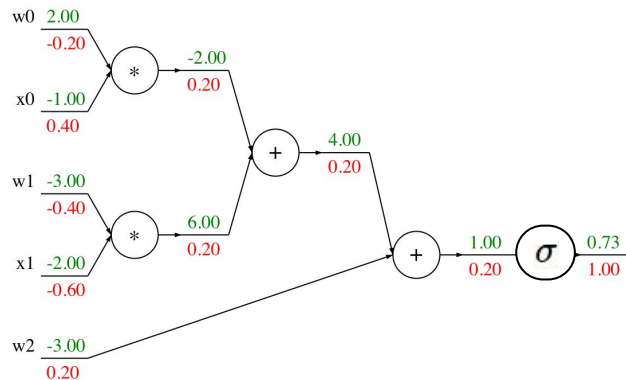
# “Flat” Backprop: Do this for assignment 1!

E.g. for two-layer neural net:

```
# receive W1,W2,b1,b2 (weights/biases), X (data)
# forward pass:
h1 = #... function of X,W1,b1
scores = #... function of h1,W2,b2
loss = #... (several lines of code to evaluate Softmax loss)
# backward pass:
dscores = #...
dh1,dW2,db2 = #...
dW1,db1 = #...
```

# Backprop Implementation: Modularized API

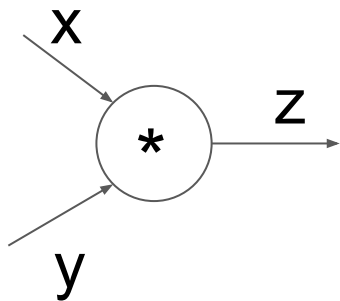
Graph (or Net) object (*rough pseudo code*)



```
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

Gate / Node / Function object: Actual PyTorch code



(x,y,z are scalars)

```
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 stash  
some values for  
use in backward

Upstream  
gradient

Multiply upstream  
and local gradients

# Example: PyTorch operators

pytorch / pytorch

Watch

1,221

★ Unstar

26,770

Y Fork

6,340

Code

Issues 2,286

Pull requests 561

Projects 4

Wiki

Insights

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

BCECriterion.c

ClassNLLCriterion.c

Col2Im.c

ELU.c

FeatureLPPooling.c

GatedLinearUnit.c

HardTanh.c

Im2Col.c

IndexLinear.c

LeakyReLU.c

LogSigmoid.c

MSECriterion.c

MultiLabelMarginCriterion.c

MultiMarginCriterion.c

RRReLU.c

Sigmoid.c

SmoothL1Criterion.c

SoftMarginCriterion.c

SoftPlus.c

SoftShrink.c

SparseLinear.c

SpatialAdaptiveAveragePooling.c

SpatialAdaptiveMaxPooling.c

SpatialAveragePooling.c

SpatialClassNLLCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialConvolutionMM.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialDilatedMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialFractionalMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialMaxUnpooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialReflectionPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialUpSamplingBilinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
THNN.h	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Tanh.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalReflectionPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalRowConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalUpSamplingLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricAdaptiveAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricAdaptiveMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricConvolutionMM.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricDilatedMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricFractionalMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricMaxUnpooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricUpSamplingTrilinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
linear_upsampling.h	Implement nn.functional.interpolate based on upsample. (#8591)	9 months ago
pooling_shape.h	Use integer math to compute output size of pooling operations (#14405)	4 months ago
unfold.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago

# PyTorch sigmoid layer

Forward

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



```
void THNN_(Sigmoid_updateOutput)(
    THNNState *state,
    THTensor *input,
    THTensor *output)
{
    THTensor_(sigmoid)(output, input);
}
```

```
void THNN_(Sigmoid_updateGradInput)(
    THNNState *state,
    THTensor *gradOutput,
    THTensor *gradInput,
    THTensor *output)
{
    THNN_CHECK_NELEMENT(output, gradOutput);
    THTensor_(resizeAs)(gradInput, output);
    TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
        scalar_t z = *output_data;
        *gradInput_data = *gradOutput_data * (1. - z) * z;
    );
}
```

[Source](#)



# PyTorch sigmoid layer

```
1 #ifndef TH_GENERIC_FILE
2 #define TH_GENERIC_FILE "THNN/generic/Sigmoid.c"
3 #else
4
5 void THNN_(Sigmoid_updateOutput)(
6     THNNState *state,
7     THTensor *input,
8     THTensor *output)
9 {
10     THTensor_(sigmoid)(output, input);
11 }
```

Forward

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

```
13 void THNN_(Sigmoid_updateGradInput)(
14     THNNState *state,
15     THTensor *gradOutput,
16     THTensor *gradInput,
17     THTensor *output)
18 {
19     THNN_CHECK_NELEMENT(output, gradOutput);
20     THTensor_(resizeAs)(gradInput, output);
21     TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
22         scalar_t z = *output_data;
23         *gradInput_data = *gradOutput_data * (1. - z) * z;
24     );
25 }
26
27 #endif
```

```
static void sigmoid_kernel(TensorIterator& iter) {
    AT_DISPATCH_FLOATING_TYPES(iter.dtype(), "sigmoid_cpu", [&]() {
        unary_kernel_vec(
            iter,
            [=](scalar_t a) -> scalar_t { return (1 / (1 + std::exp((-a)))); },
            [=](Vec256<scalar_t> a) {
                a = Vec256<scalar_t>((scalar_t)(0)) - a;
                a = a.exp();
                a = Vec256<scalar_t>((scalar_t)(1)) + a;
                a = a.reciprocal();
                return a;
            });
    });
}
```

Forward actually  
defined elsewhere...

```
return (1 / (1 + std::exp((-a))));
```

[Source](#)

# PyTorch sigmoid layer

```
1 #ifndef TH_GENERIC_FILE
2 #define TH_GENERIC_FILE "THNN/generic/Sigmoid.c"
3 #else
```

```
4
5 void THNN_(Sigmoid_updateOutput)(
6     THNNState *state,
7     THTensor *input,
8     THTensor *output)
9 {
10     THTensor_(sigmoid)(output, input);
11 }
```

Forward

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

```
12
13 void THNN_(Sigmoid_updateGradInput)(
14     THNNState *state,
15     THTensor *gradOutput,
16     THTensor *gradInput,
17     THTensor *output)
18 {
19     THNN_CHECK_NELEMENT(output, gradOutput);
20     THTensor_(resizeAs)(gradInput, output);
21     TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
22         scalar_t z = *output_data;
23         *gradInput_data = *gradOutput_data * (1. - z) * z;
24     );
25 }
```

```
static void sigmoid_kernel(TensorIterator& iter) {
    AT_DISPATCH_FLOATING_TYPES(iter.dtype(), "sigmoid_cpu", [&]() {
        unary_kernel_vec(
            iter,
            [=](scalar_t a) -> scalar_t { return (1 / (1 + std::exp((-a)))); },
            [=](Vec256<scalar_t> a) {
                a = Vec256<scalar_t>((scalar_t)(0)) - a;
                a = a.exp();
                a = Vec256<scalar_t>((scalar_t)(1)) + a;
                a = a.reciprocal();
                return a;
            });
    });
}
```

Forward actually defined [elsewhere...](#)

Backward

$$(1 - \sigma(x)) \sigma(x)$$

[Source](#)

So far: backprop with scalars

What about vector-valued functions?

# Recap: 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?

# Recap: 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?

# Recap: Vector derivatives

## Scalar to Scalar

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

Regular derivative:

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

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## 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

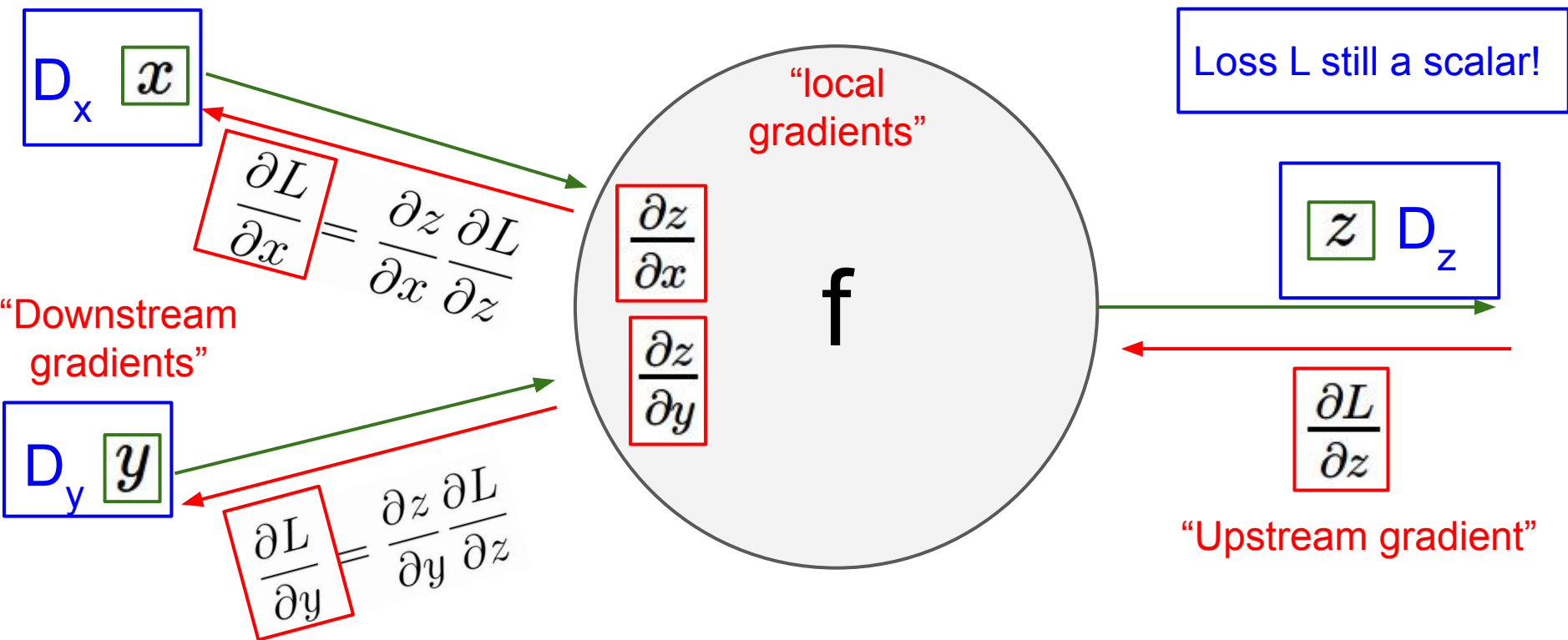
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

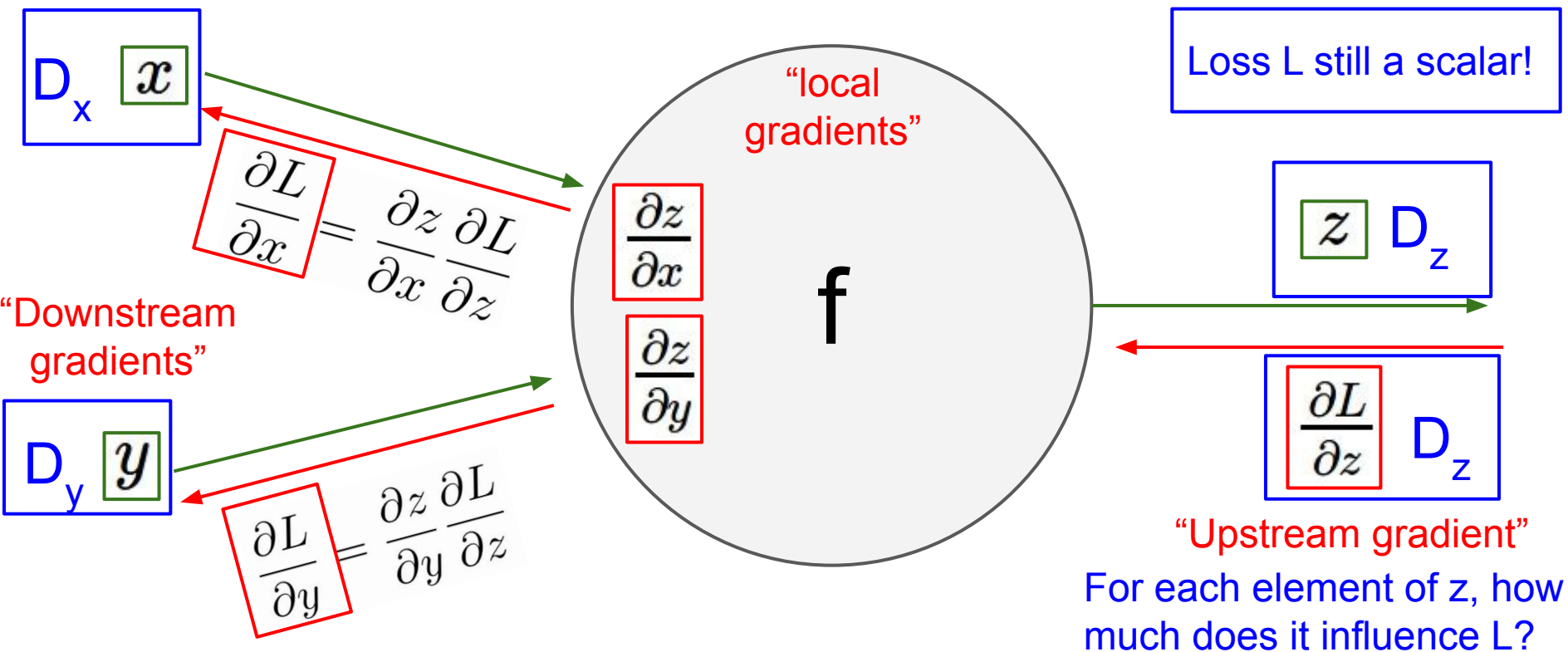
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left( \frac{\partial y}{\partial x} \right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

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

# Backprop with Vectors

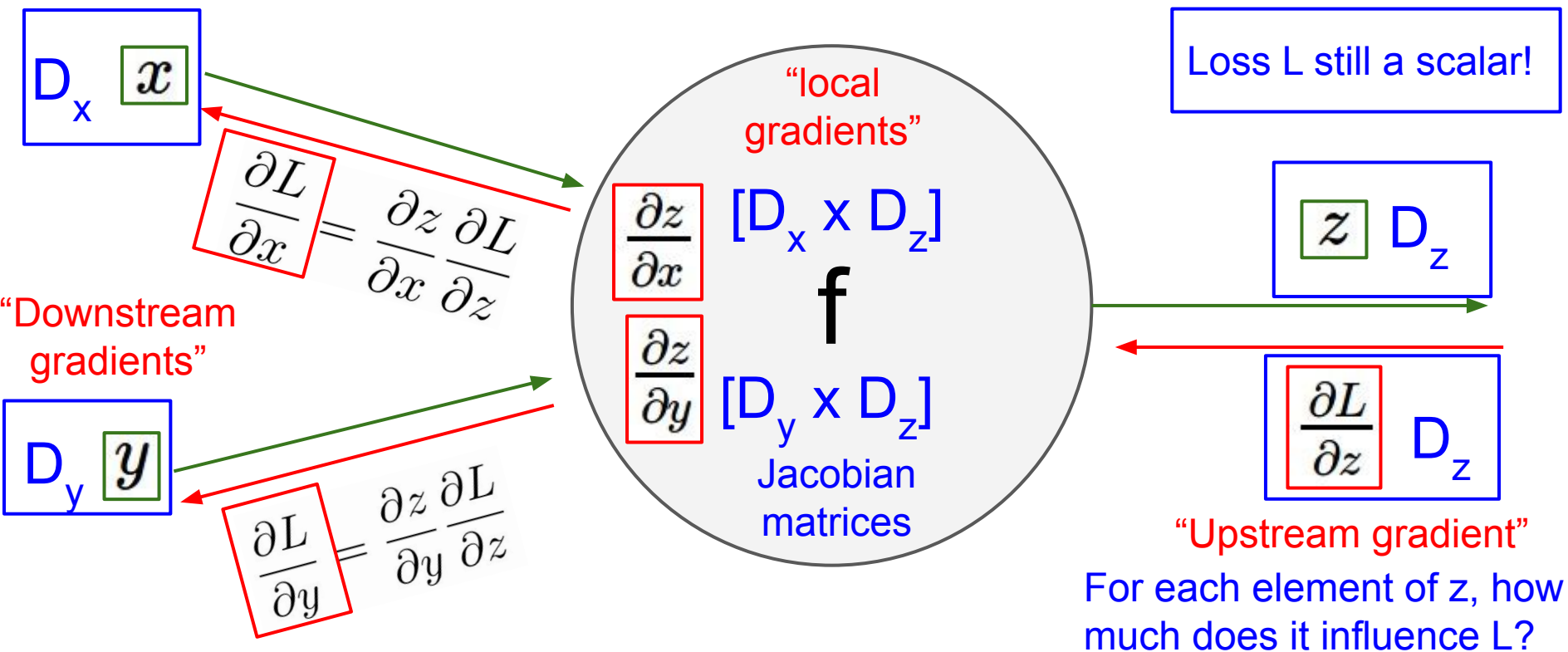


# Backprop with Vectors

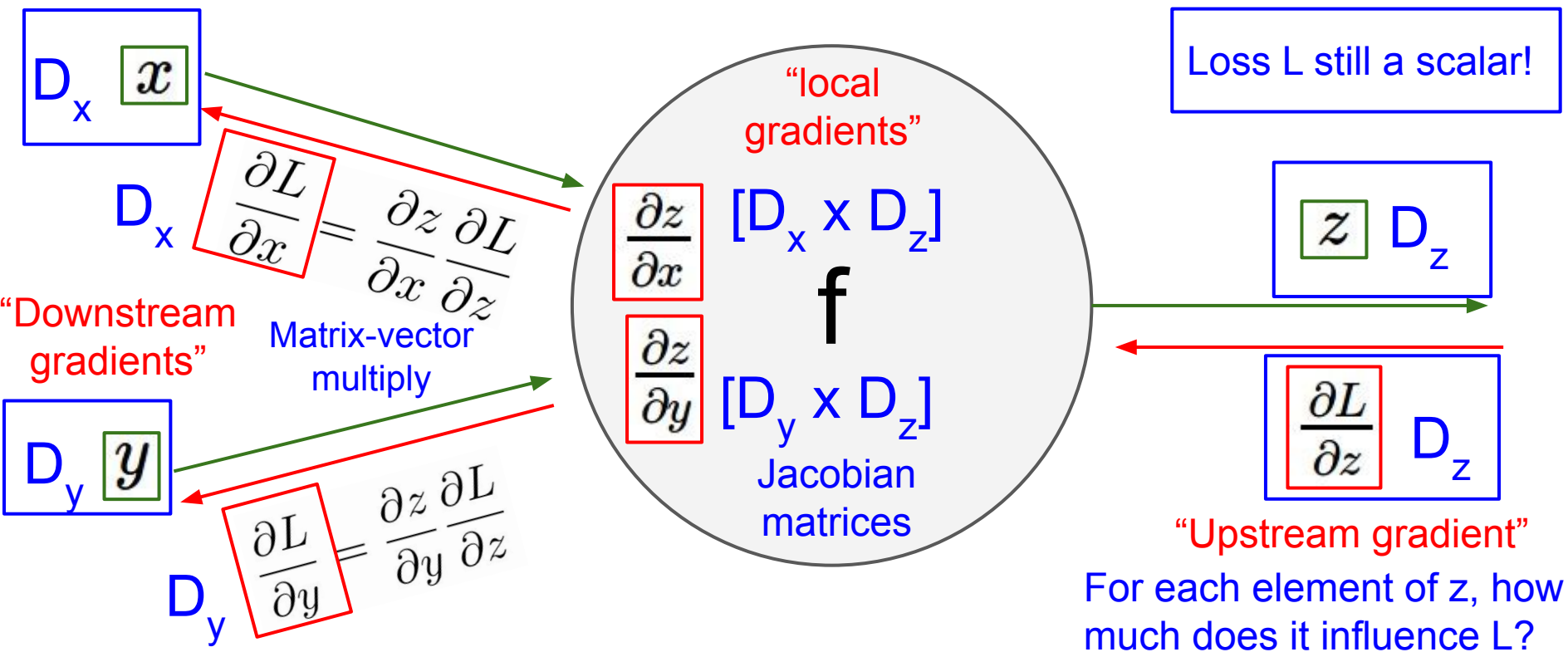




# Backprop with Vectors



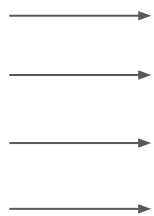
# Backprop with Vectors



# Backprop with Vectors

4D input x:

$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$

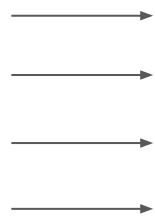


$$f(x) = \max(0, x)$$

*(elementwise)*

4D output y:

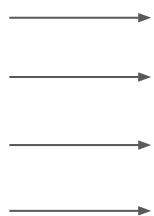
$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$



# Backprop with Vectors

4D input x:

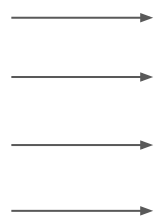
$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$



$$f(x) = \max(0, x) \\ (\textit{elementwise})$$

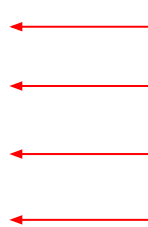
4D output y:

$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$



4D dL/dy:

$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$

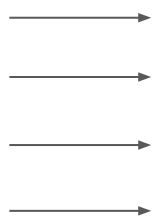


Upstream  
gradient

# Backprop with Vectors

4D input x:

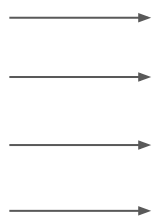
$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$



$f(x) = \max(0, x)$   
(*elementwise*)

4D output y:

$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$



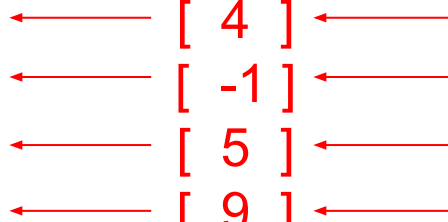
Jacobian  $dy/dx$

$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$

4D  $dL/dy$ :

$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$

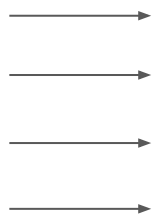
Upstream  
gradient



# Backprop with Vectors

4D input x:

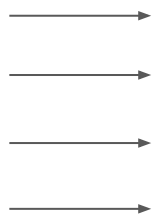
$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$



$f(x) = \max(0, x)$   
(*elementwise*)

4D output y:

$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$



$[dy/dx] \ [dL/dy]$

$\begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \end{bmatrix}$

$\begin{bmatrix} 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} -1 \end{bmatrix}$

$\begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 5 \end{bmatrix}$

$\begin{bmatrix} 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 9 \end{bmatrix}$

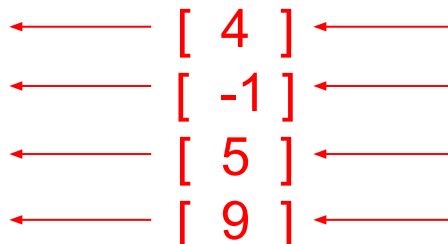
4D dL/dy:

$\begin{bmatrix} 4 \end{bmatrix}$

$\begin{bmatrix} -1 \end{bmatrix}$

$\begin{bmatrix} 5 \end{bmatrix}$

$\begin{bmatrix} 9 \end{bmatrix}$

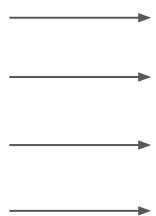


Upstream  
gradient

# Backprop with Vectors

4D input x:

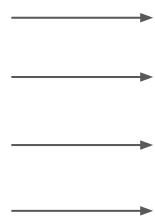
$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$



$$f(x) = \max(0, x) \\ (\textit{elementwise})$$

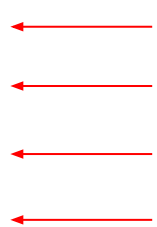
4D output y:

$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$



4D dL/dx:

$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix}$

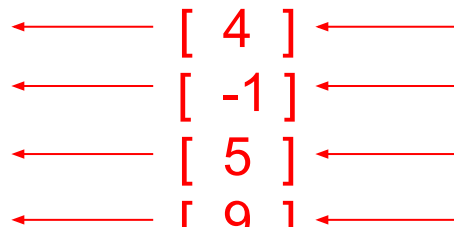


$\begin{bmatrix} dy/dx \\ dL/dy \end{bmatrix}$

$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$

4D dL/dy:

$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$



Upstream  
gradient

# Backprop with Vectors

4D input x:

$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$

$$f(x) = \max(0, x) \quad (\text{elementwise})$$

4D output y:

$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$

Jacobian is **sparse**:  
off-diagonal entries  
always zero! Never  
**explicitly** form  
Jacobian -- instead  
use **implicit**  
multiplication

4D  $dL/dx$ :

$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix}$

$[dy/dx] [dL/dy]$

$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$

4D  $dL/dy$ :

$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$

Upstream  
gradient



# Backprop with Vectors

4D input x:

$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$

$$f(x) = \max(0, x) \quad (\text{elementwise})$$

4D output y:

$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$

Jacobian is **sparse**:  
off-diagonal entries  
always zero! Never  
**explicitly** form  
Jacobian -- instead  
use **implicit**  
multiplication

4D  $dL/dx$ :

$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix}$

$[dy/dx] [dL/dy]$

$$\left( \frac{\partial L}{\partial x} \right)_i = \begin{cases} \left( \frac{\partial L}{\partial y} \right)_i & \text{if } x_i > 0 \\ 0 & \text{otherwise} \end{cases}$$

4D  $dL/dy$ :

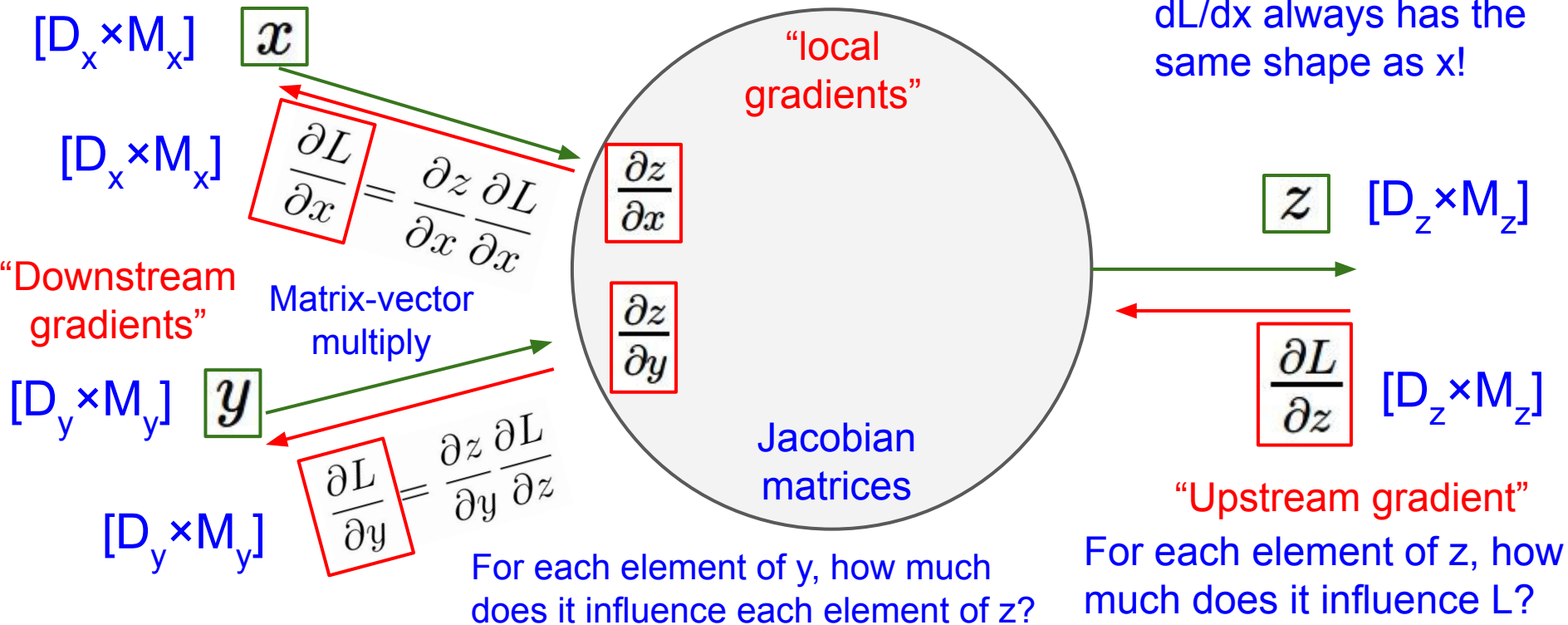
$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$

Upstream  
gradient

# Backprop with Matrices (or Tensors)

Loss L still a scalar!

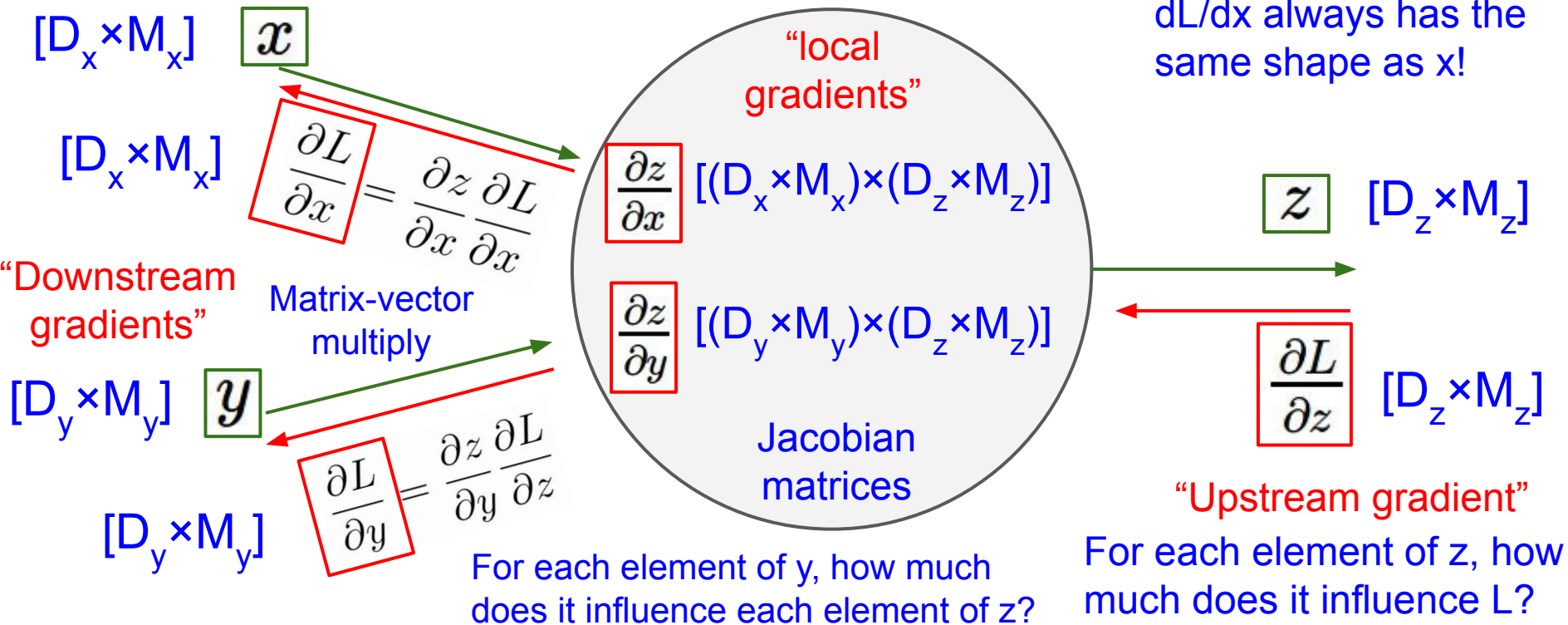
$dL/dx$  always has the same shape as  $x$ !



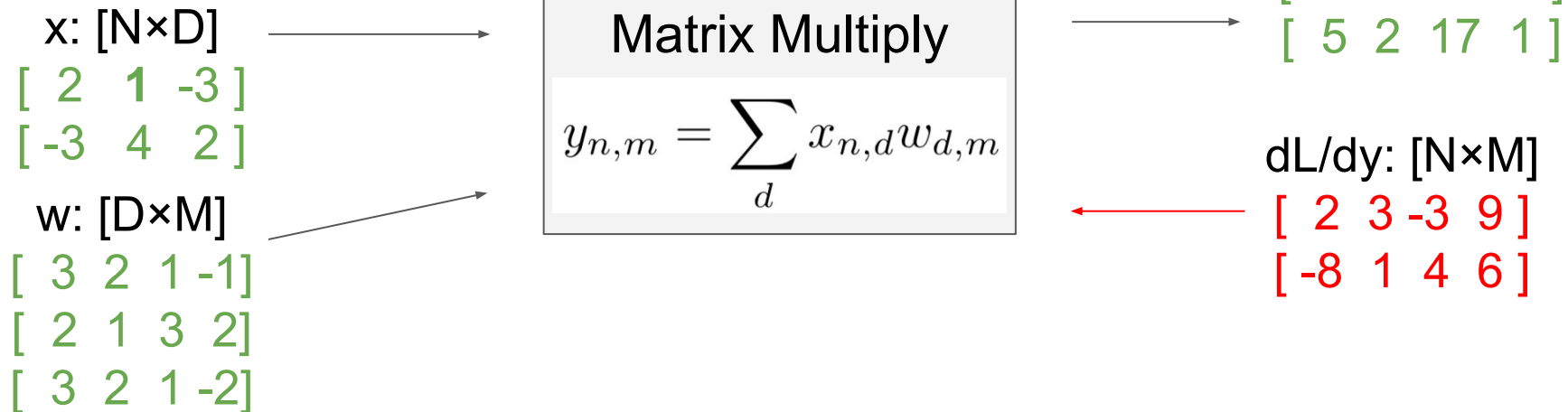
# Backprop with Matrices (or Tensors)

Loss L still a scalar!

$dL/dx$  always has the same shape as  $x$ !



# Backprop with Matrices



Also see derivation in the course notes:

<http://cs231n.stanford.edu/handouts/linear-backprop.pdf>

# Backprop with Matrices

x: [N×D]

[ 2 1 -3 ]

[ -3 4 2 ]

w: [D×M]

[ 3 2 1 -1 ]

[ 2 1 3 2 ]

[ 3 2 1 -2 ]

Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

**Jacobians:**

dy/dx: [(N×D)×(N×M)]

dy/dw: [(D×M)×(N×M)]

y: [N×M]

[13 9 -2 -6]

[ 5 2 17 1 ]

dL/dy: [N×M]

[ 2 3 -3 9 ]

[ -8 1 4 6 ]

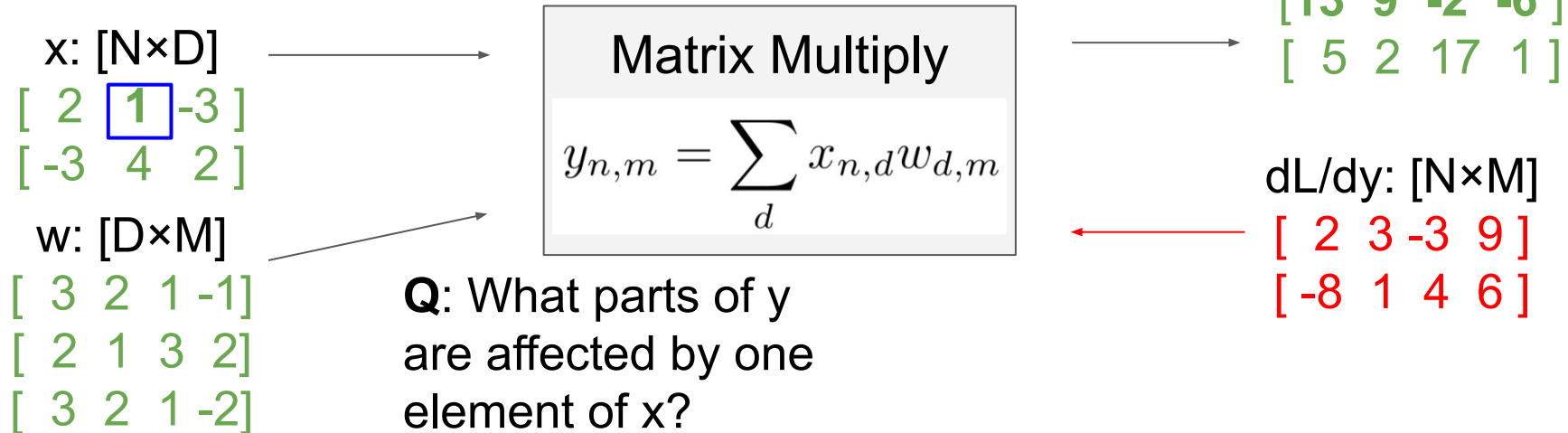
For a neural net we may have

N=64, D=M=4096

Each Jacobian takes 256 GB of memory!

Must work with them implicitly!

# Backprop with Matrices



# Backprop with Matrices

$x: [N \times D]$   
 $\begin{bmatrix} 2 & \boxed{1} & -3 \\ -3 & 4 & 2 \end{bmatrix}$

$w: [D \times M]$   
 $\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$

Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

$y: [N \times M]$   
 $\begin{bmatrix} \boxed{13} & 9 & -2 & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$

$dL/dy: [N \times M]$   
 $\begin{bmatrix} \boxed{2} & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$

**Q:** What parts of  $y$  are affected by one element of  $x$ ?

**A:**  $x_{n,d}$  affects the whole row  $y_{n,\cdot}$ .

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}}$$

# Backprop with Matrices

$x: [N \times D]$   
 $\begin{bmatrix} 2 & \boxed{1} & -3 \\ -3 & 4 & 2 \end{bmatrix}$

$w: [D \times M]$   
 $\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$

Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

$y: [N \times M]$   
 $\begin{bmatrix} \boxed{13} & 9 & \boxed{-2} & \boxed{-6} \\ 5 & 2 & 17 & 1 \end{bmatrix}$

$dL/dy: [N \times M]$   
 $\begin{bmatrix} \boxed{2} & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$

**Q:** What parts of  $y$  are affected by one element of  $x$ ?

**A:**  $x_{n,d}$  affects the whole row  $y_{n,\cdot}$ .

**Q:** How much does  $x_{n,d}$  affect  $y_{n,m}$ ?

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}}$$



# Backprop with Matrices

$x: [N \times D]$   
 $\begin{bmatrix} 2 & \boxed{1} & -3 \\ -3 & 4 & 2 \end{bmatrix}$

$w: [D \times M]$   
 $\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & \boxed{3} & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$

Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

$y: [N \times M]$   
 $\begin{bmatrix} \boxed{13} & 9 & \boxed{-2} & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$

$dL/dy: [N \times M]$   
 $\begin{bmatrix} \boxed{2} & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$

**Q:** What parts of  $y$  are affected by one element of  $x$ ?

**A:**  $x_{n,d}$  affects the whole row  $y_n$ .

**Q:** How much does  $x_{n,d}$  affect  $y_{n,m}$ ?

**A:**  $w_{d,m}$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} w_{d,m}$$

# Backprop with Matrices

$$x: [N \times D]$$

$$\begin{bmatrix} 2 & \boxed{1} & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

$$w: [D \times M]$$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & \boxed{3} & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$[N \times D] \quad [N \times M] \quad [M \times D]$$

$$\frac{\partial L}{\partial x} = \left( \frac{\partial L}{\partial y} \right) w^T$$

Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

$$y: [N \times M]$$

$$\begin{bmatrix} \boxed{13} & 9 & \boxed{-2} & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

$$dL/dy: [N \times M]$$

$$\begin{bmatrix} \boxed{2} & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

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**A:**  $w_{d,m}$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} w_{d,m}$$

# Backprop with Matrices

$$x: [N \times D]$$

$$\begin{bmatrix} 2 & \boxed{1} & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

$$w: [D \times M]$$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & \boxed{3} & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

$$y: [N \times M]$$

$$\begin{bmatrix} \boxed{13} & 9 & \boxed{-2} & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

$$dL/dy: [N \times M]$$

$$\begin{bmatrix} \boxed{2} & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

By similar logic:

$$[N \times D] \quad [N \times M] \quad [M \times D]$$

$$\frac{\partial L}{\partial x} = \left( \frac{\partial L}{\partial y} \right) w^T$$

$$[D \times M] \quad [D \times N] \quad [N \times M]$$

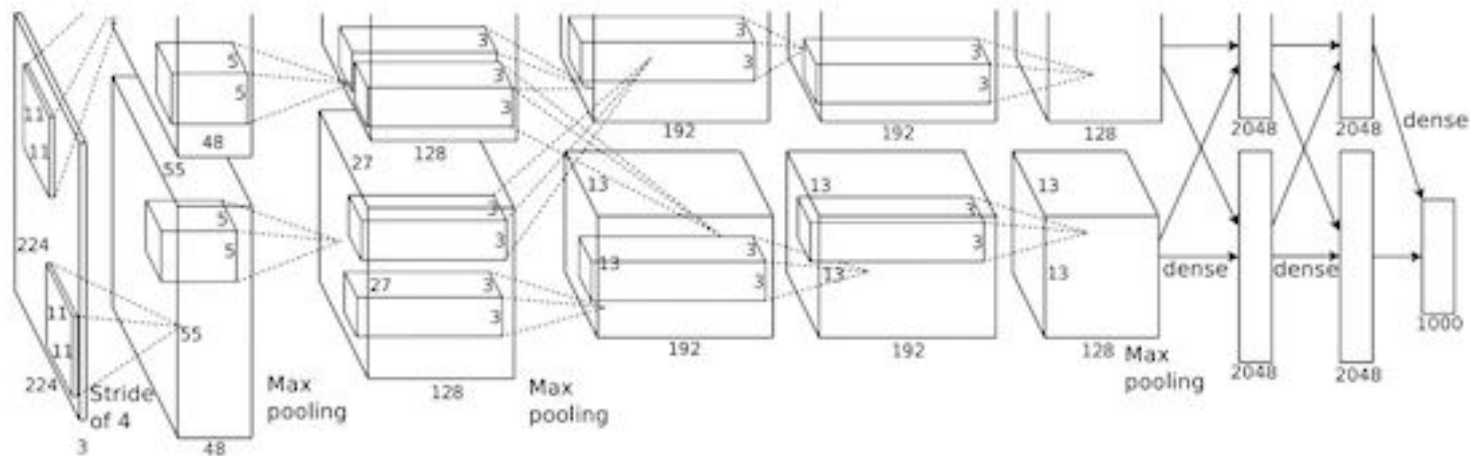
$$\frac{\partial L}{\partial w} = x^T \left( \frac{\partial L}{\partial y} \right)$$

These formulas are easy to remember: they are the only way to make shapes match up!

# Summary for today:

- **(Fully-connected) Neural Networks** are stacks of linear functions and nonlinear activation functions; they have much more representational power than linear classifiers
- **backpropagation** = recursive application of the chain rule along a computational graph to compute the gradients of all inputs/parameters/intermediates
- 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

# Next Time: Convolutional Networks!



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

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

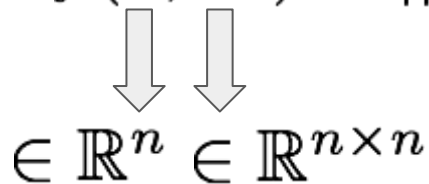
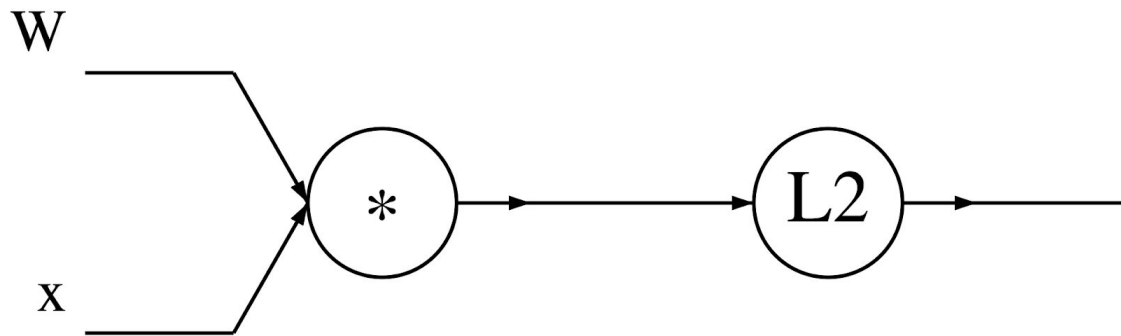


Diagram illustrating the vectorization of the variables  $x$  and  $W$  in the function  $f(x, W)$ . Two gray arrows point downwards from the variables  $x$  and  $W$  in the equation above to their respective spaces below.

$$\begin{matrix} \downarrow & \downarrow \\ \in \mathbb{R}^n & \in \mathbb{R}^{n \times n} \end{matrix}$$

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

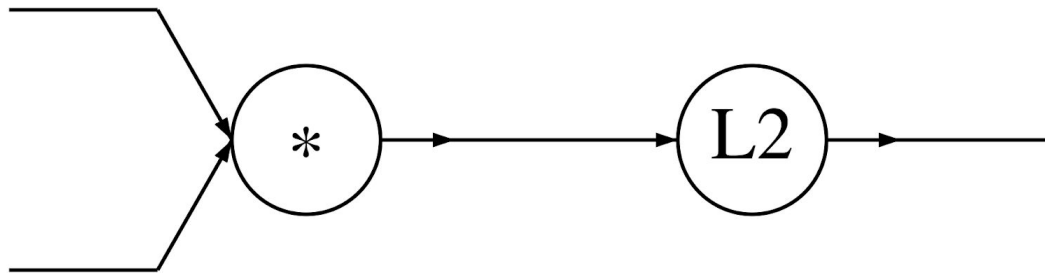




A vectorized example:  $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$

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

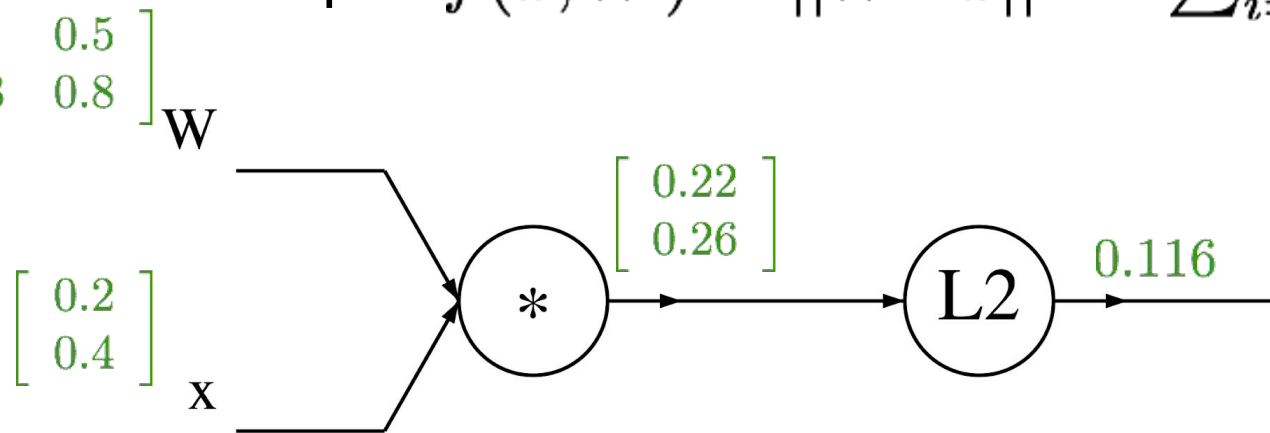
$$\begin{bmatrix} 0.2 \\ 0.4 \end{bmatrix} \mathbf{x}$$



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

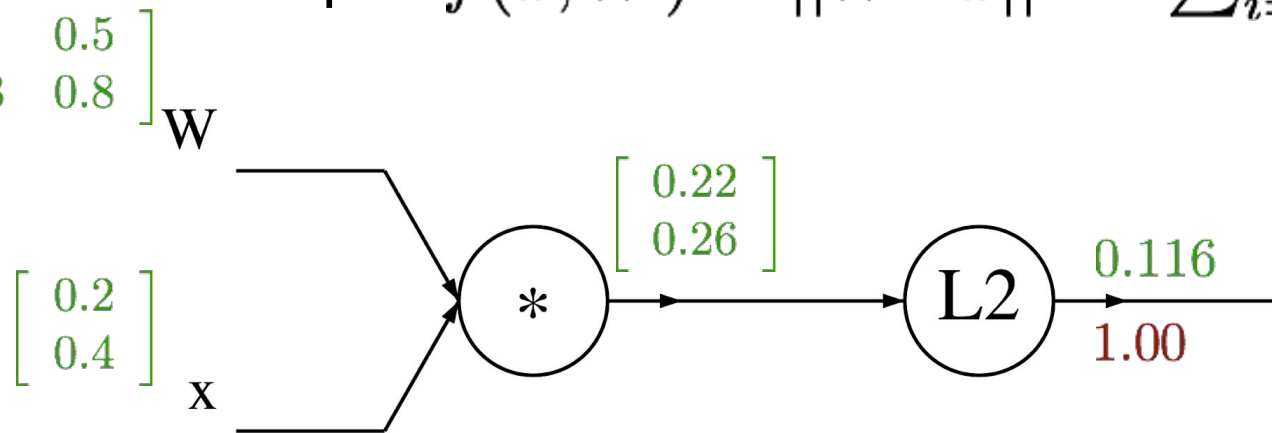
$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

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



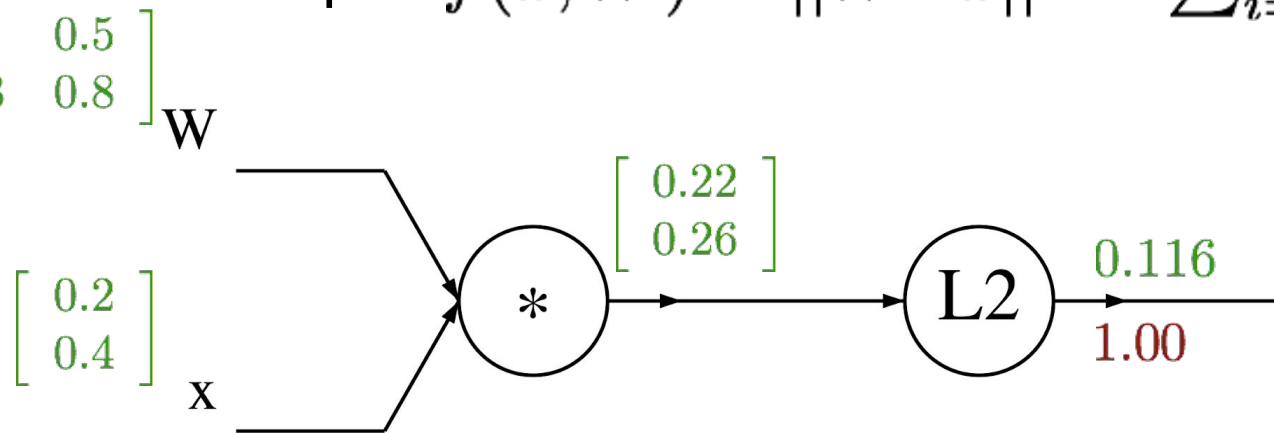
$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$
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A vectorized example:  $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$



$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$
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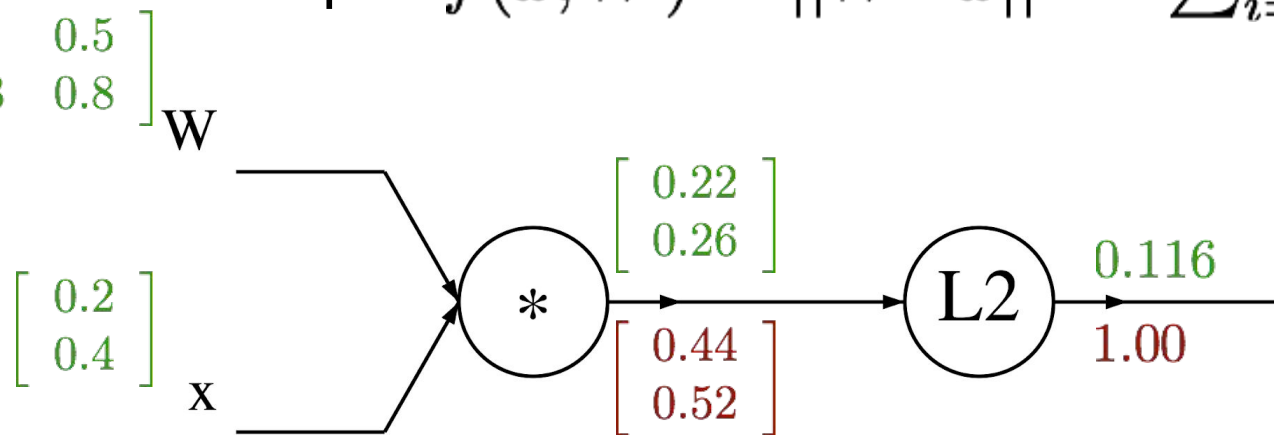
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$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

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

$$\nabla_q f = 2q$$

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



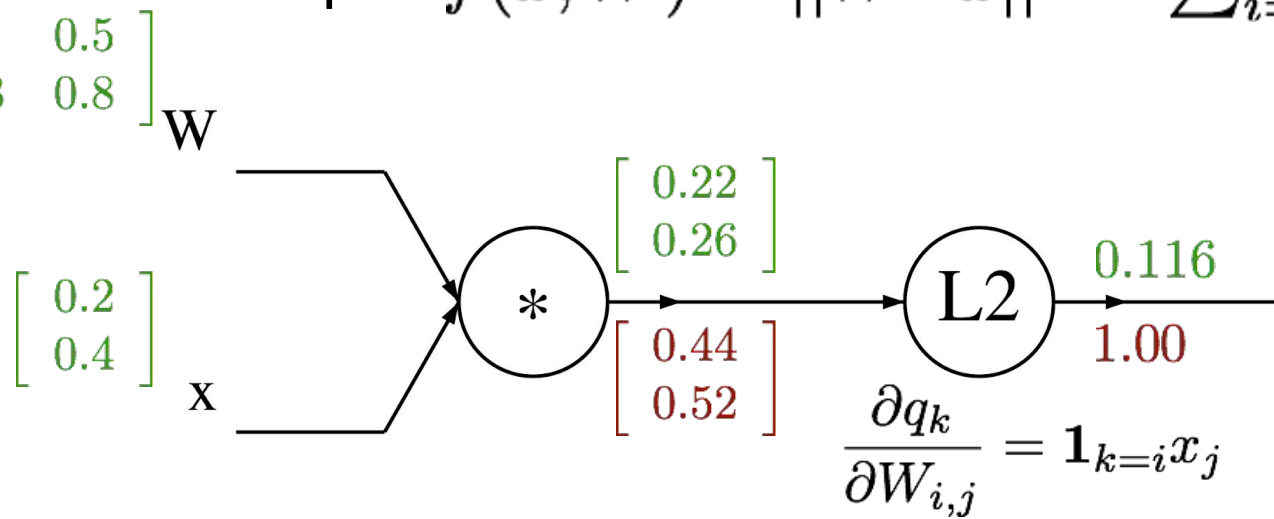
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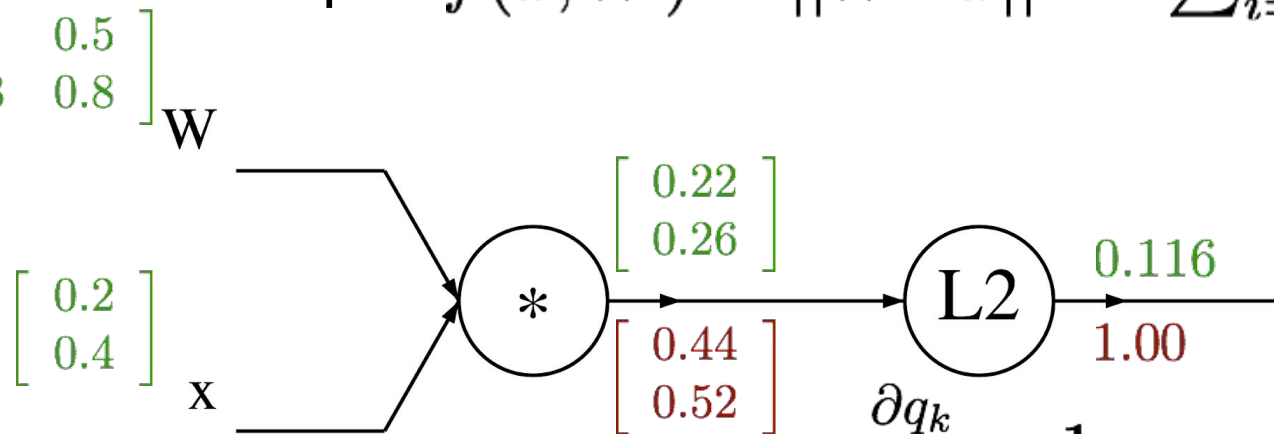
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$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

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

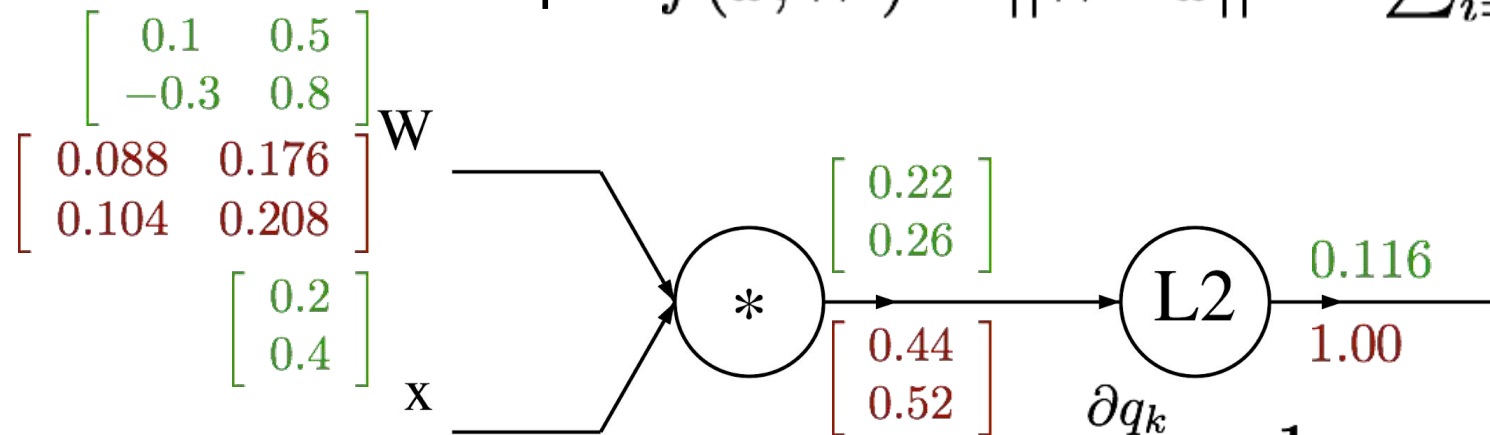


$$\begin{aligned} \frac{\partial q_k}{\partial W_{i,j}} &= \mathbf{1}_{k=i} x_j \\ \frac{\partial f}{\partial W_{i,j}} &= \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}} \\ &= \sum_k (2q_k) (\mathbf{1}_{k=i} x_j) \\ &= 2q_i x_j \end{aligned}$$

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

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

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



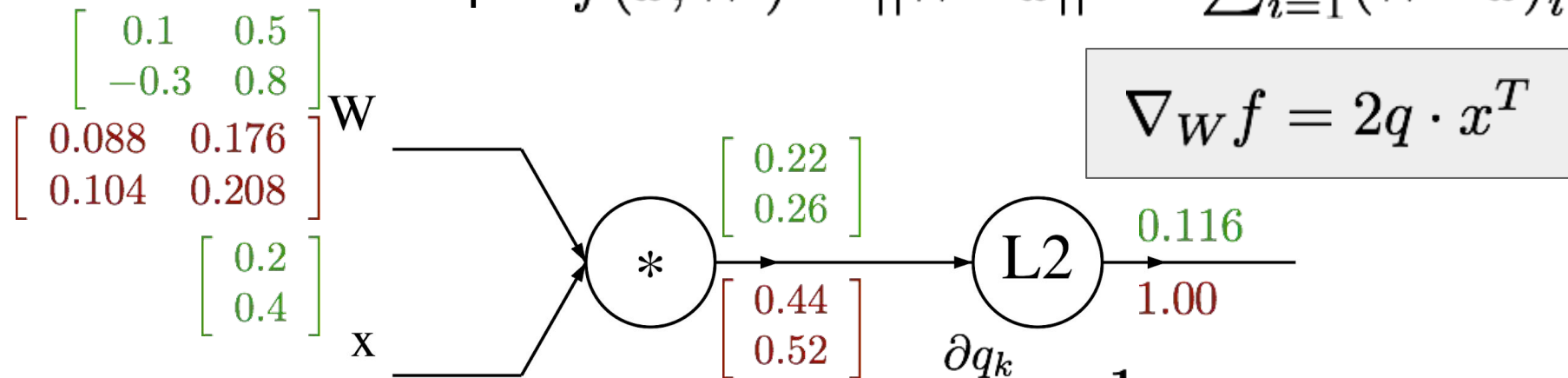
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$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$



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

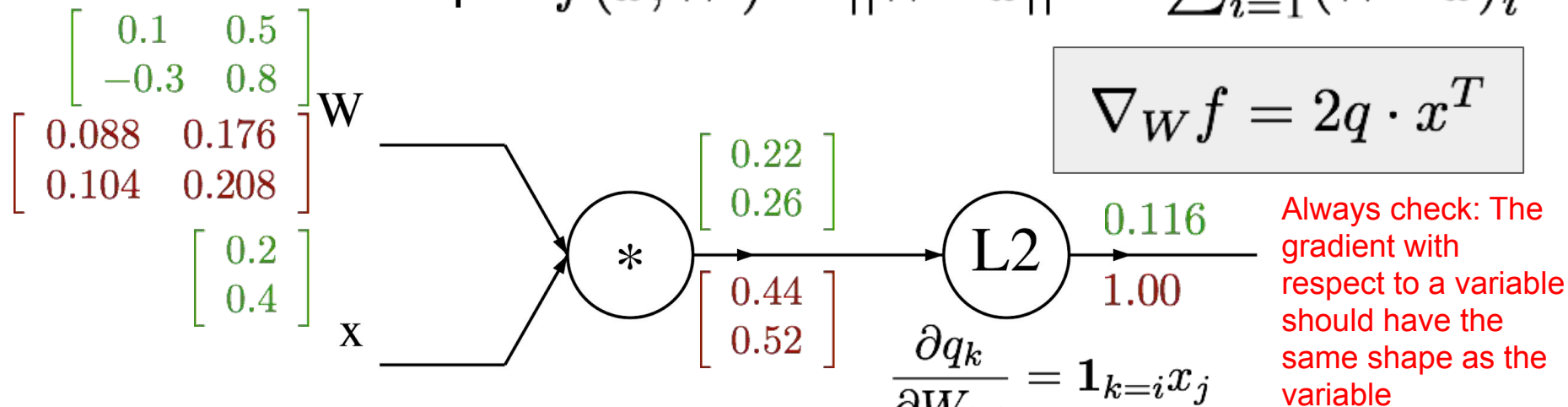


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$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

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

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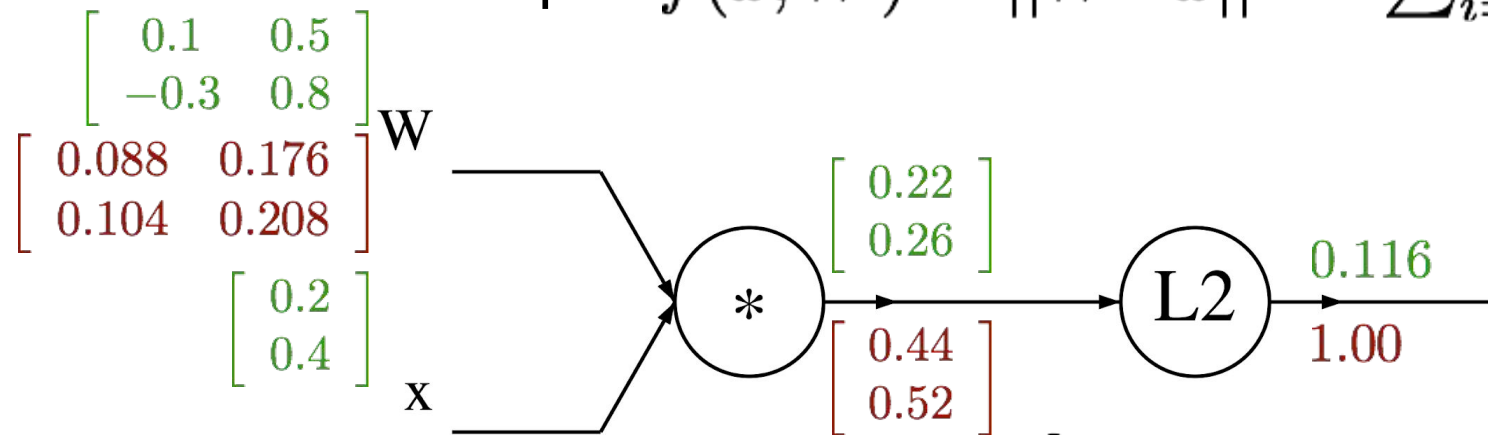


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

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

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

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

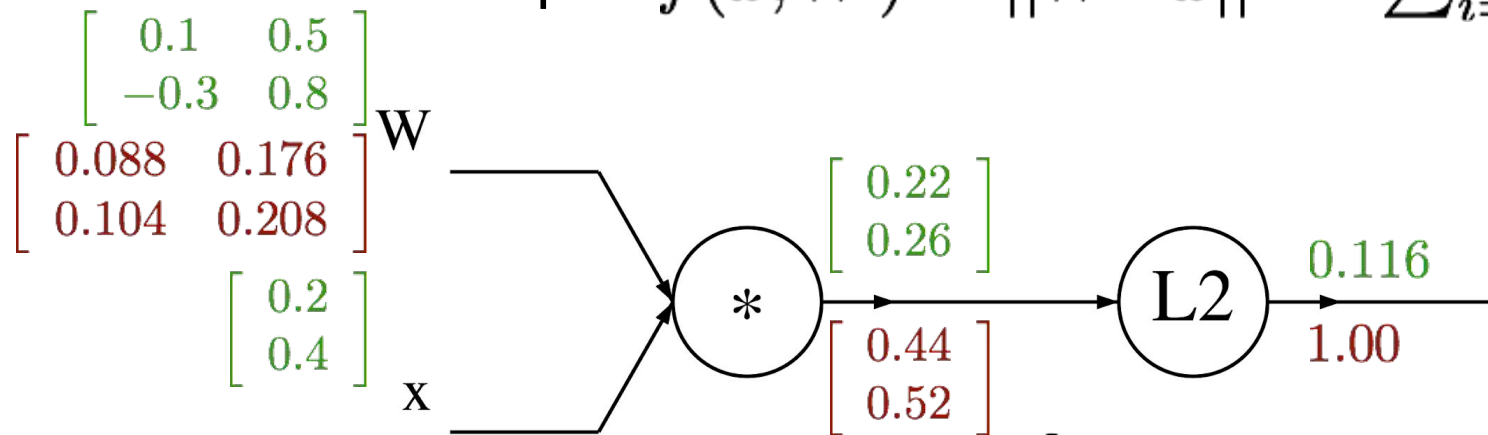


$$\frac{\partial q_k}{\partial x_i} = W_{k,i}$$

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

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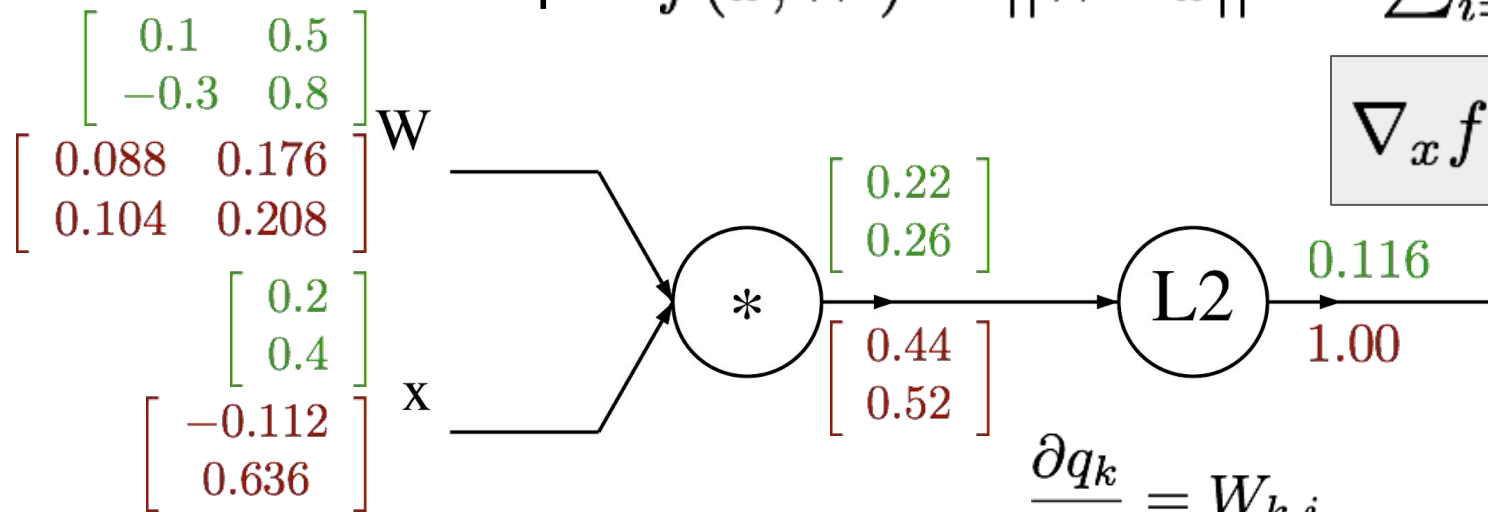


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

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



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

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

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

$$\begin{aligned} \frac{\partial q_k}{\partial x_i} &= W_{k,i} \\ \frac{\partial f}{\partial x_i} &= \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial x_i} \\ &= \sum_k 2q_k W_{k,i} \end{aligned}$$

In discussion section: A matrix example...

$$z_1 = XW_1$$

$$h_1 = \text{ReLU}(z_1)$$

$$\hat{y} = h_1 W_2$$

$$L = ||\hat{y}||_2^2$$

$$\frac{\partial L}{\partial W_2} = ?$$

$$\frac{\partial L}{\partial W_1} = ?$$

