

# Lecture 4: Neural Networks and Backpropagation

# Administrative: Assignment 1

Due 10/20 11:59pm

- K-Nearest Neighbor
- Linear classifiers: SVM, Softmax
- Two-layer neural network
- Image features

# Administrative: Project proposal

Due **Friday 10/27**

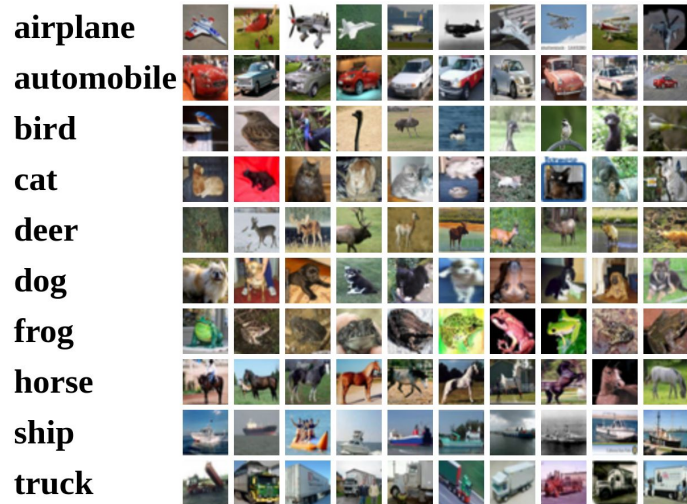
Come to office hours to talk about potential ideas.

Use EdStem to find teammates

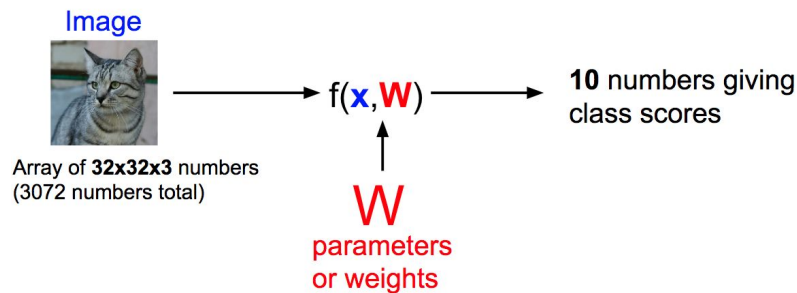
# Administrative: EdStem

Please make sure to check and read all pinned EdStem posts.

# Recap: from last time



$$f(x, W) = Wx + b$$



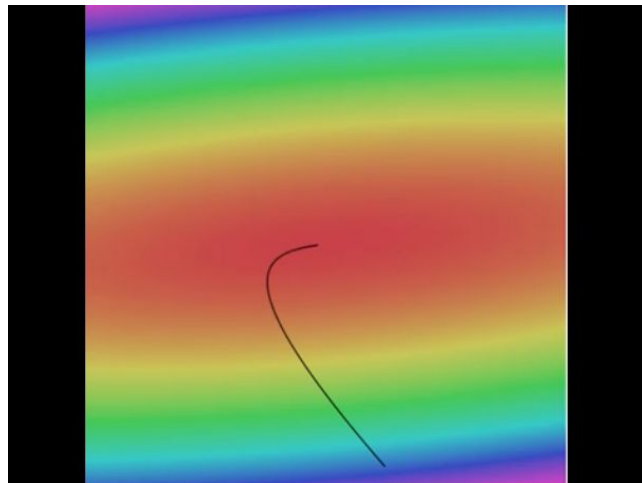
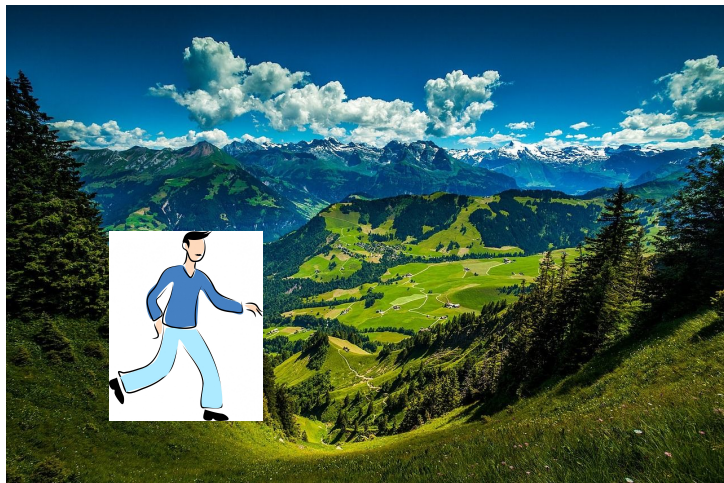
# Recap: loss functions

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

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

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

# 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



# Stochastic Gradient Descent (SGD)

$$L(W) = \frac{1}{N} \sum_{i=1}^N L_i(x_i, y_i, W) + \lambda R(W)$$

$$\nabla_W L(W) = \frac{1}{N} \sum_{i=1}^N \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

Full sum expensive  
when N is large!

Approximate sum  
using a **minibatch** of  
examples  
32 / 64 / 128 common

```
# Vanilla Minibatch Gradient Descent
```

```
while True:
```

```
    data_batch = sample_training_data(data, 256) # sample 256 examples
```

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

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

# What we are going to discuss today!

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

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

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

How to find the best  $W$ ?

$$\nabla_W L$$

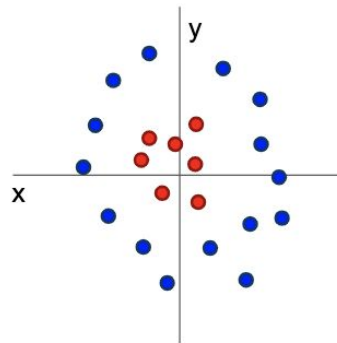
# Problem: Linear Classifiers are not very powerful

## Visual Viewpoint



Linear classifiers learn  
one template per class

## Geometric Viewpoint



Linear classifiers  
can only draw linear  
decision boundaries

# Pixel Features

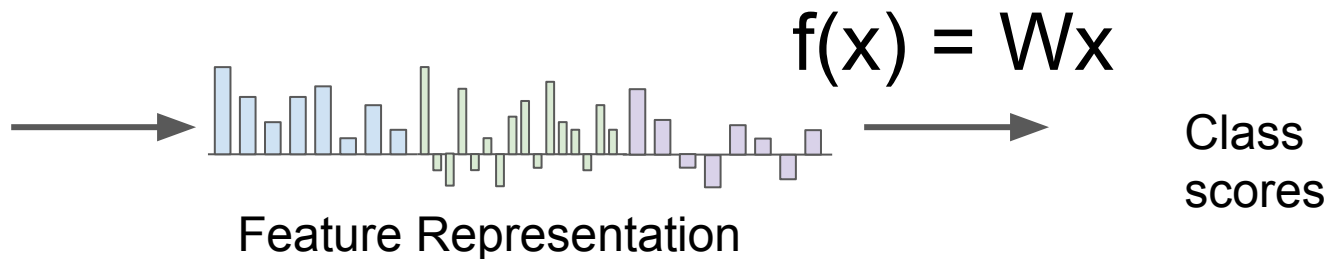


$$f(x) = Wx$$

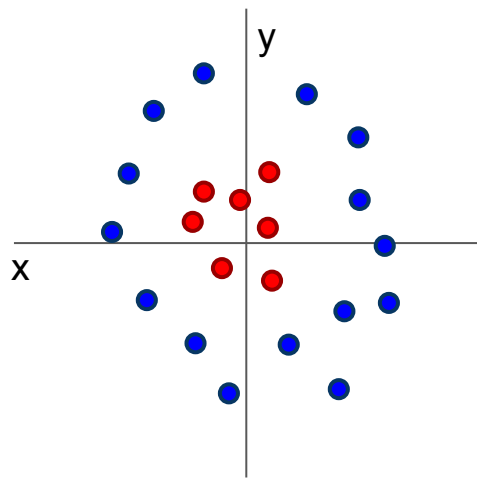
Class  
scores



# Image Features

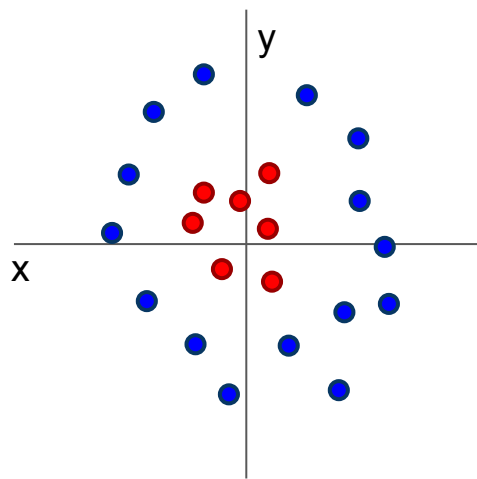


# Image Features: Motivation



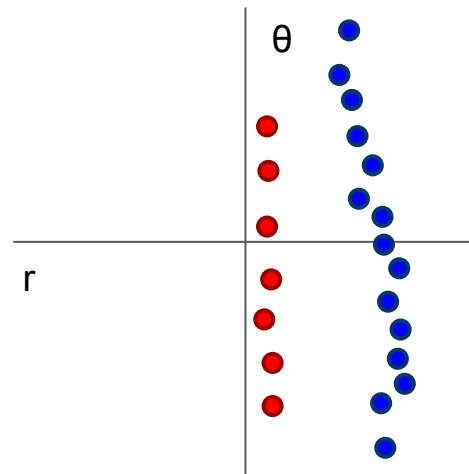
Cannot separate red  
and blue points with  
linear classifier

# Feature become linearly separable through a non-linear transformation



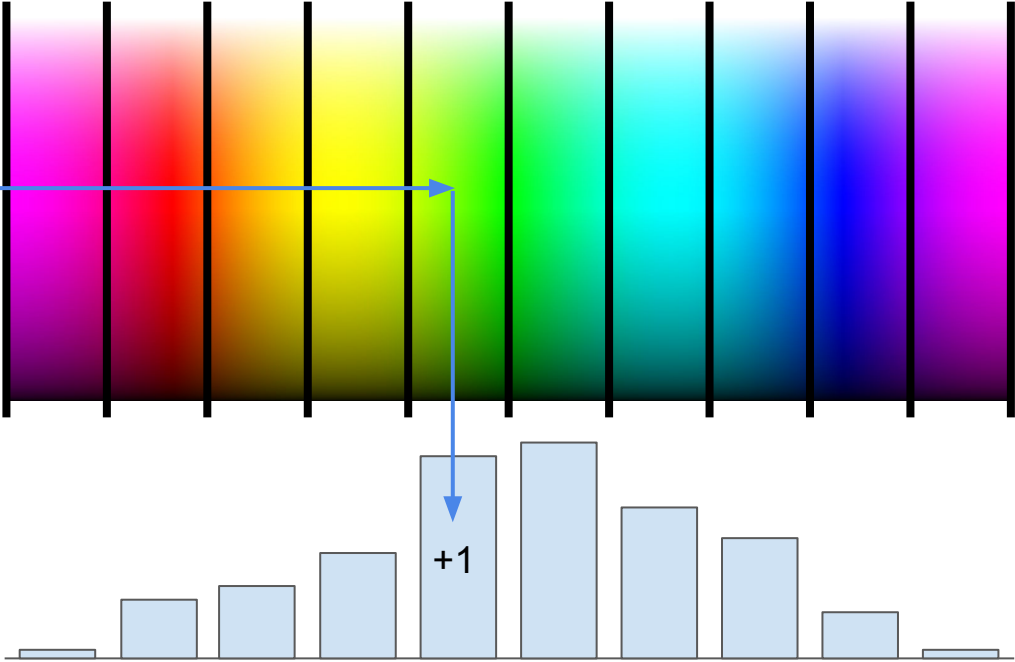
Cannot separate red and blue points with linear classifier

$$f(x, y) = (r(x, y), \theta(x, y))$$



After applying feature transform, points can be separated by linear classifier

# Example: Color Histogram

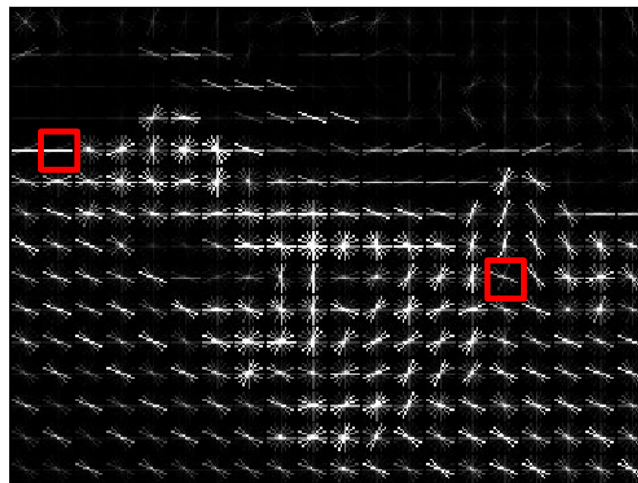




# Example: Histogram of Oriented Gradients (HoG)



Divide image into 8x8 pixel regions  
Within each region quantize edge  
direction into 9 bins



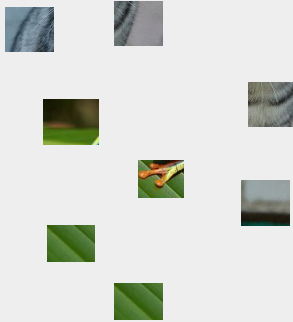
Example: 320x240 image gets divided  
into 40x30 bins; in each bin there are  
9 numbers so feature vector has  
 $30 \times 40 \times 9 = 10,800$  numbers

# Example: Bag of Words

## Step 1: Build codebook



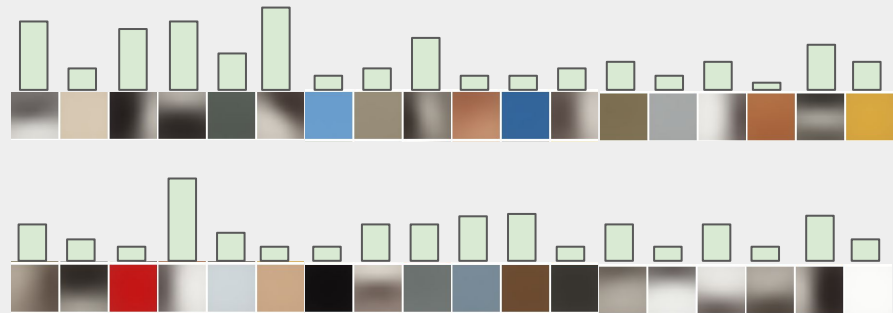
Extract random patches



Cluster patches to form "codebook" of "visual words"

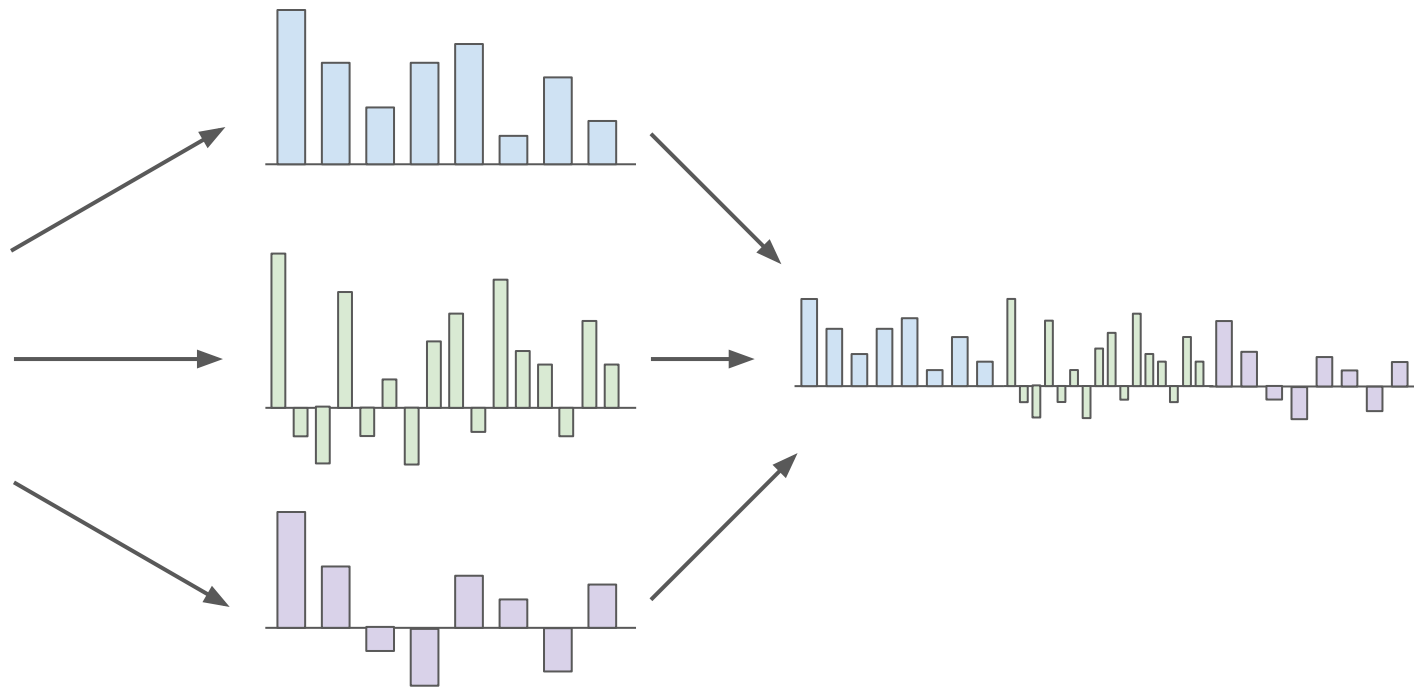


## Step 2: Encode images

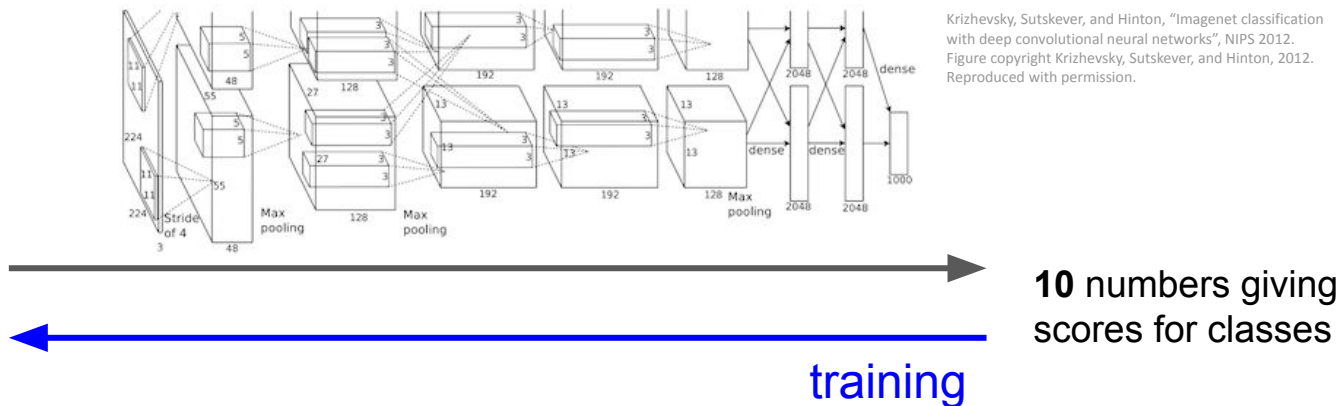
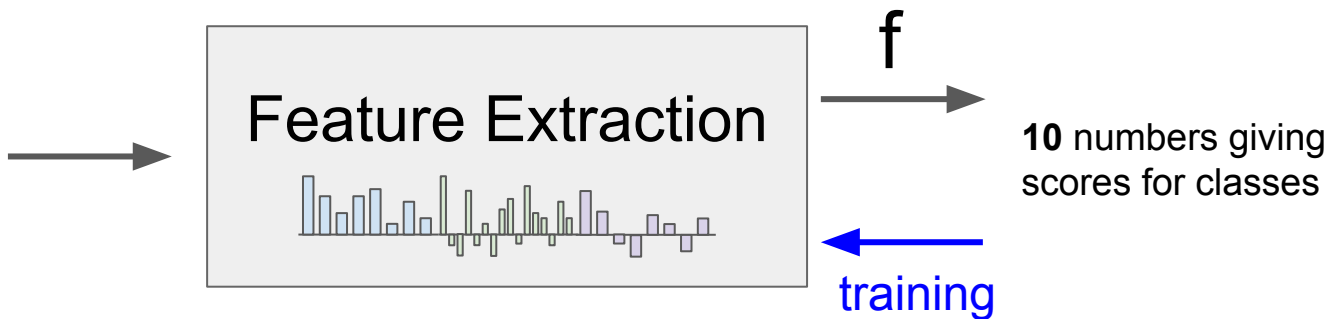


Fei-Fei and Perona, "A bayesian hierarchical model for learning natural scene categories", CVPR 2005

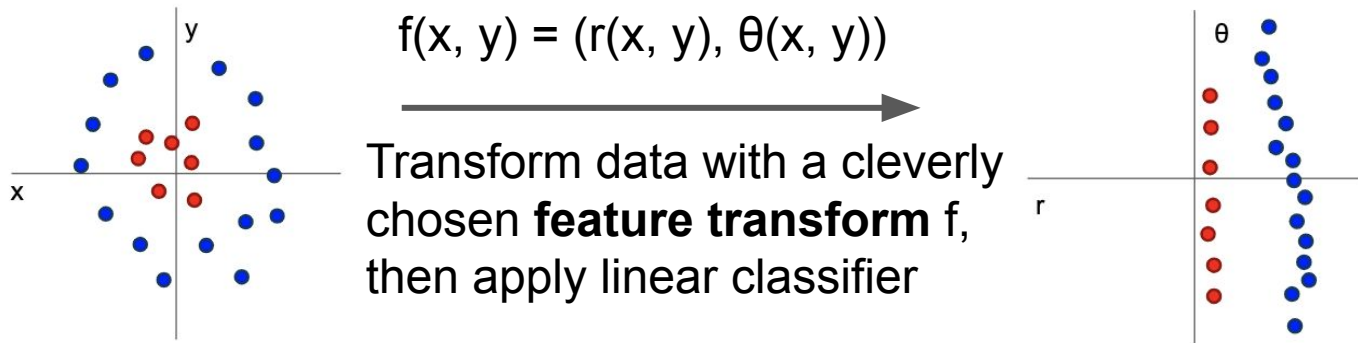
# Combine many different features if unsure which features are better



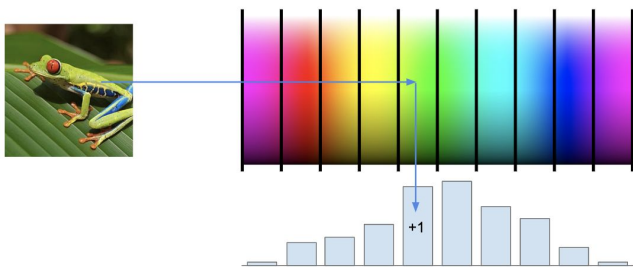
# Image features vs neural networks



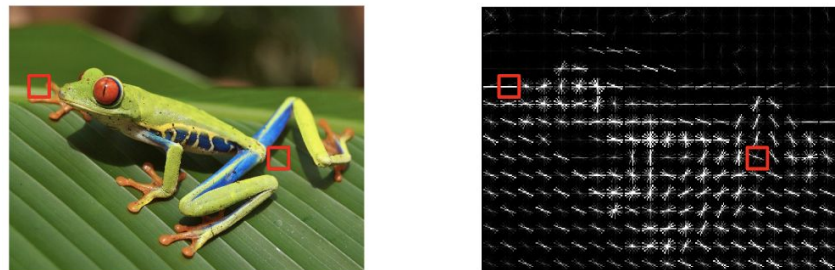
# One Solution: Non-linear feature transformation



Color Histogram



Histogram of Oriented Gradients (HoG)



# Today: Neural Networks

# Neural networks: the original linear classifier

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

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

# Neural networks: 2 layers

(**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: also called fully connected network

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

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

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

“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: 3 layers

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

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

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

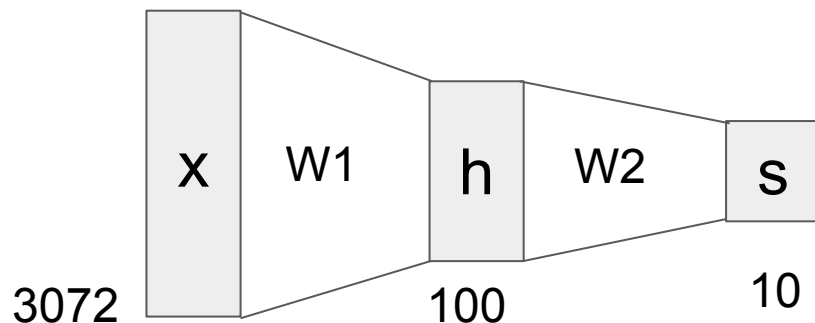
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

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

# Neural networks: hierarchical computation

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

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

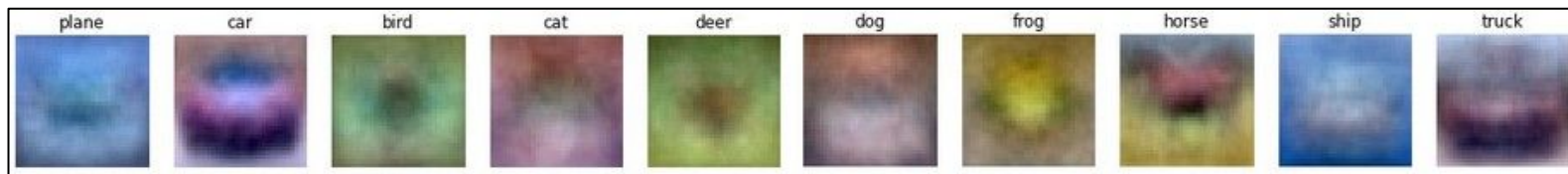
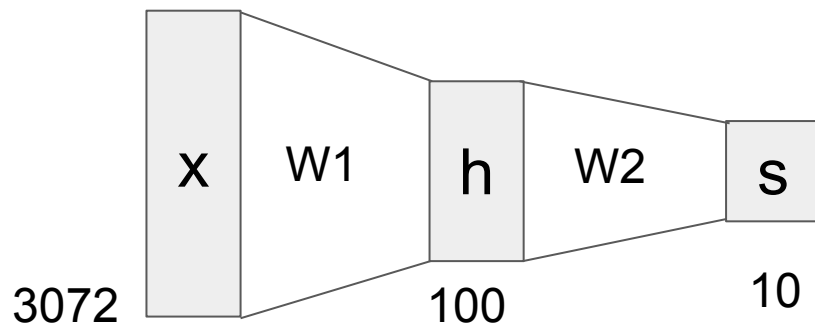


$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

# Neural networks: learning 100s of templates

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

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



Learn 100 templates instead of 10.

Share templates between classes

# Neural networks: why is max operator important?

(**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: why is max operator important?

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

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

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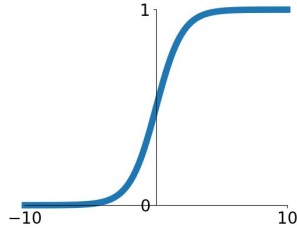
$$f = W_2 W_1 x \quad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

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

# Activation functions

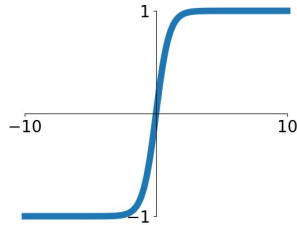
## Sigmoid

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



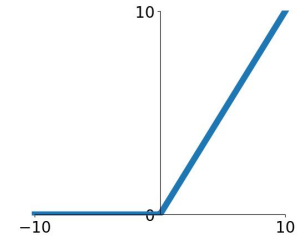
## tanh

$$\tanh(x)$$



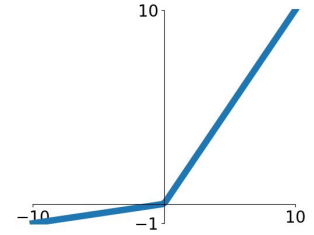
## ReLU

$$\max(0, x)$$



## Leaky ReLU

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

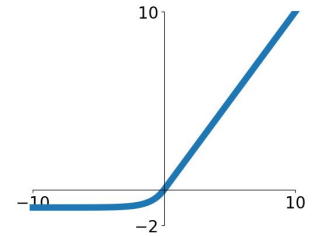


## Maxout

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

## ELU

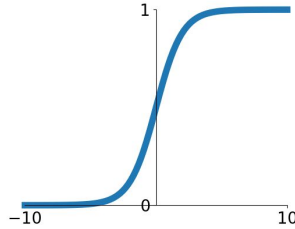
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



# Activation functions

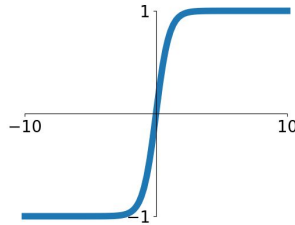
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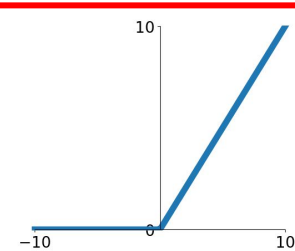
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$$\tanh(x)$$



## ReLU

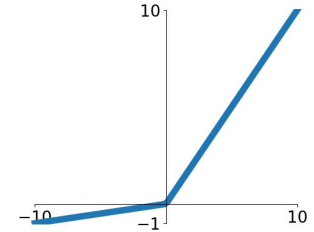
$$\max(0, x)$$



ReLU is a good default choice for most problems

## Leaky ReLU

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

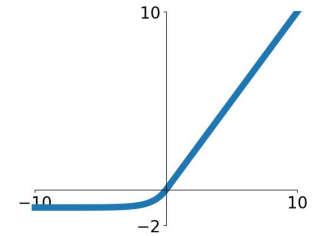


## Maxout

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

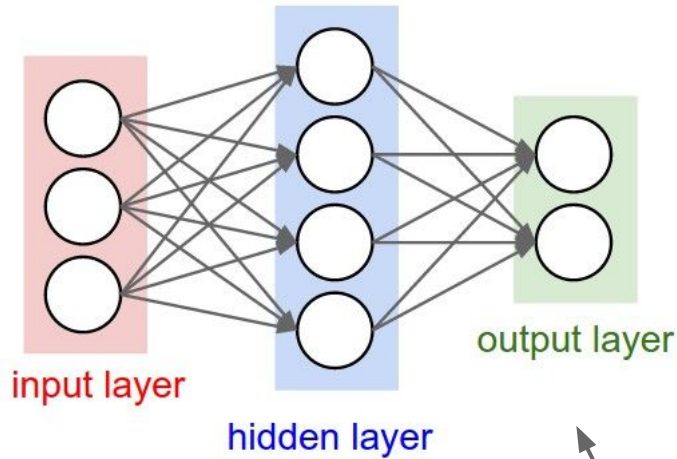
## ELU

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

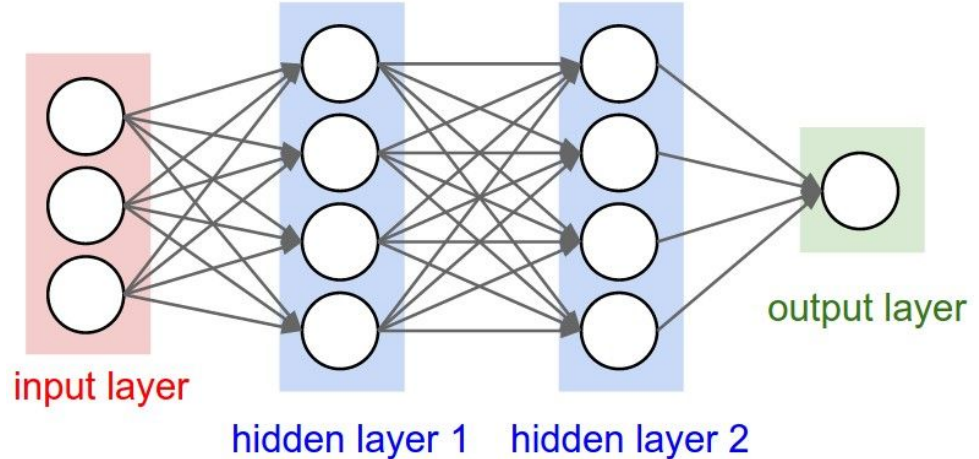




# Neural networks: Architectures



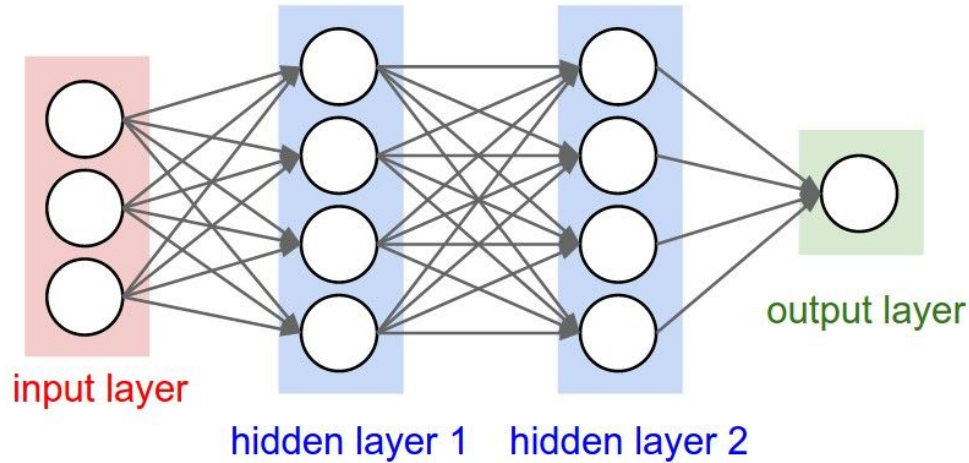
"2-layer Neural Net", or  
"1-hidden-layer Neural Net"



"3-layer Neural Net", or  
"2-hidden-layer Neural Net"

**"Fully-connected" layers**

# 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))
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19    w1 -= 1e-4 * grad_w1
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Define the network

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Forward pass

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```

Define the network

Forward pass

Calculate the analytical gradients

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```

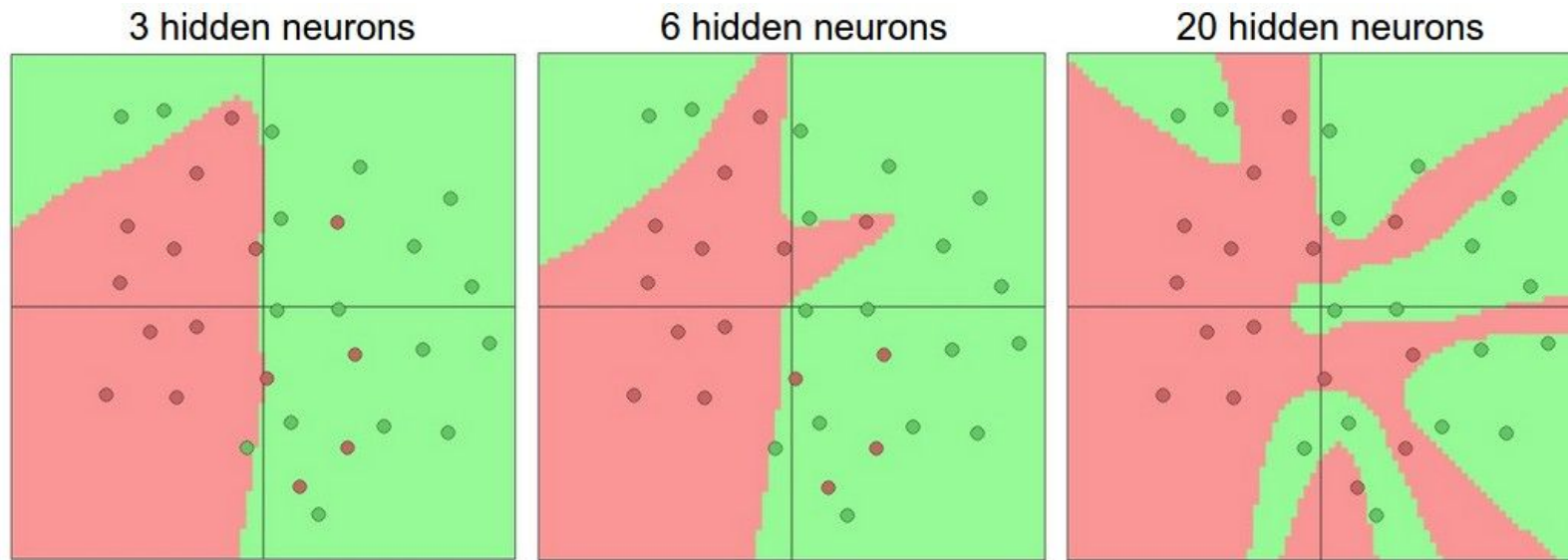
Define the network

Forward pass

Calculate the analytical gradients

Gradient descent

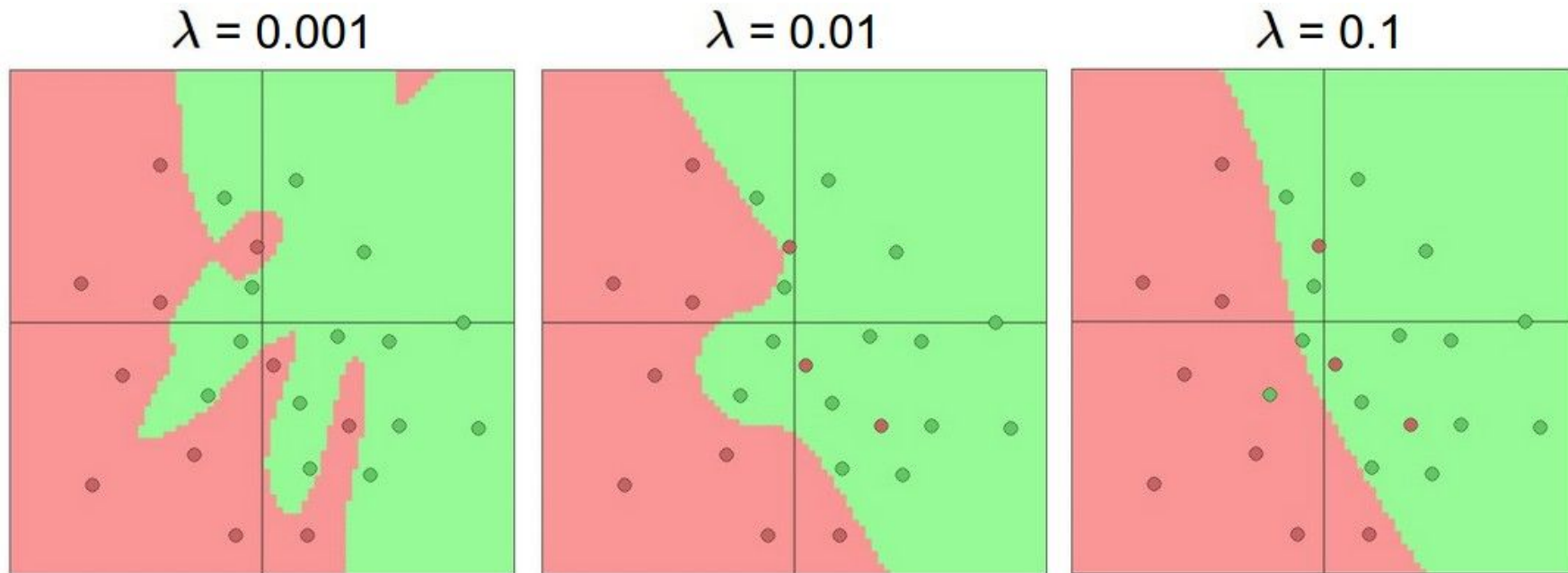
# Setting the number of layers and their sizes



more neurons = more capacity



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



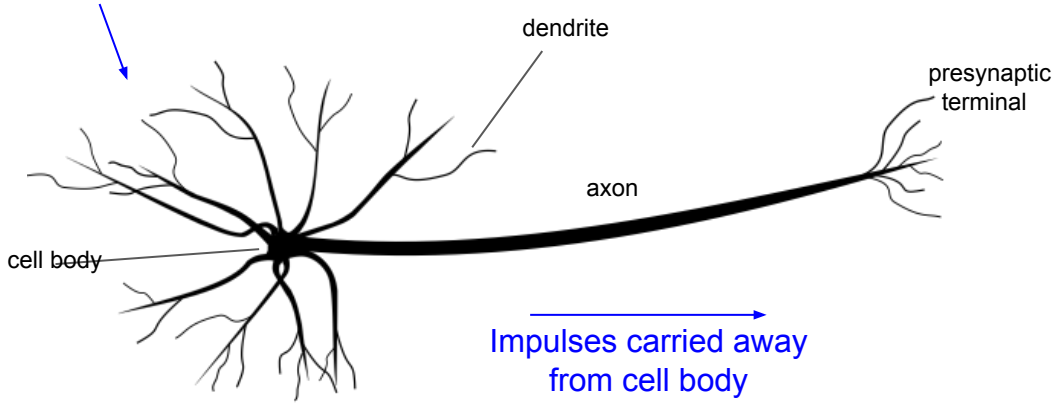
(Web demo with ConvNetJS:  
<http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html>)

$$L(W) = \frac{1}{N} \sum_{i=1}^N L_i(f(x_i, W), y_i) + \lambda R(W)$$



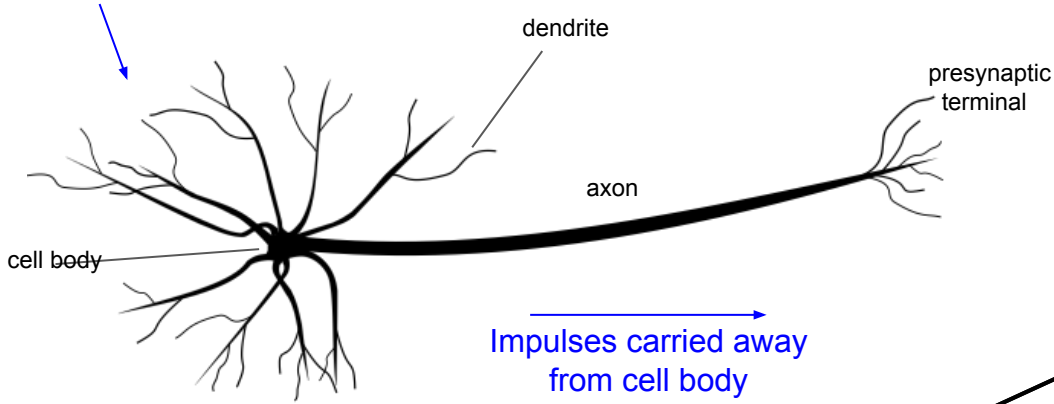
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Impulses carried toward cell body

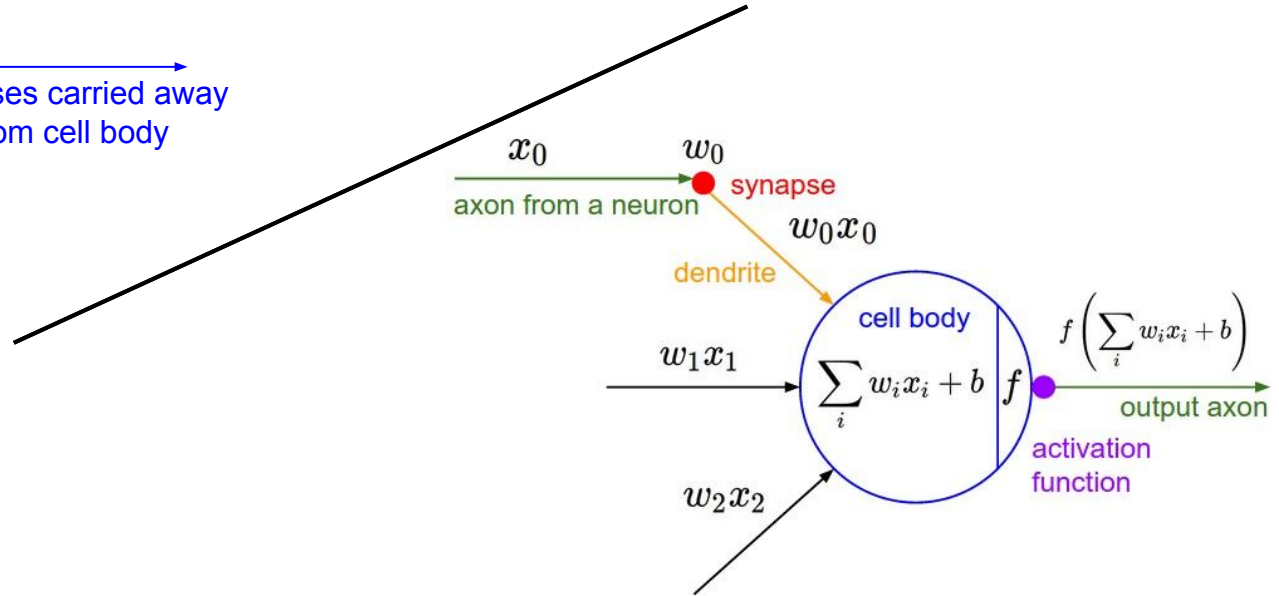


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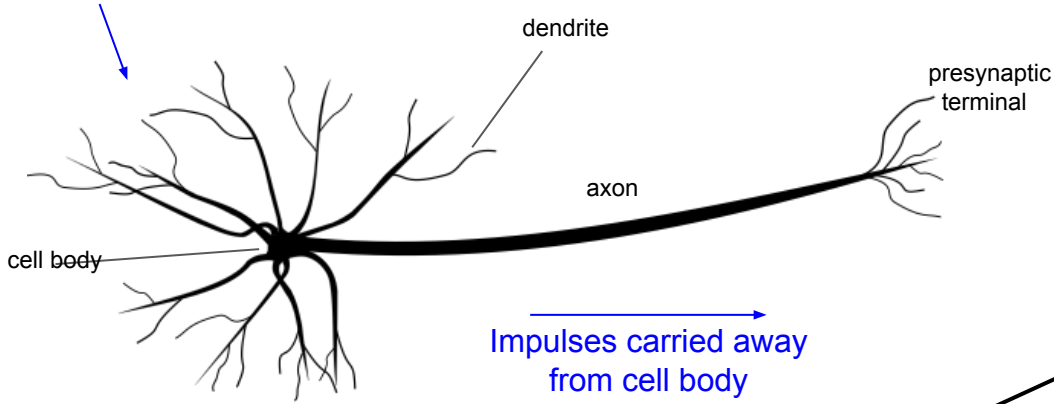
Impulses carried toward cell body



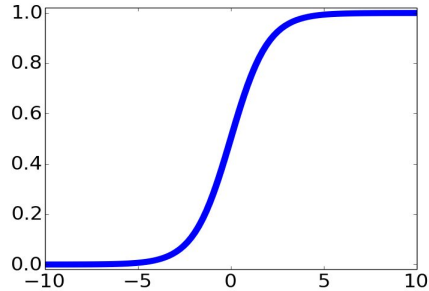
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Impulses carried toward cell body

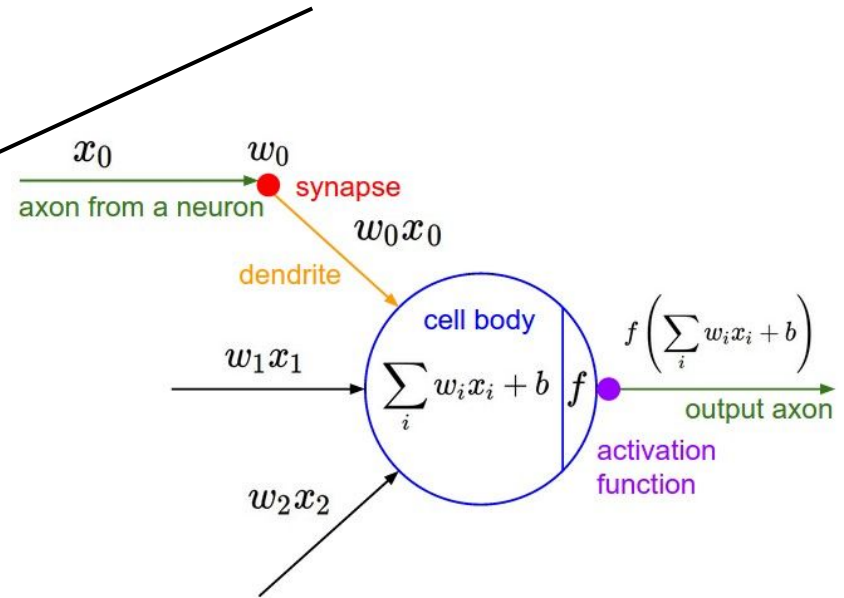


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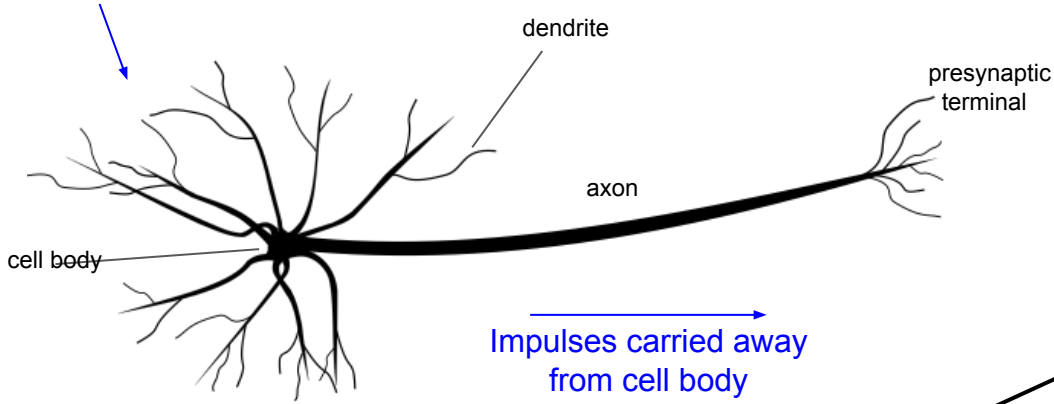


sigmoid activation function

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

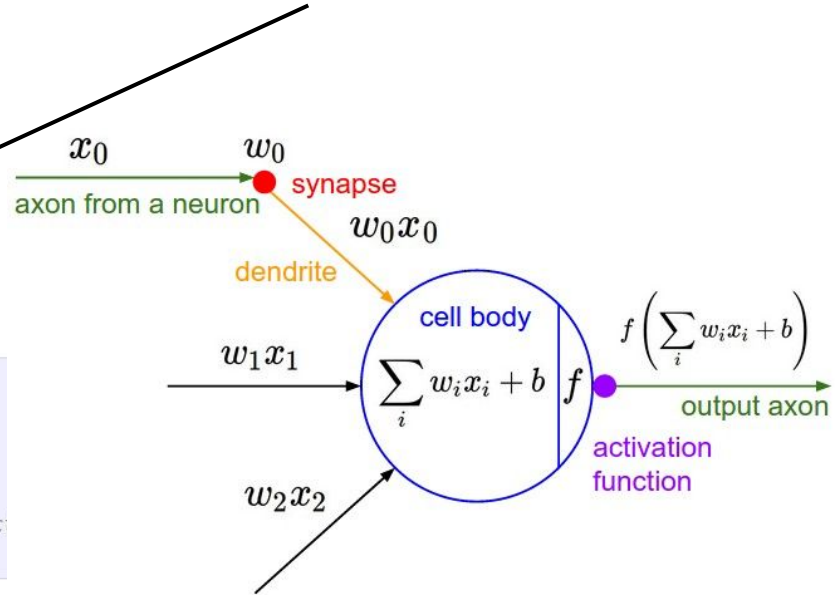


Impulses carried toward cell body

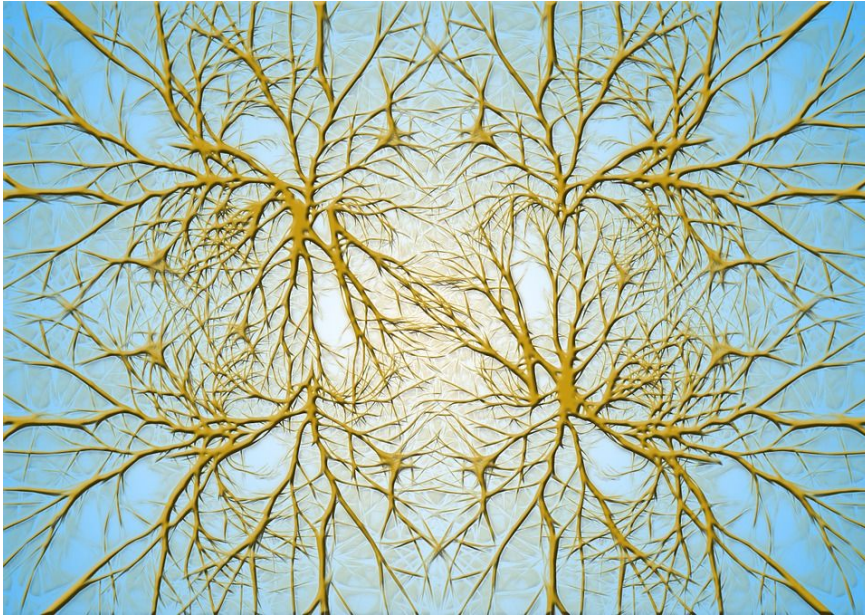


This image by Felipe Perucho is licensed under [CC-BY 3.0](https://creativecommons.org/licenses/by/3.0/)

```
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
```

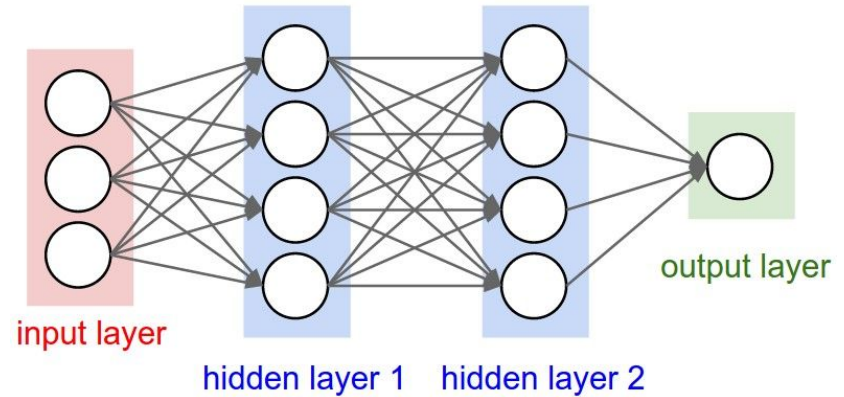


## Biological Neurons: Complex connectivity patterns

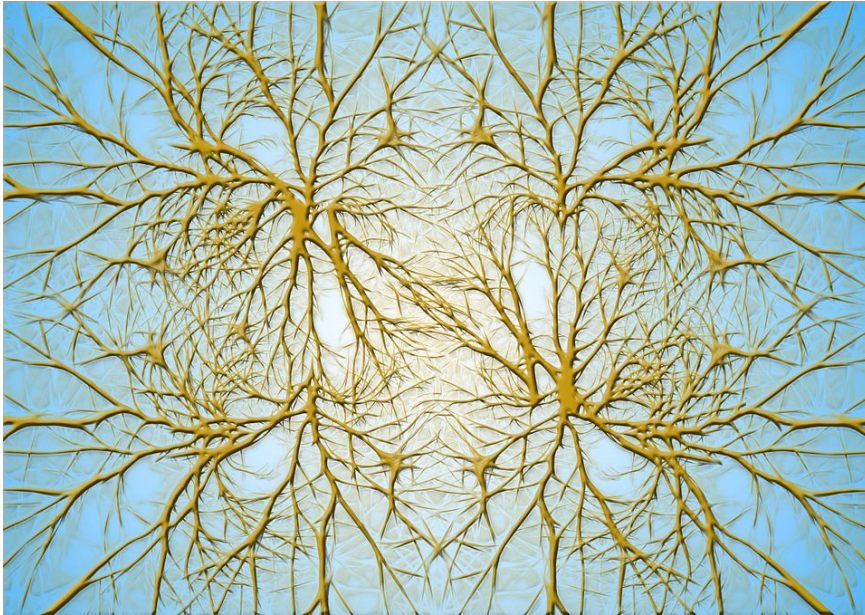


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## Neurons in a neural network: Organized into regular layers for computational efficiency

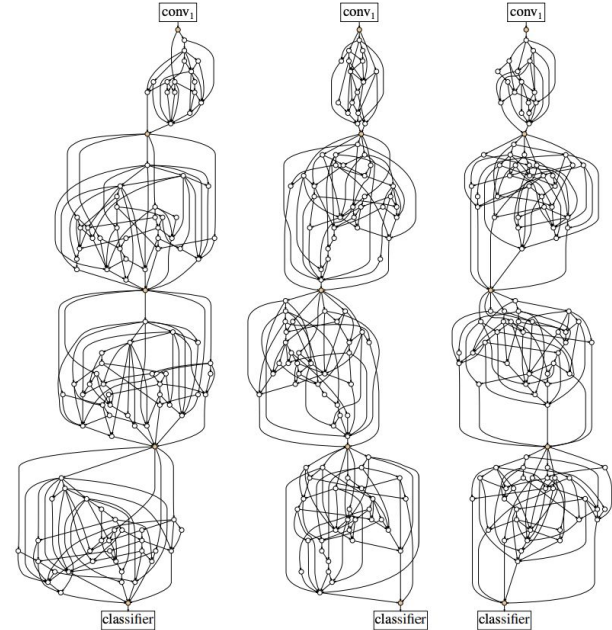


## Biological Neurons: Complex connectivity patterns



[This image](#) is [CC0 Public Domain](#)

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

[Dendritic Computation. London and Hausser]

# Plugging in neural networks with loss functions

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

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

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

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

# 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

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

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

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

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

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

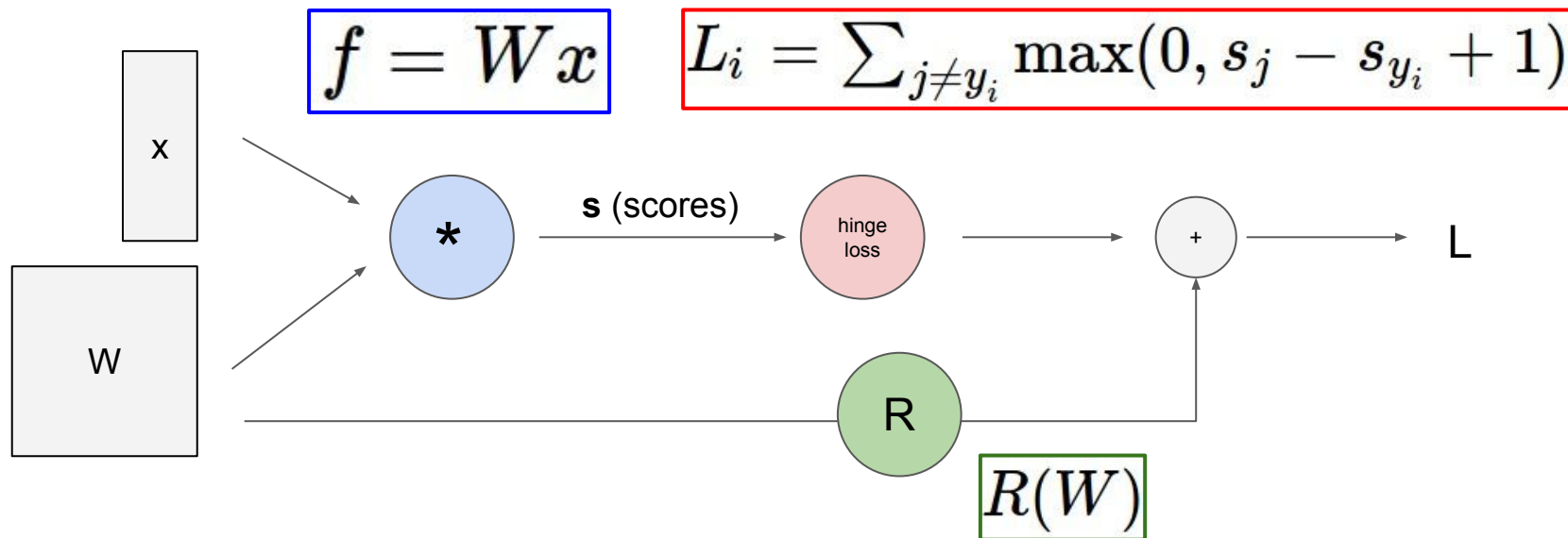
$$\nabla_W L = \nabla_W \left( \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

**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

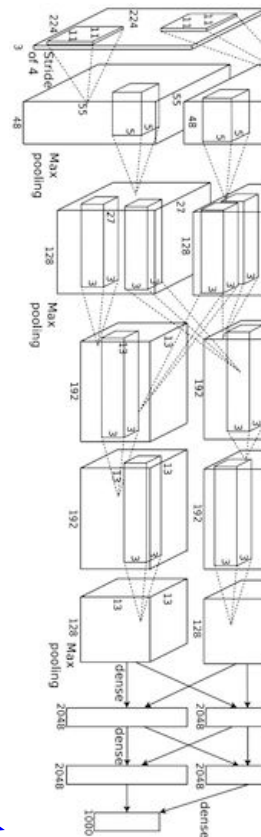


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

# Really complex neural networks!!

input image

loss

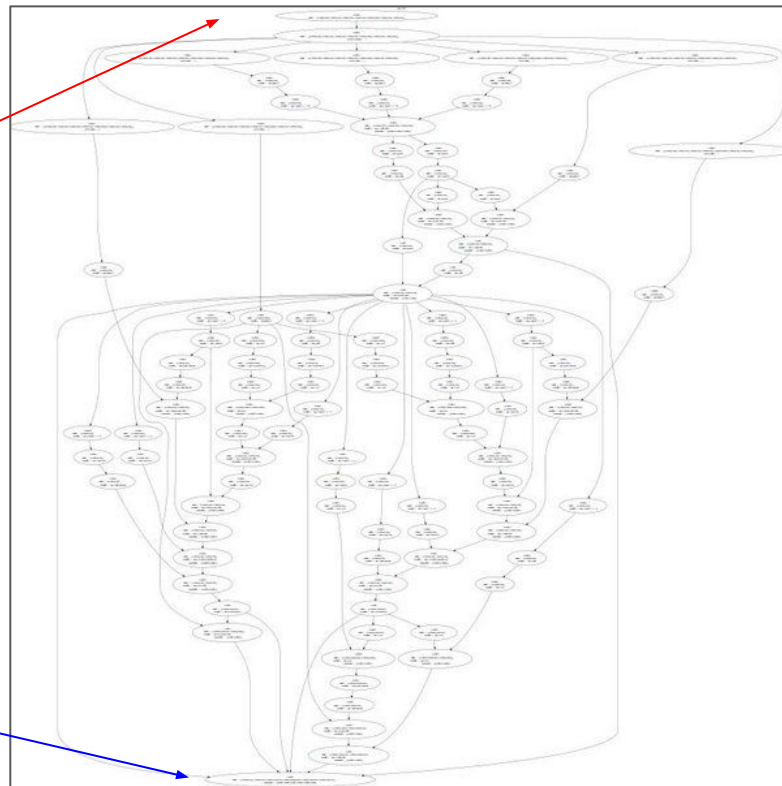


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

# Solution: Backpropagation

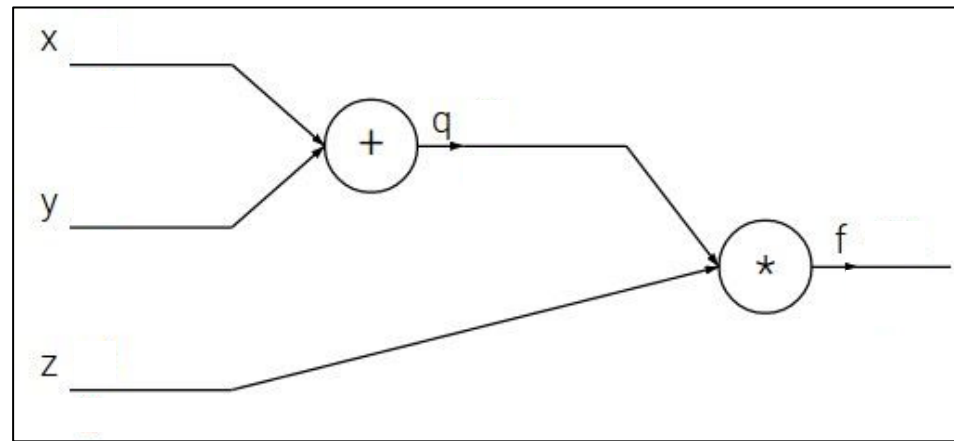


## Backpropagation: a simple example

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

# Backpropagation: a simple example

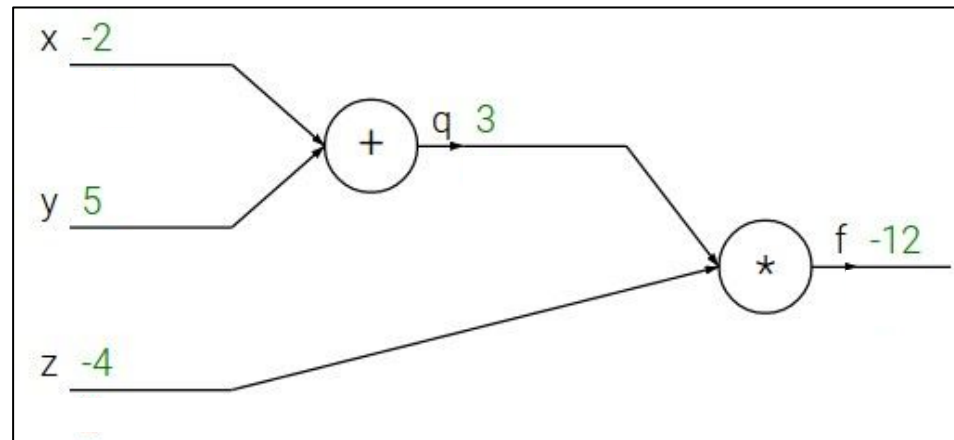
$$f(x, y, z) = (x + y)z$$



## Backpropagation: a simple example

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

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

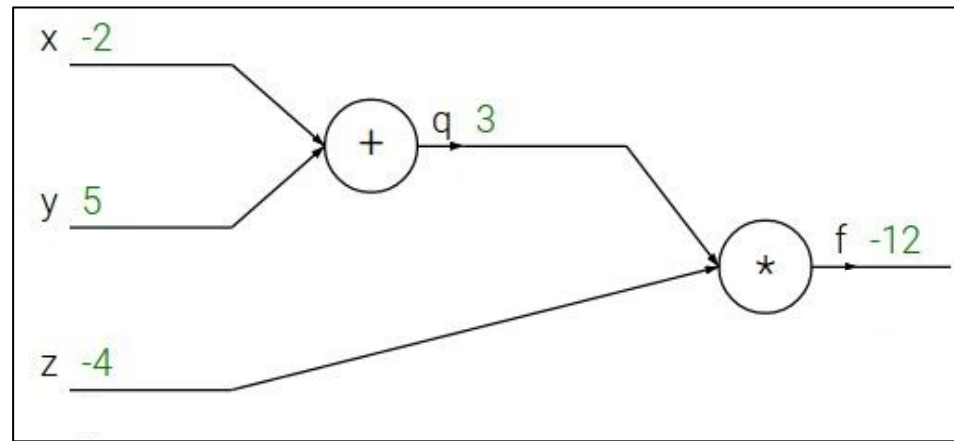


## Backpropagation: a simple example

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

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

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



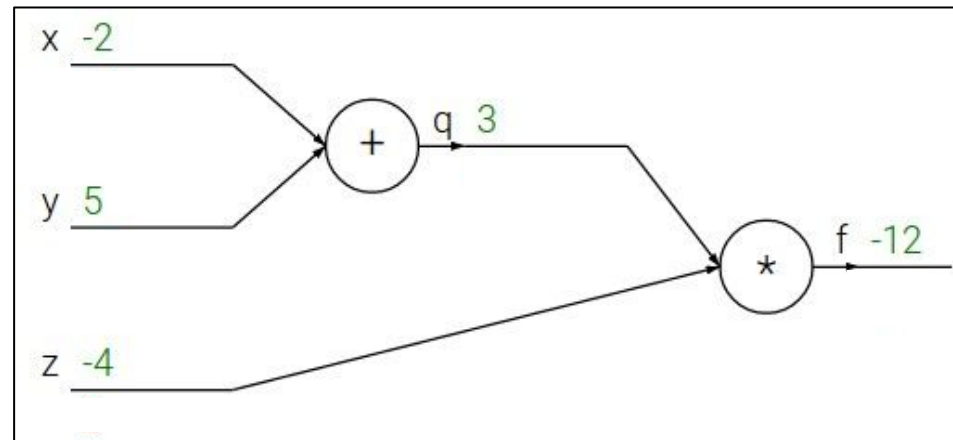
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## Backpropagation: a simple example

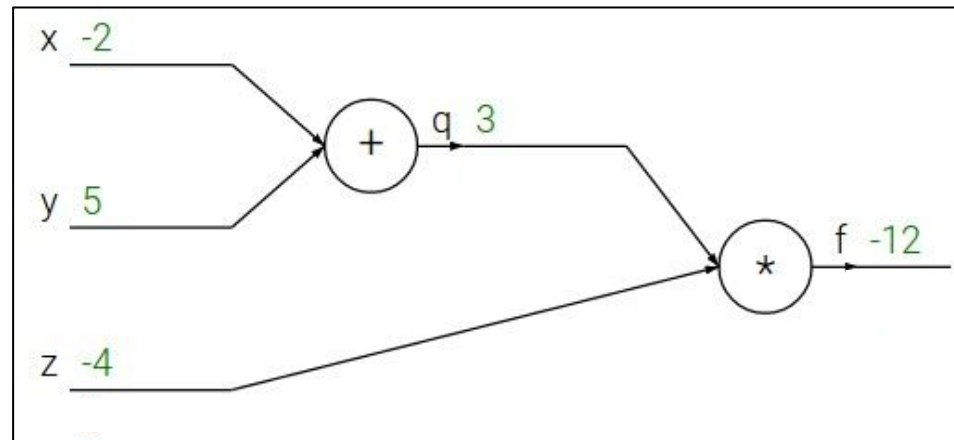
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$$\text{Want: } \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$



## Backpropagation: a simple example

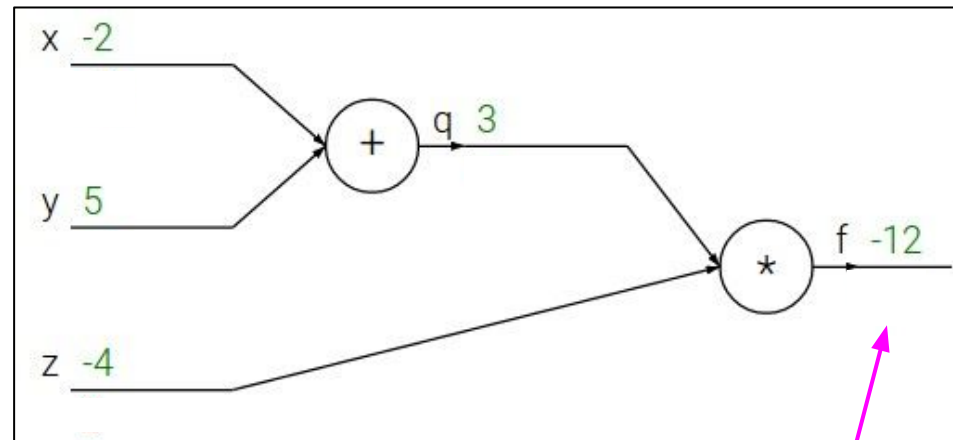
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$$\frac{\partial f}{\partial f}$$

## Backpropagation: a simple example

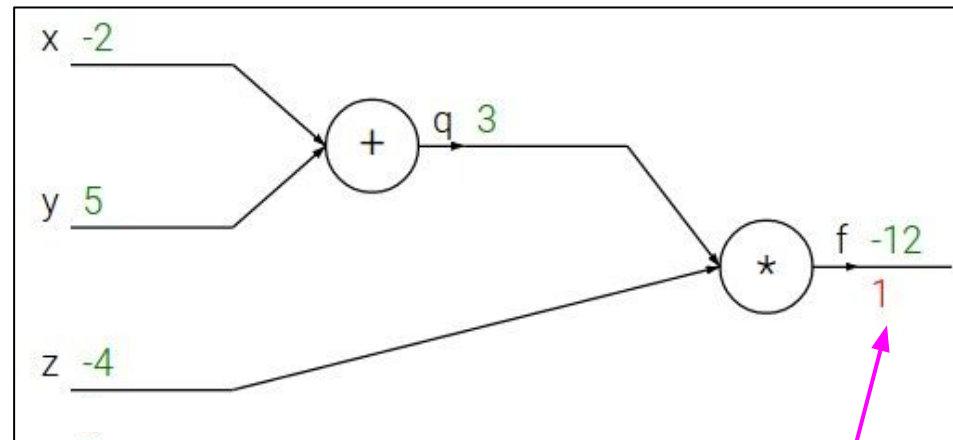
$$f(x, y, z) = (x + y)z$$

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



## Backpropagation: a simple example

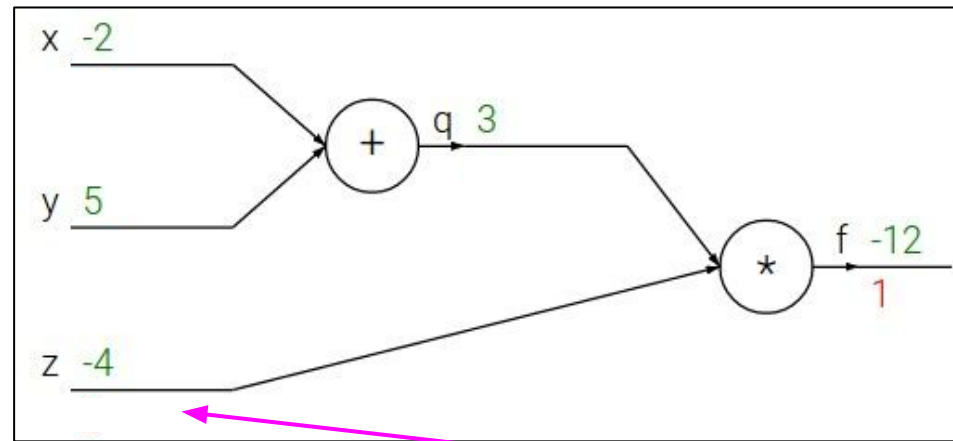
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$$\frac{\partial f}{\partial z}$$

## Backpropagation: a simple example

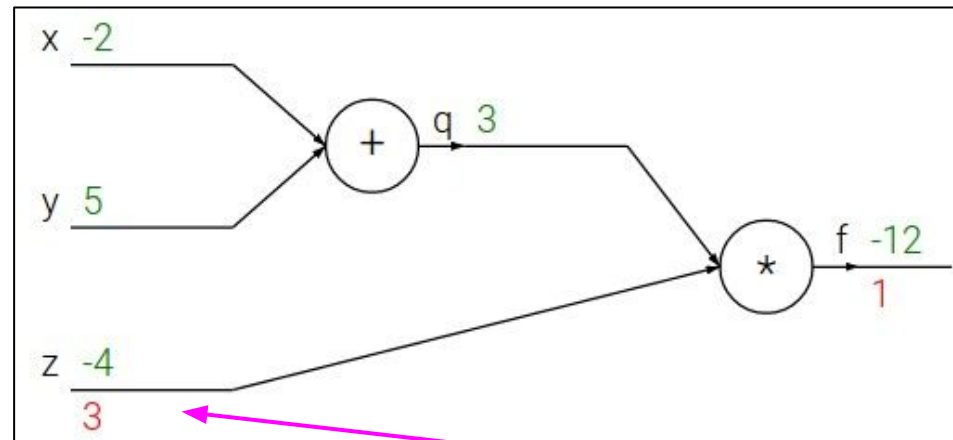
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$$\text{Want: } \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$$



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

## Backpropagation: a simple example

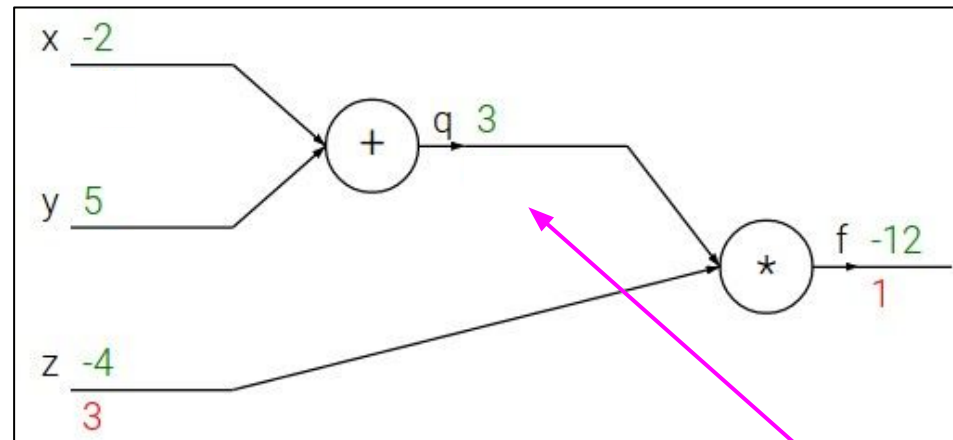
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$$\frac{\partial f}{\partial q}$$

## Backpropagation: a simple example

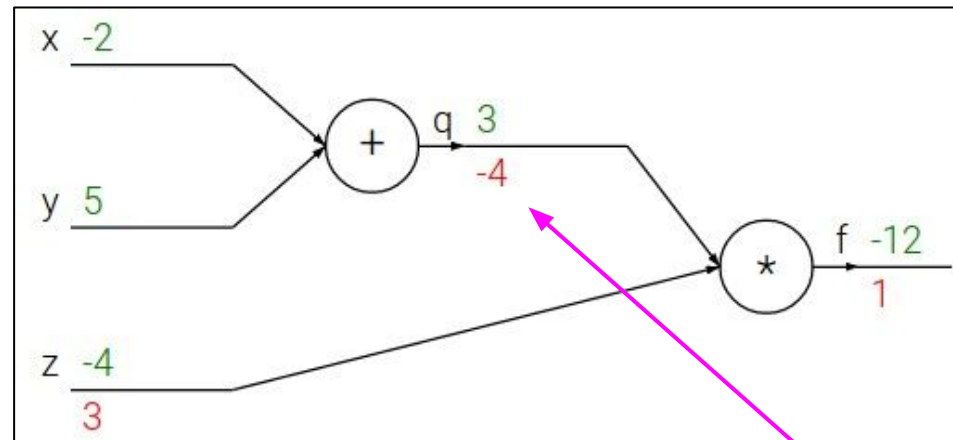
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$$\frac{\partial f}{\partial q}$$

# Backpropagation: a simple example

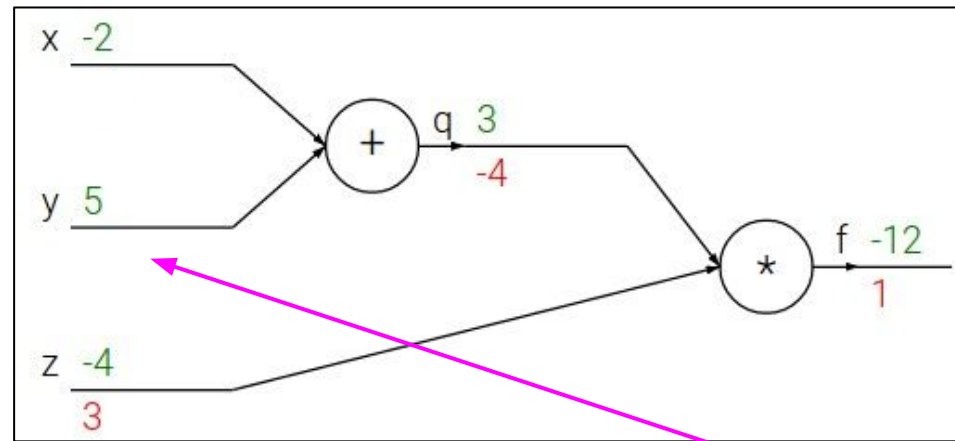
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$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

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

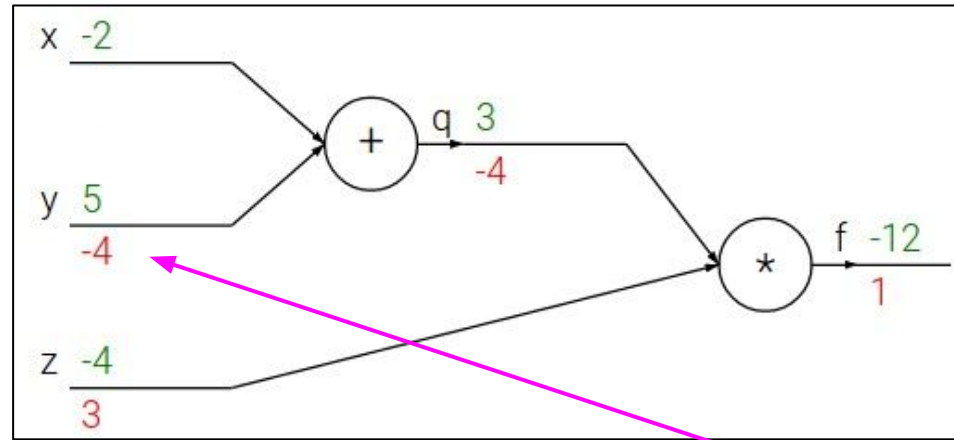
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$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

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

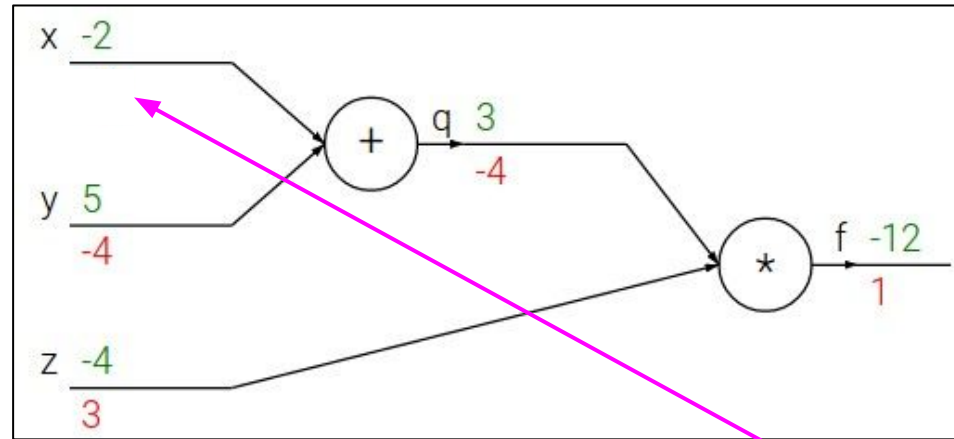
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Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

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

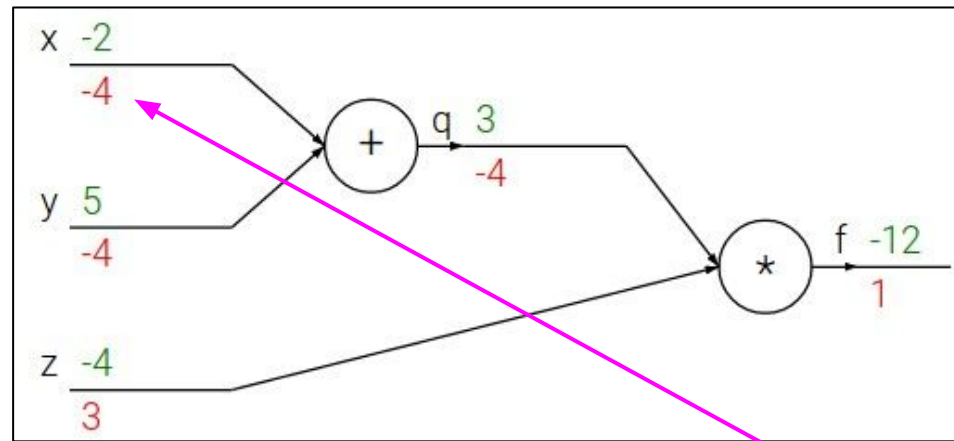
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Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

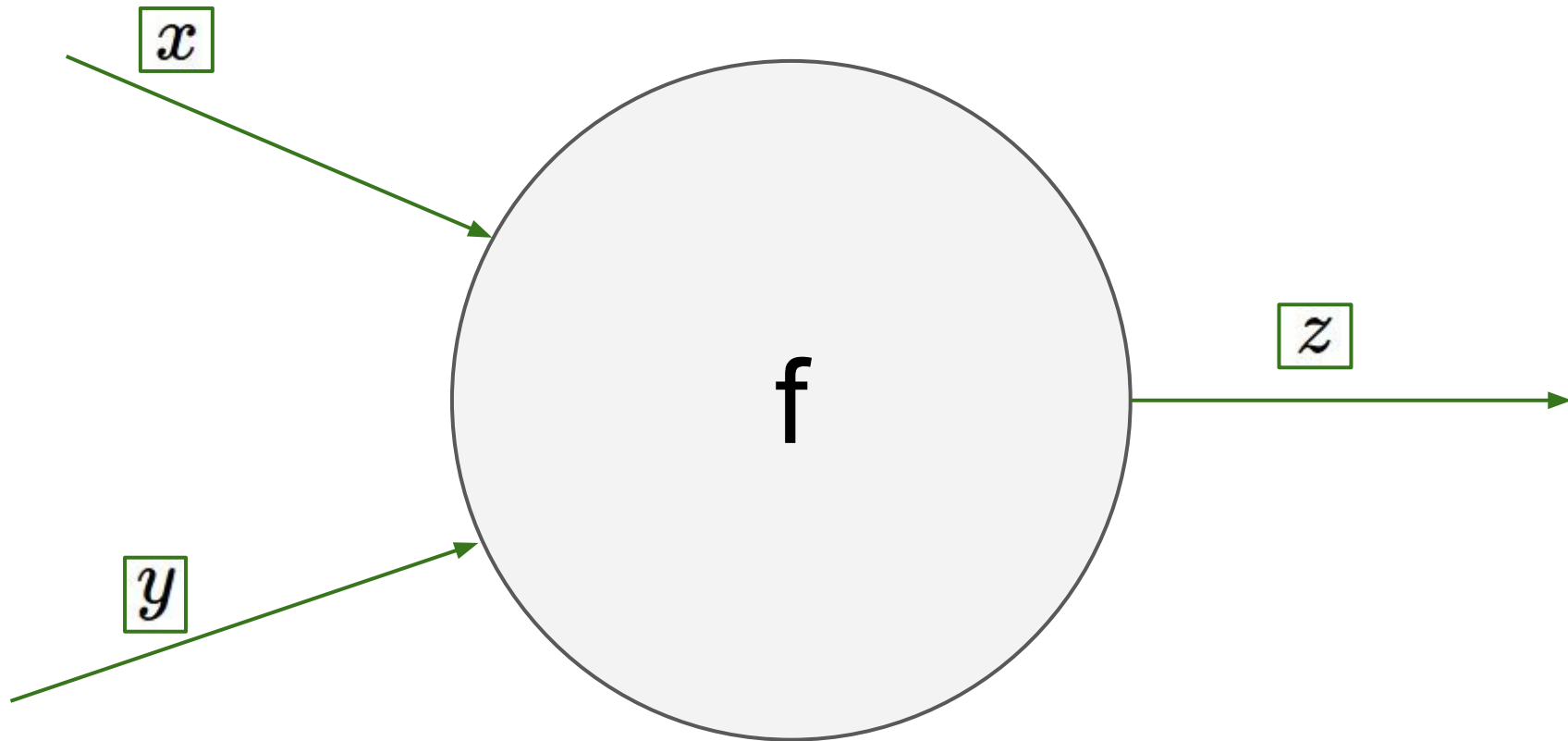
Chain rule:

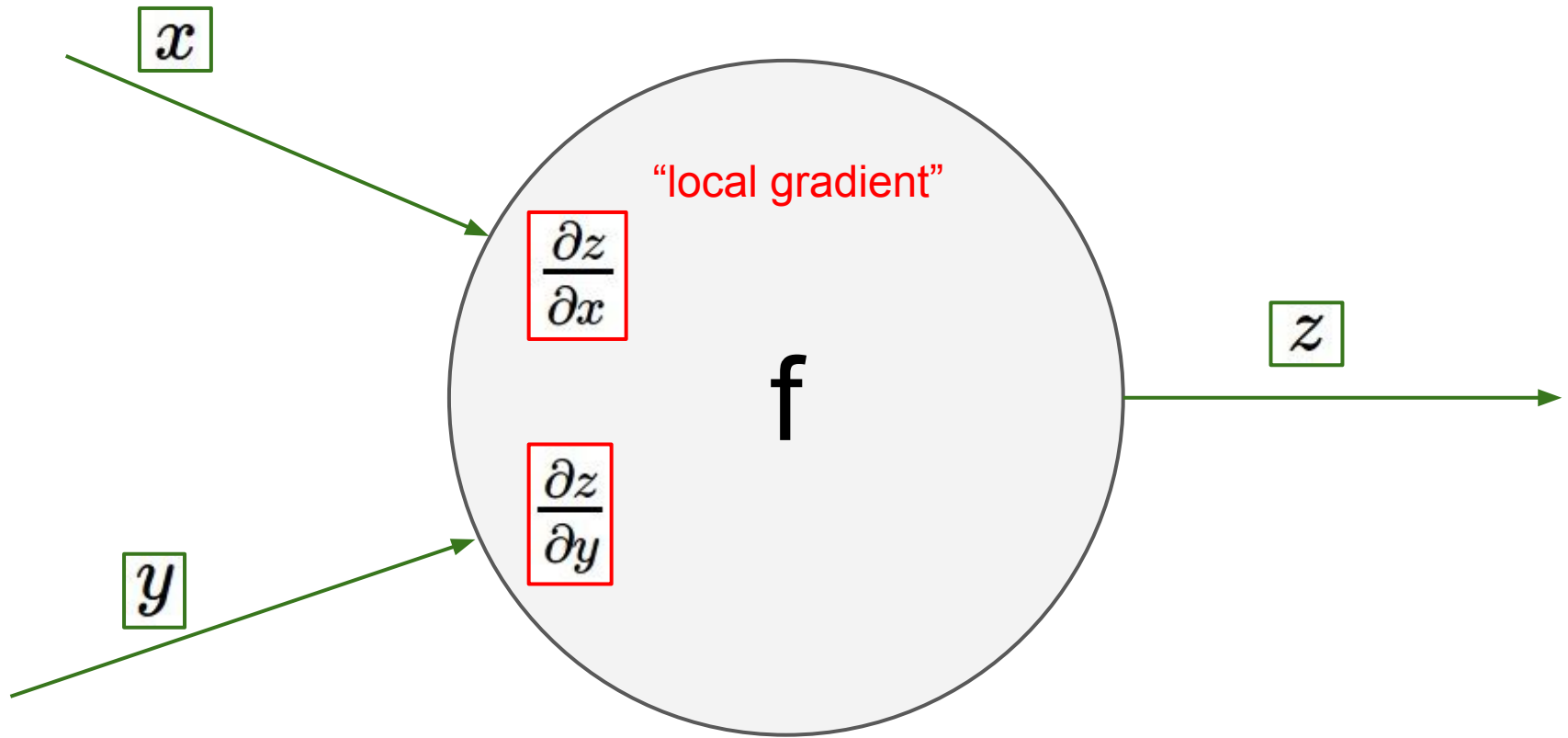
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

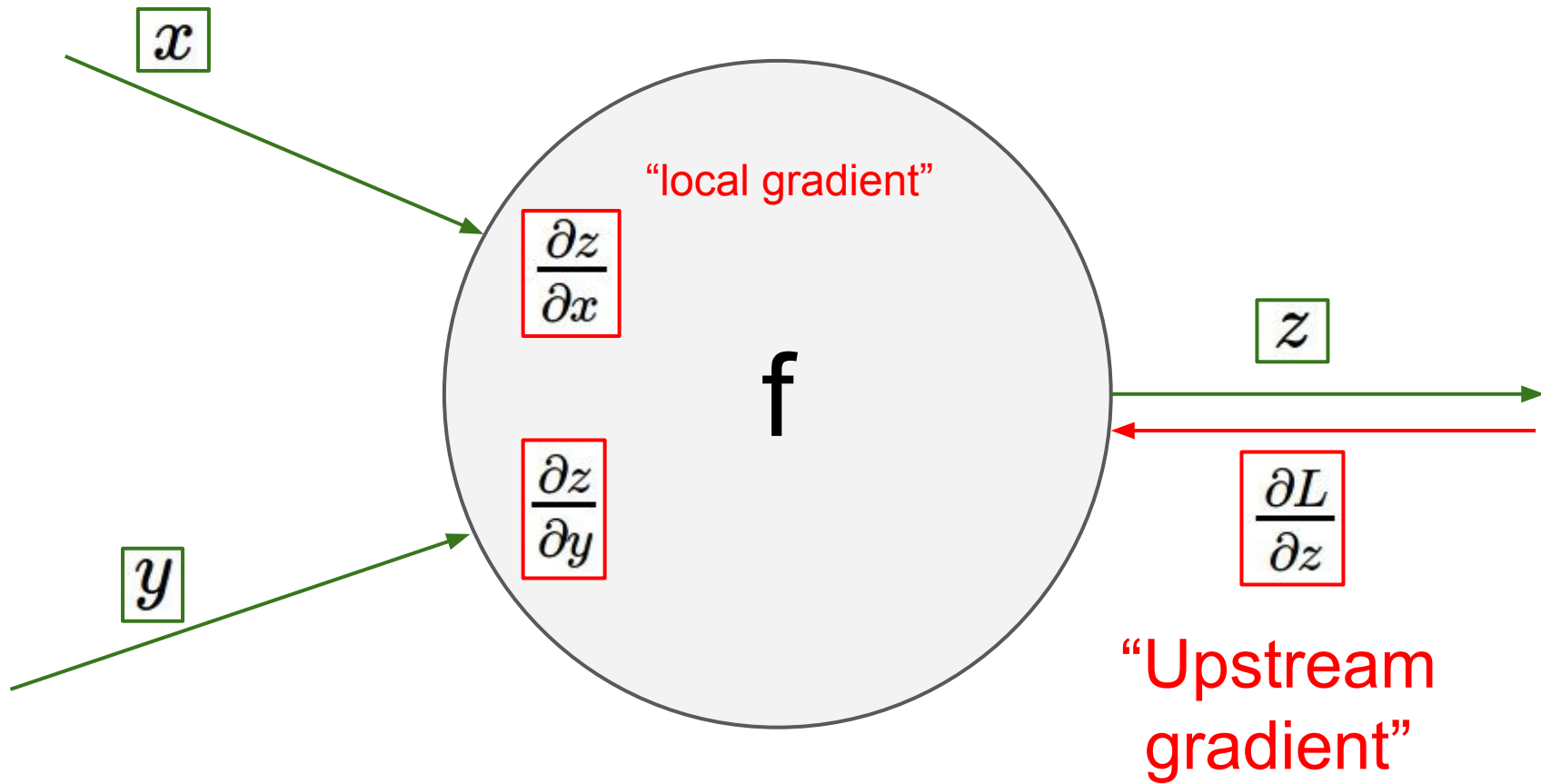
Upstream gradient

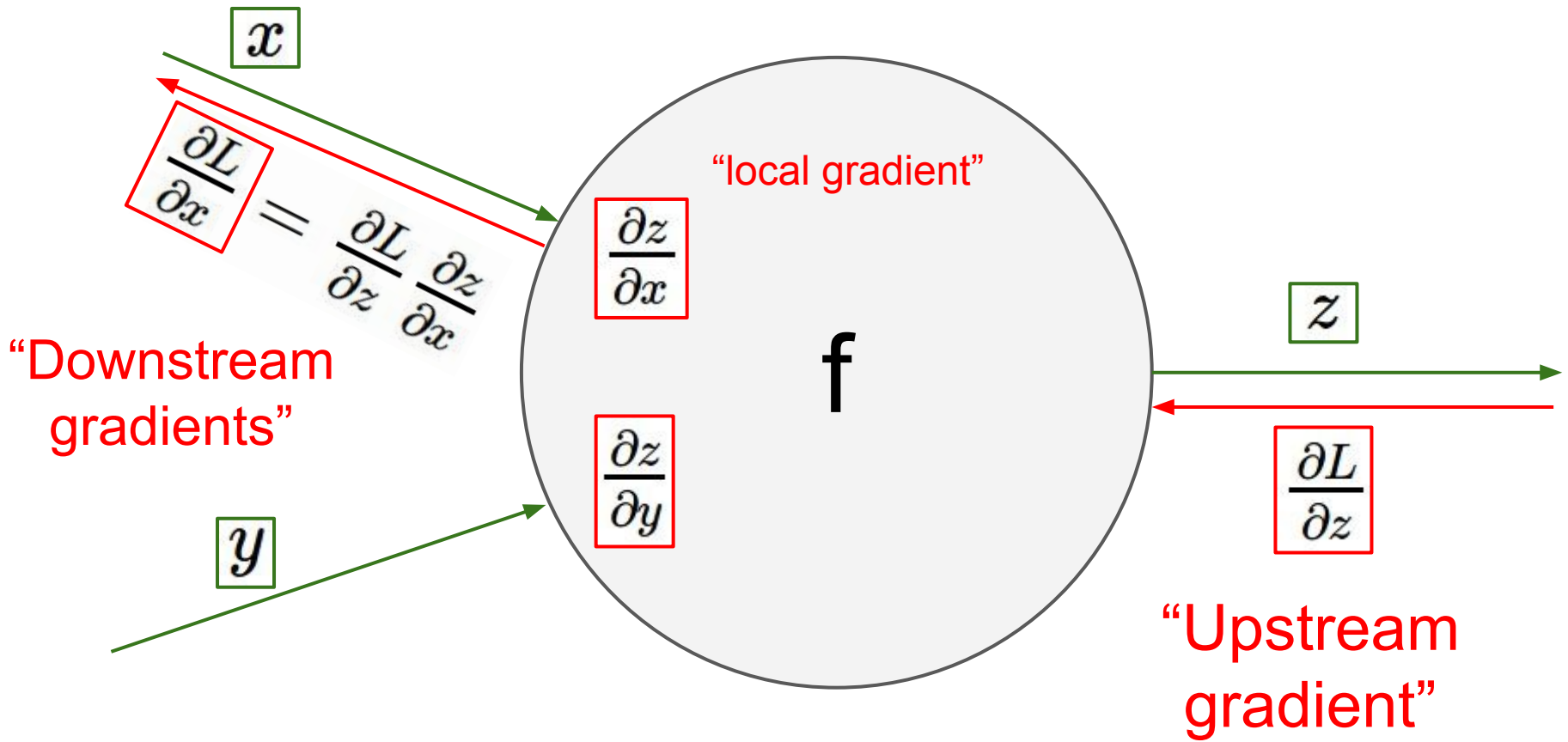
Local gradient

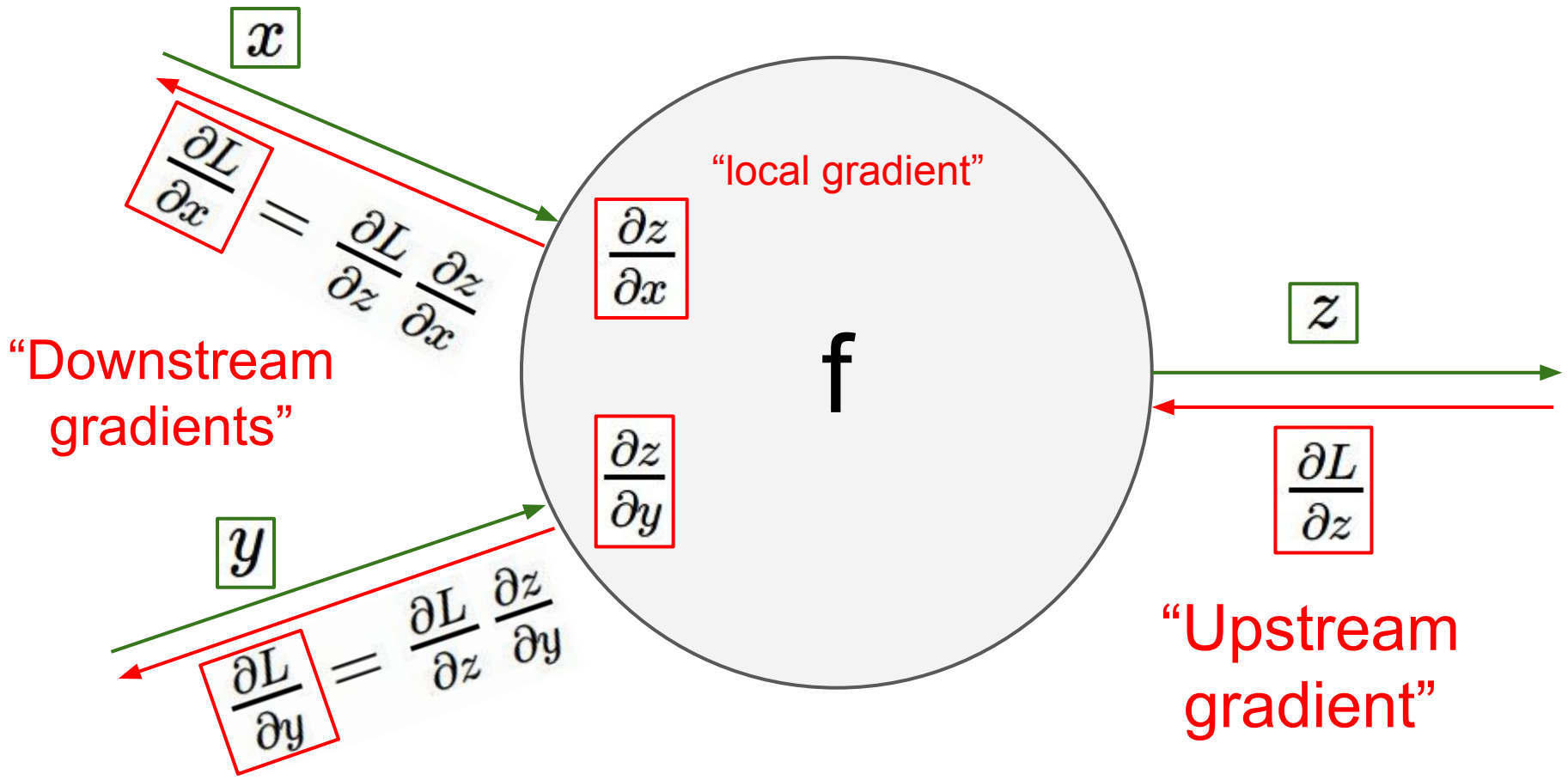


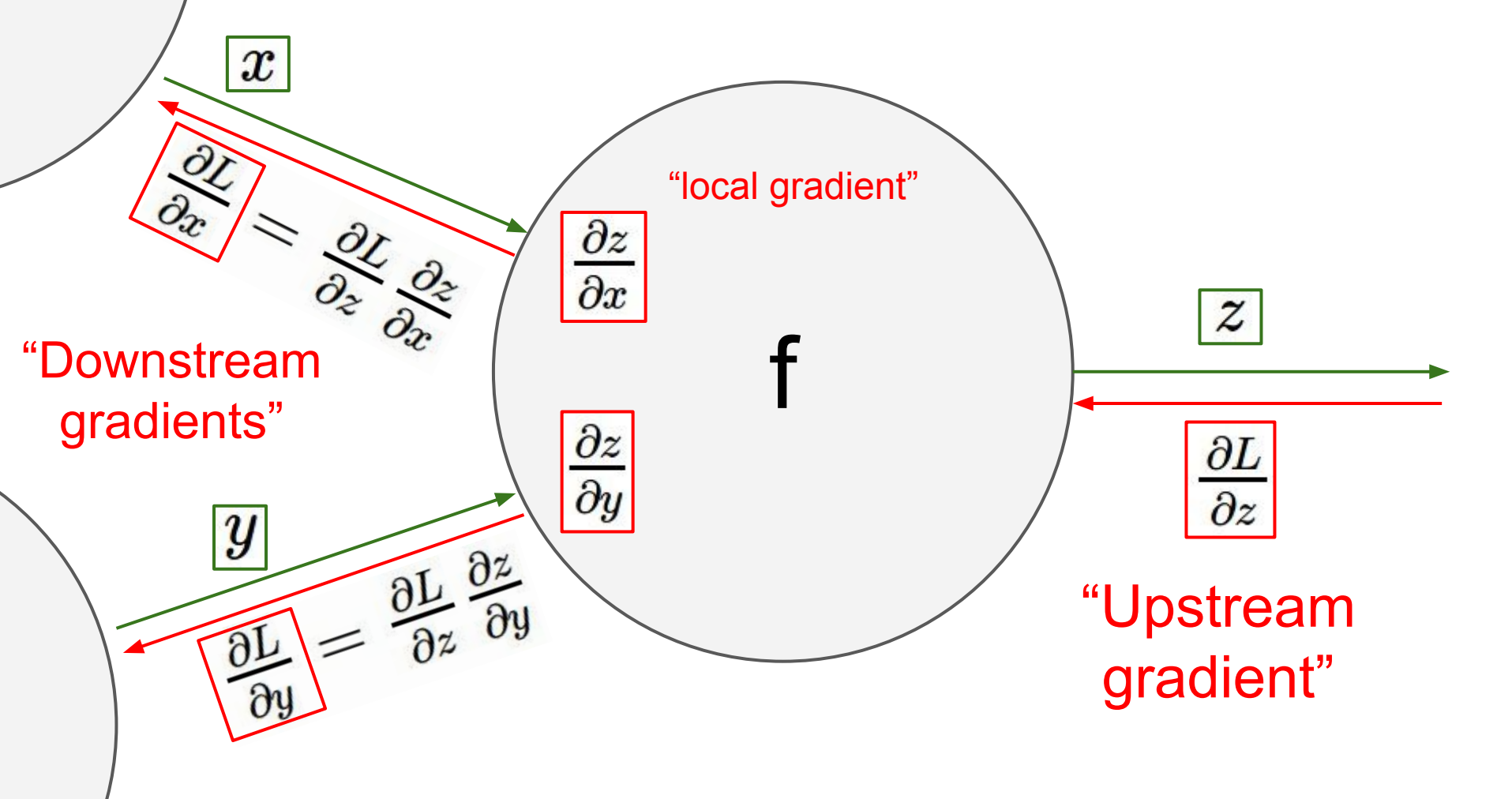






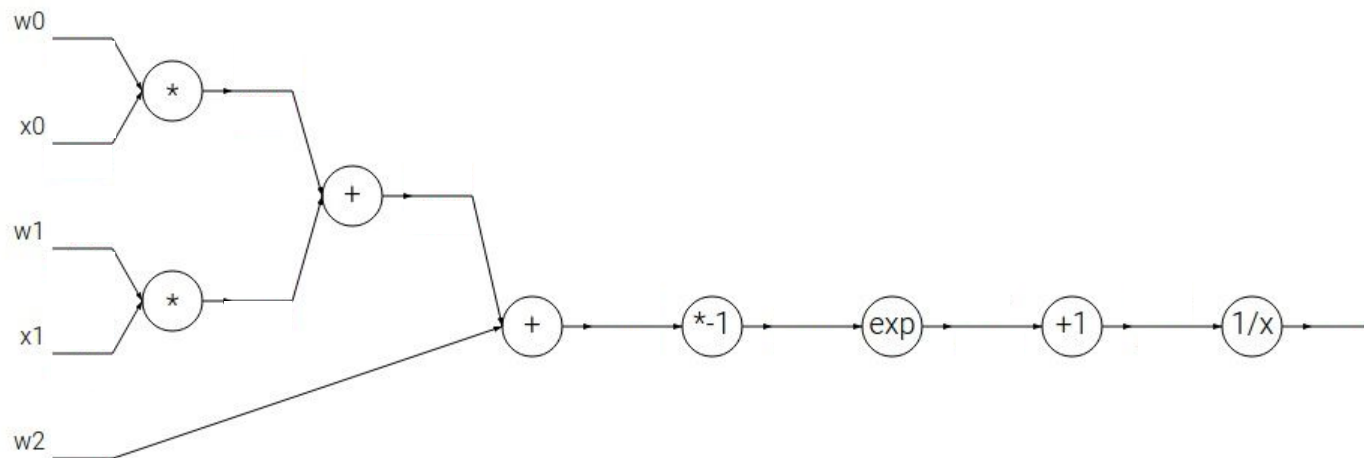






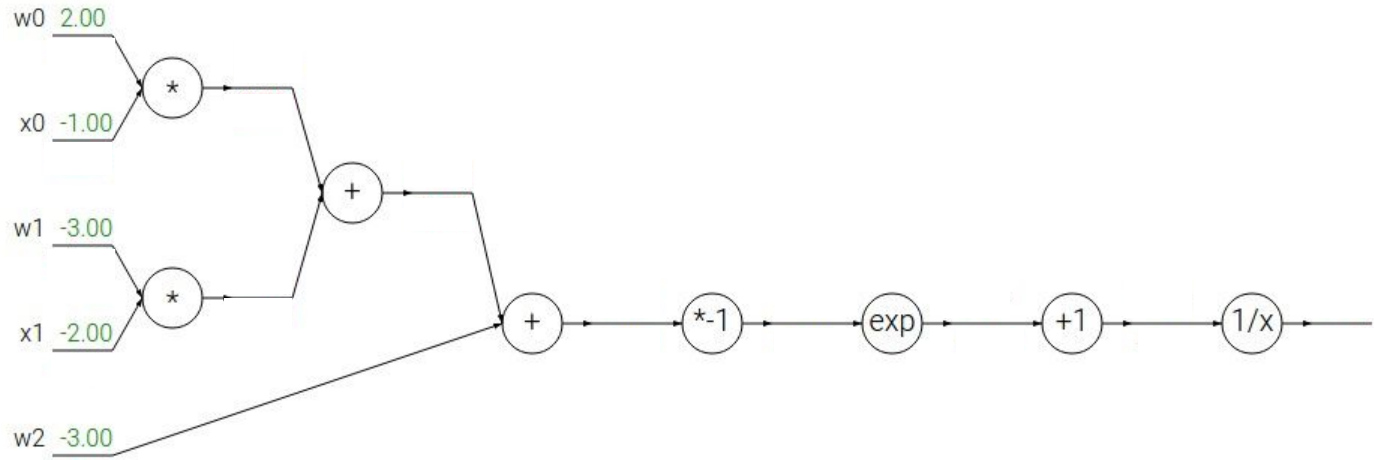
Another example:

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



Another example:

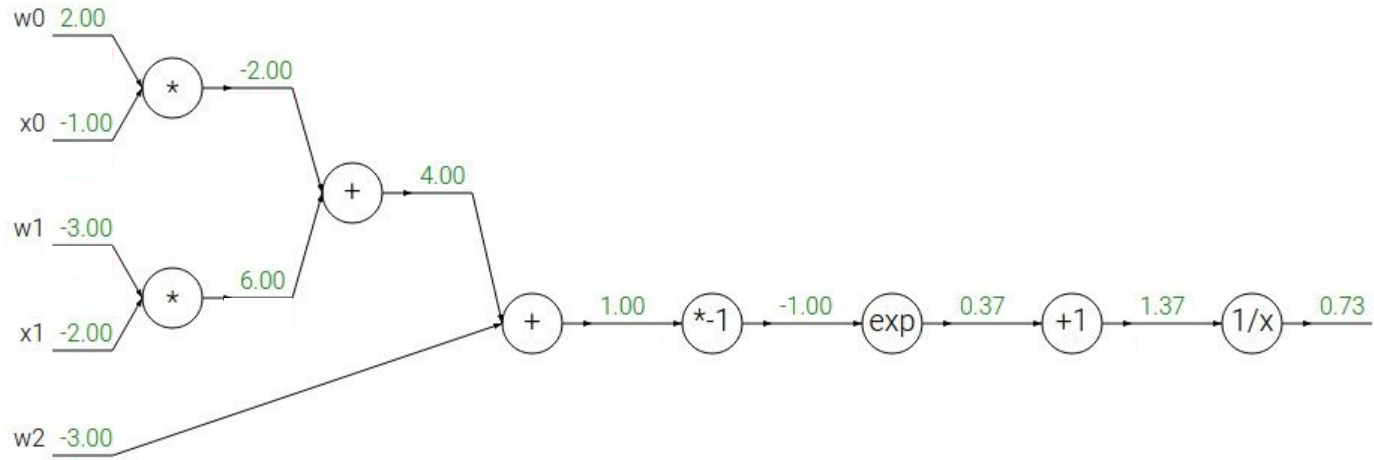
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$





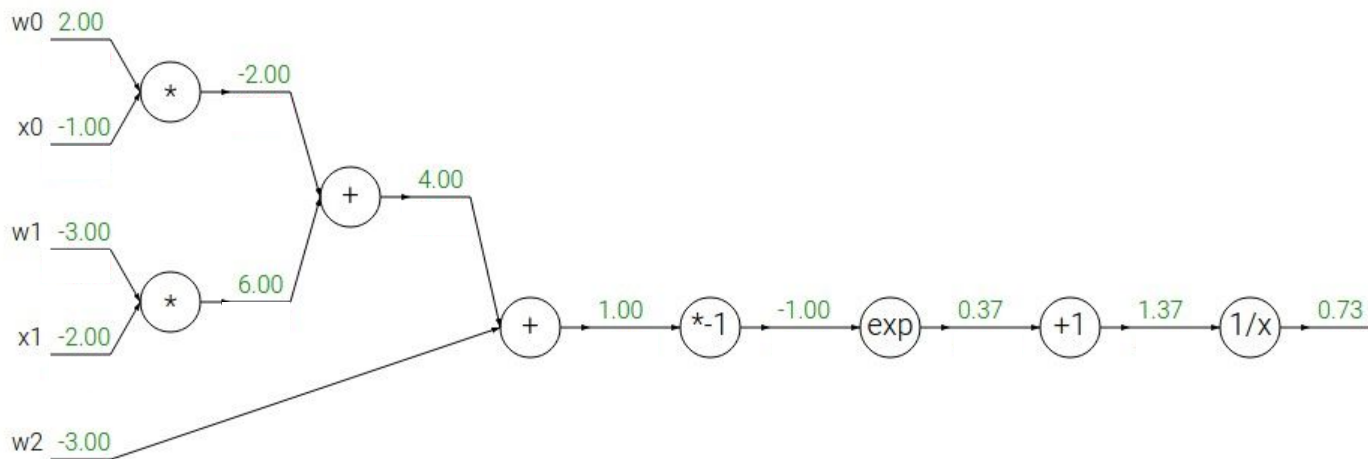
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Another example:

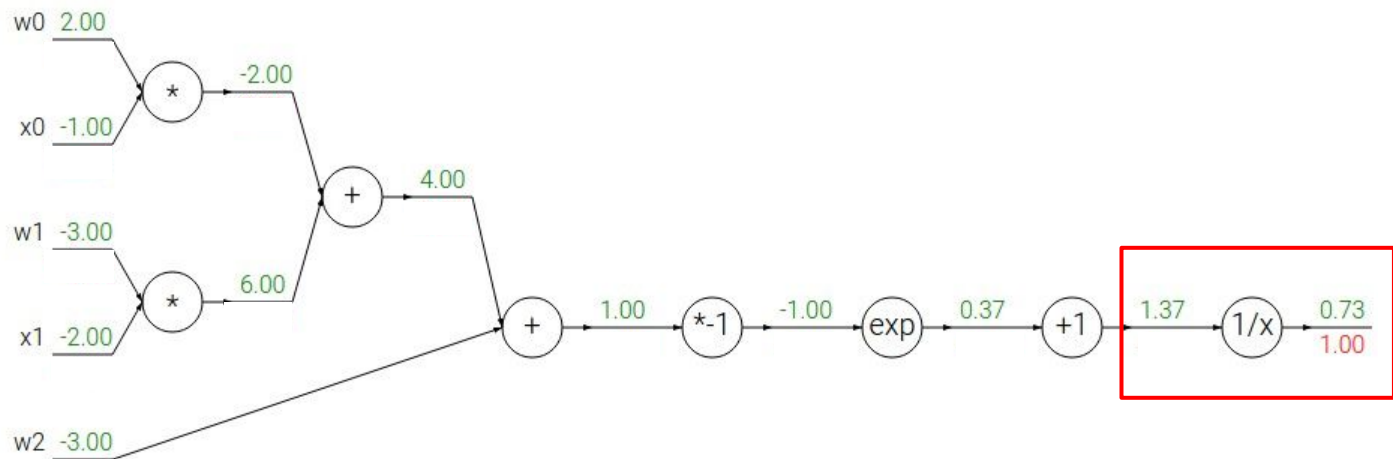
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

Another example:

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



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

→

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

$$f_a(x) = ax$$

→

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

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

→

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

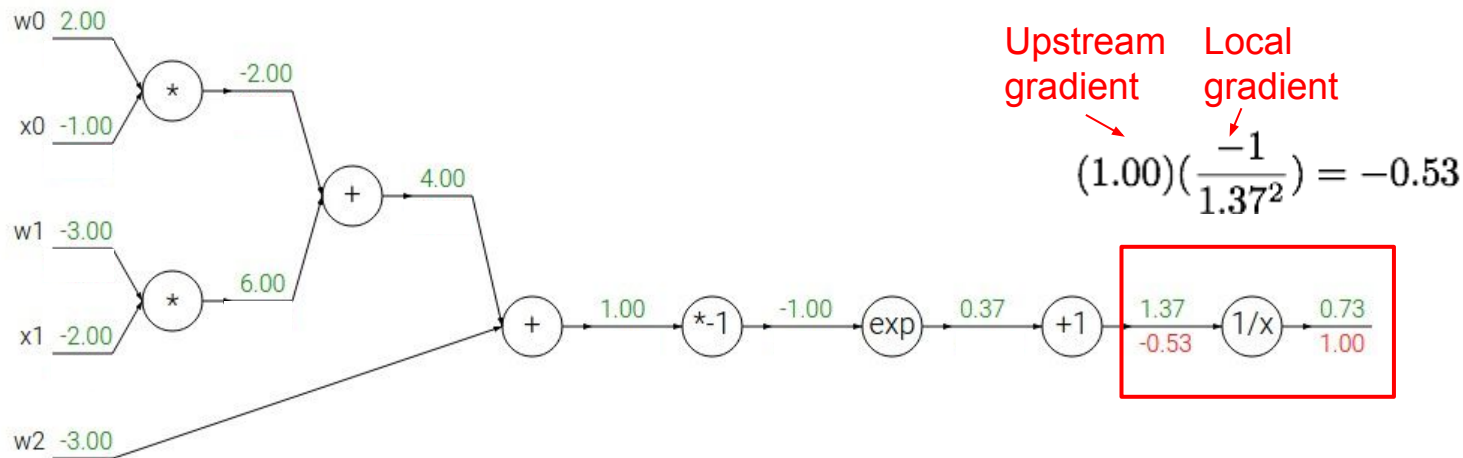
$$f_c(x) = c + x$$

→

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

Another example:

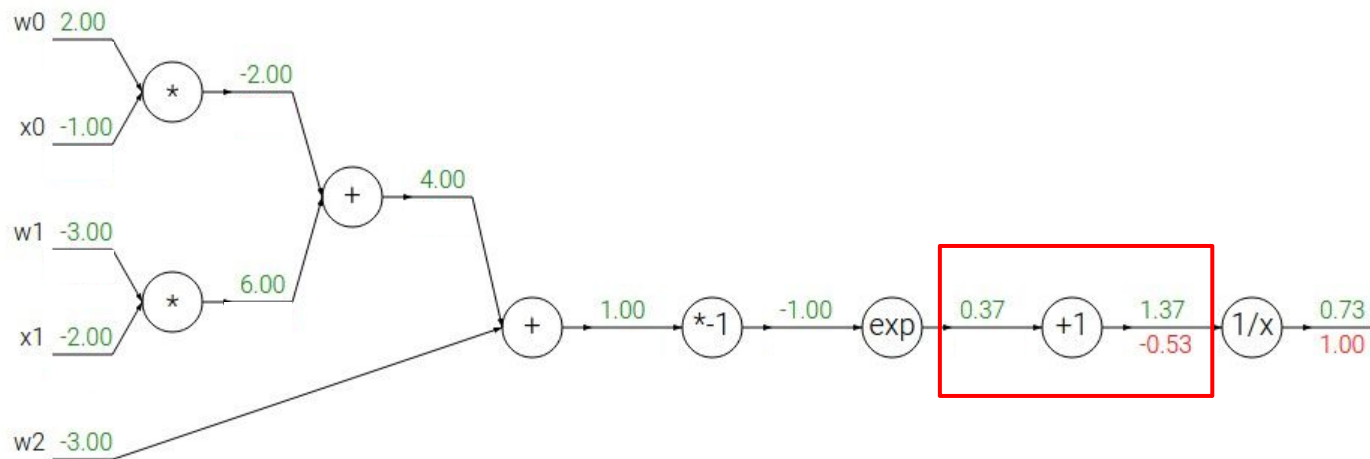
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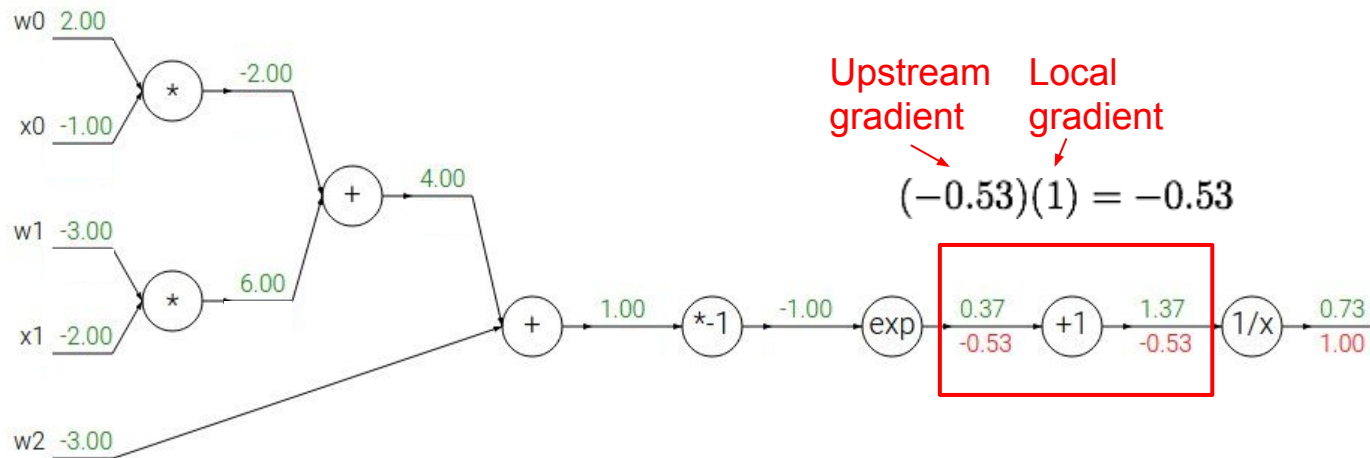
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

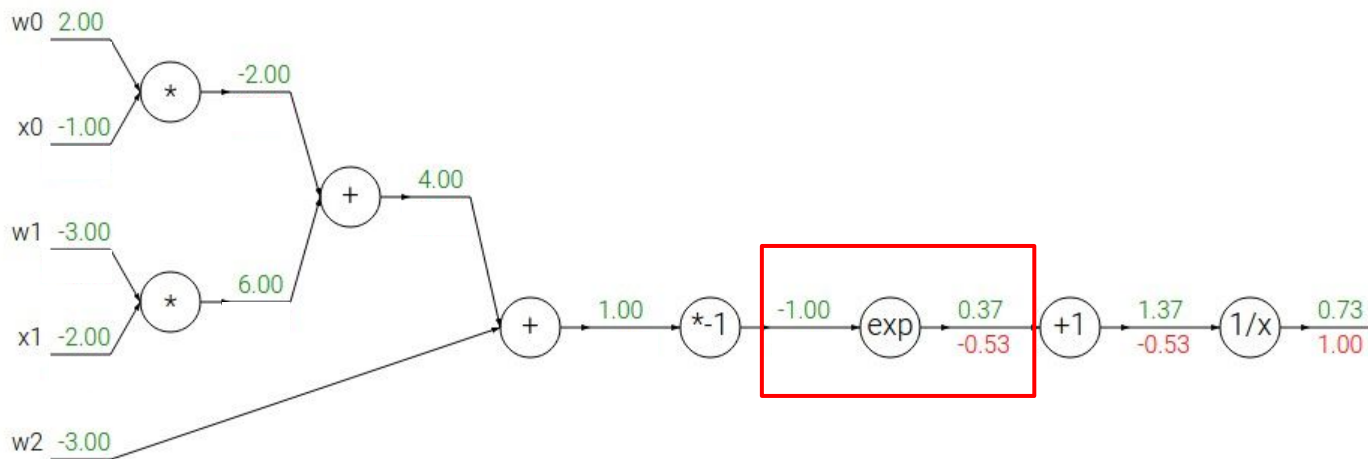
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

Another example:

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



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

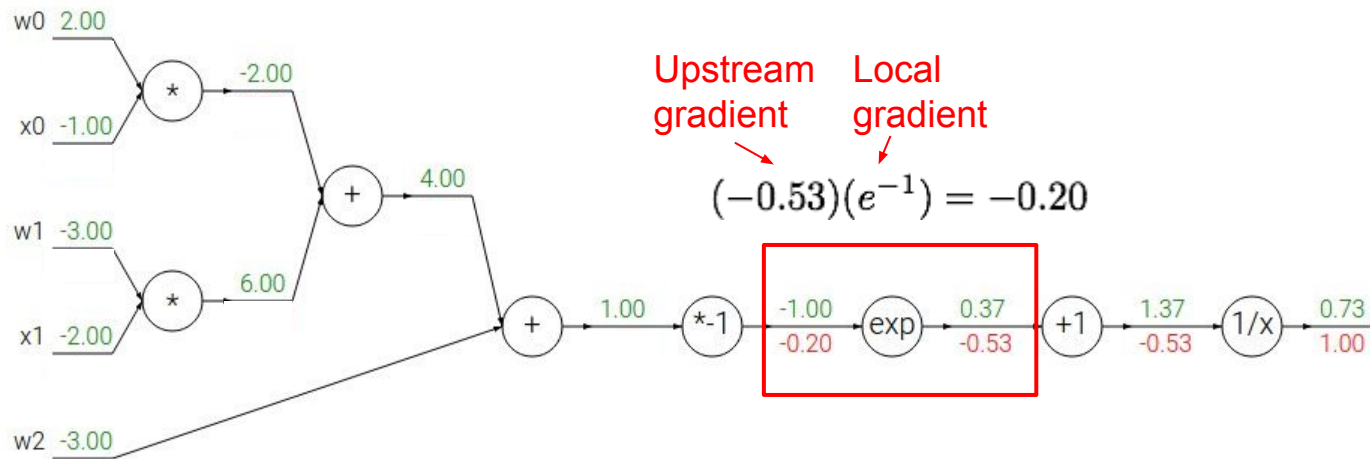
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



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

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

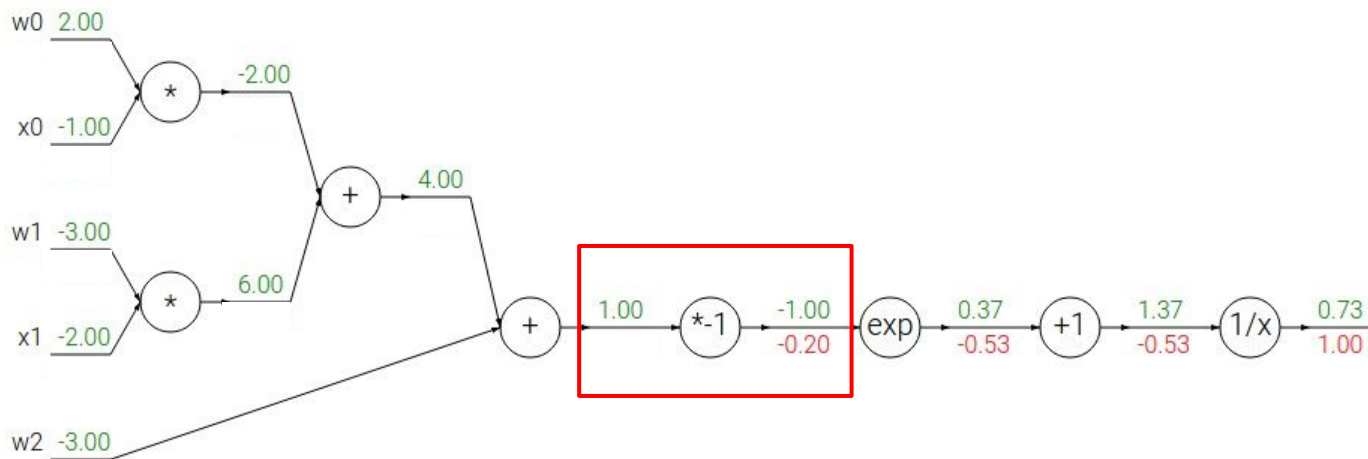
$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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



Another example:

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



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

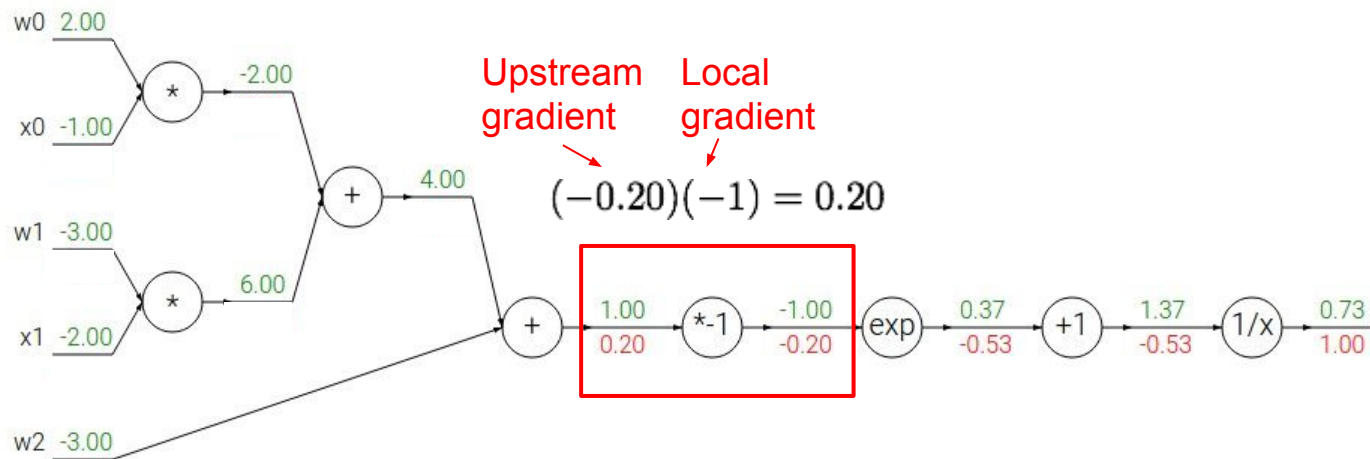
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

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

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

Another example:

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



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

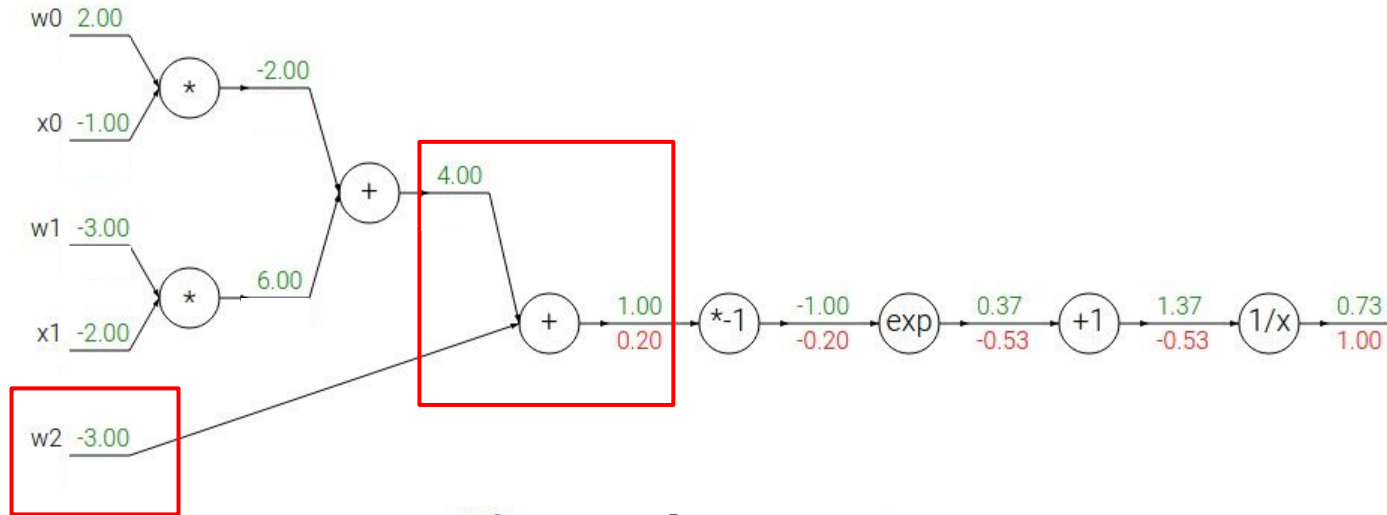
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



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

→

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

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

→

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

$$f_a(x) = ax$$

→

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

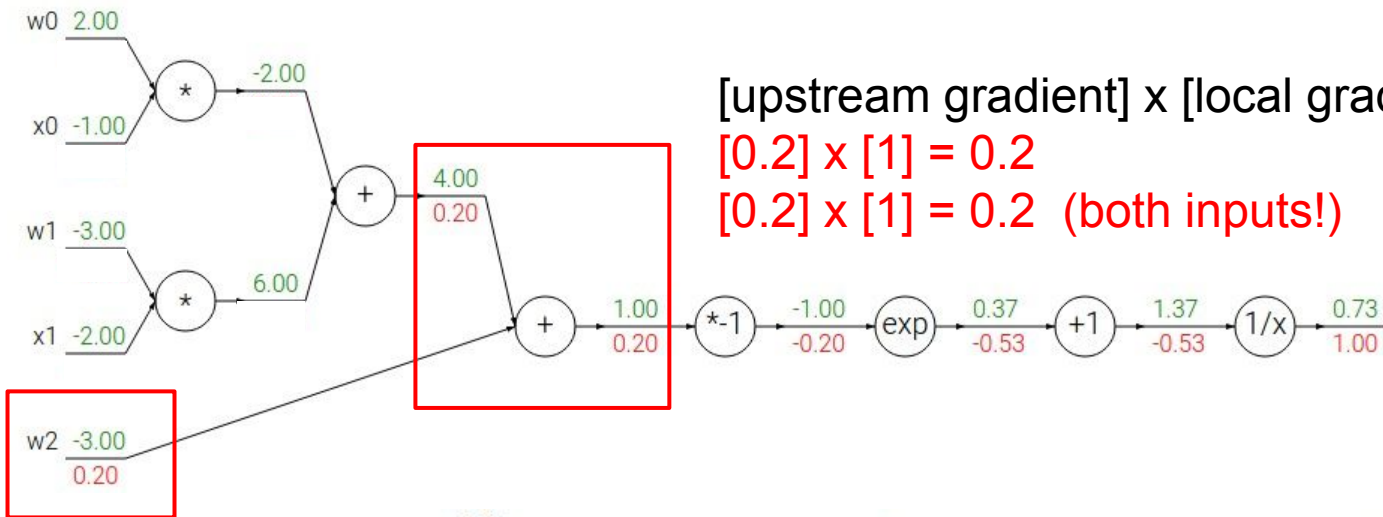
$$f_c(x) = c + x$$

→

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

Another example:

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



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

→

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

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

→

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

$$f_a(x) = ax$$

→

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

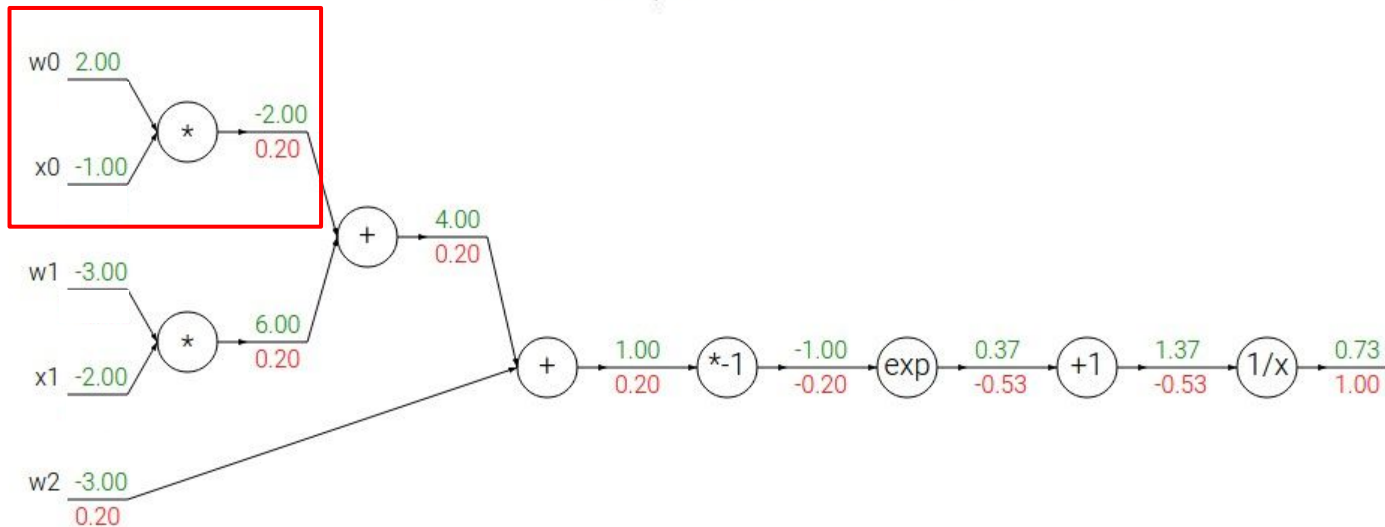
$$f_c(x) = c + x$$

→

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

Another example:

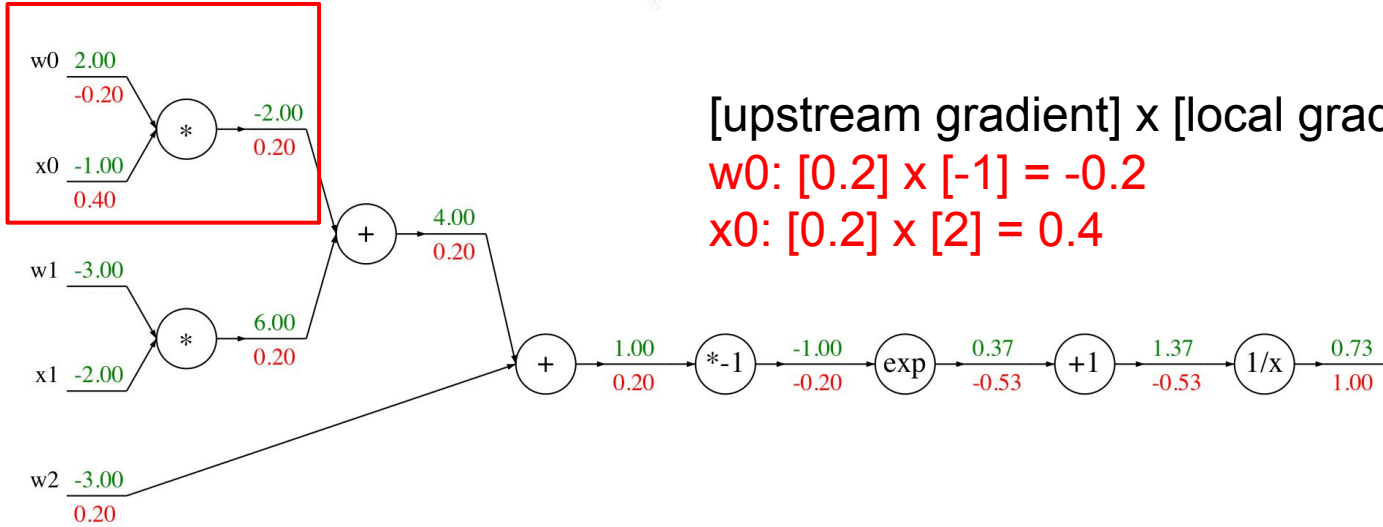
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

Another example:

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



[upstream gradient] x [local gradient]

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

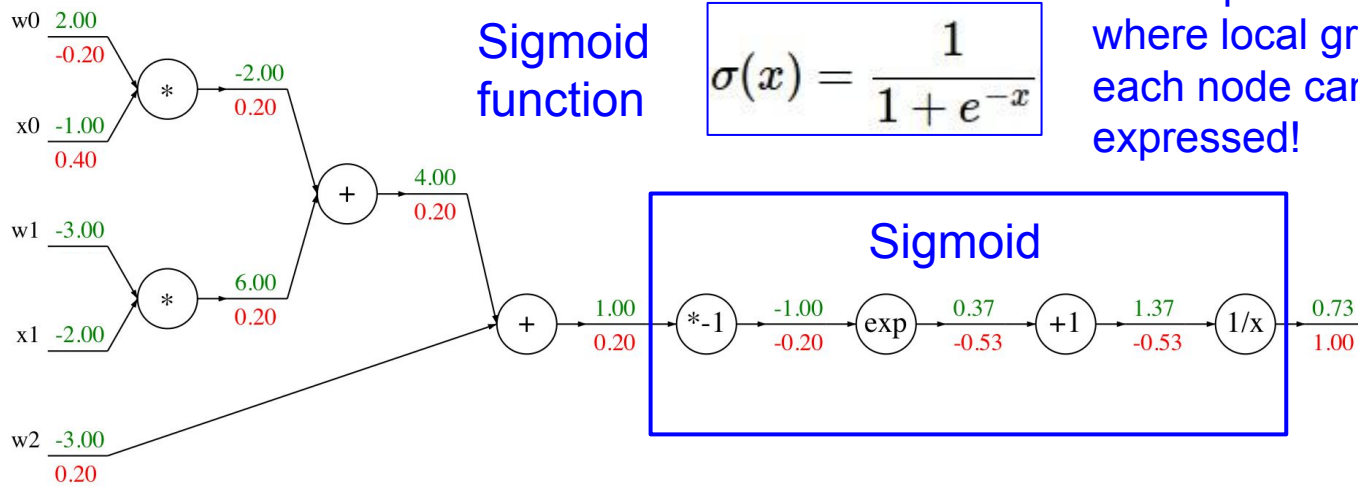
$$x_0: [0.2] \times [2] = 0.4$$

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

Another example:

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

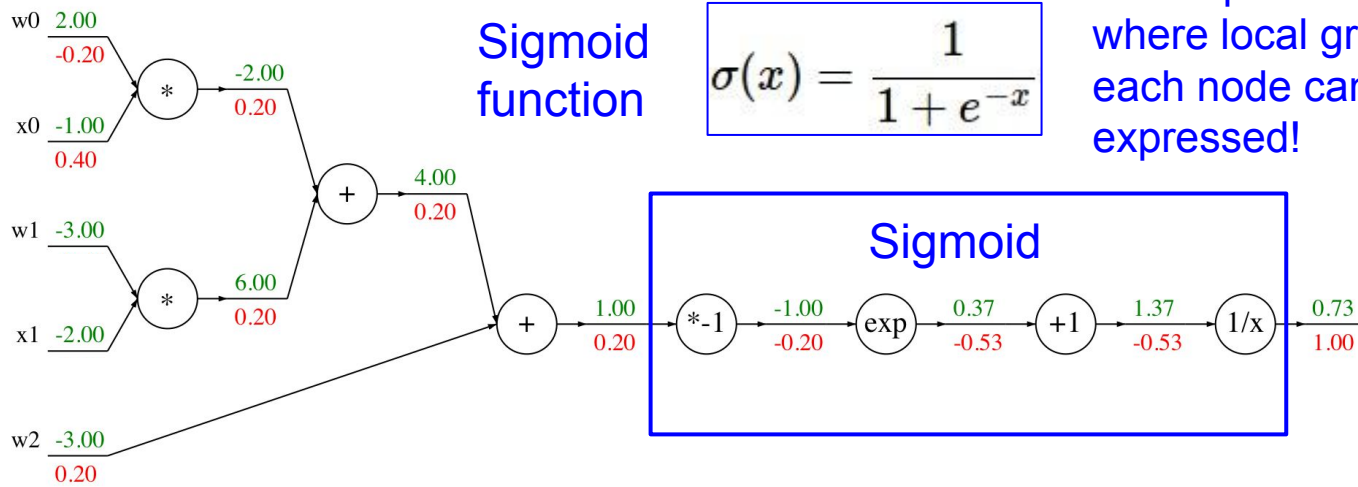
Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!



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:

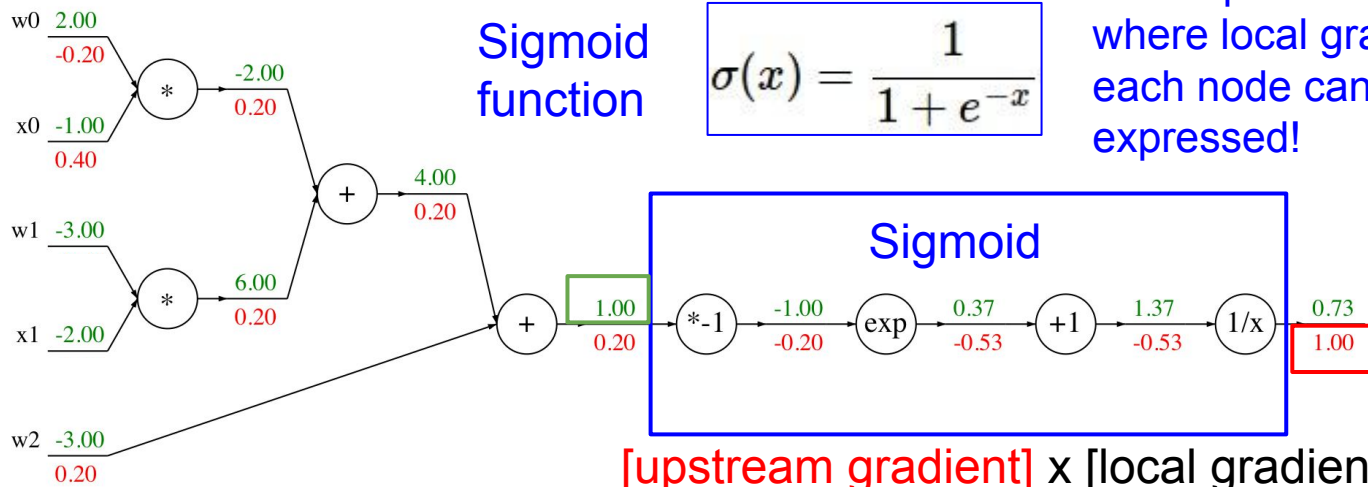
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1 + e^{-x})^2} = \left( \frac{1 + e^{-x} - 1}{1 + e^{-x}} \right) \left( \frac{1}{1 + e^{-x}} \right) = (1 - \sigma(x))\sigma(x)$$



Another example:

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

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<sup>1</sup>)) (1/(1+e<sup>1</sup>))] = 0.2

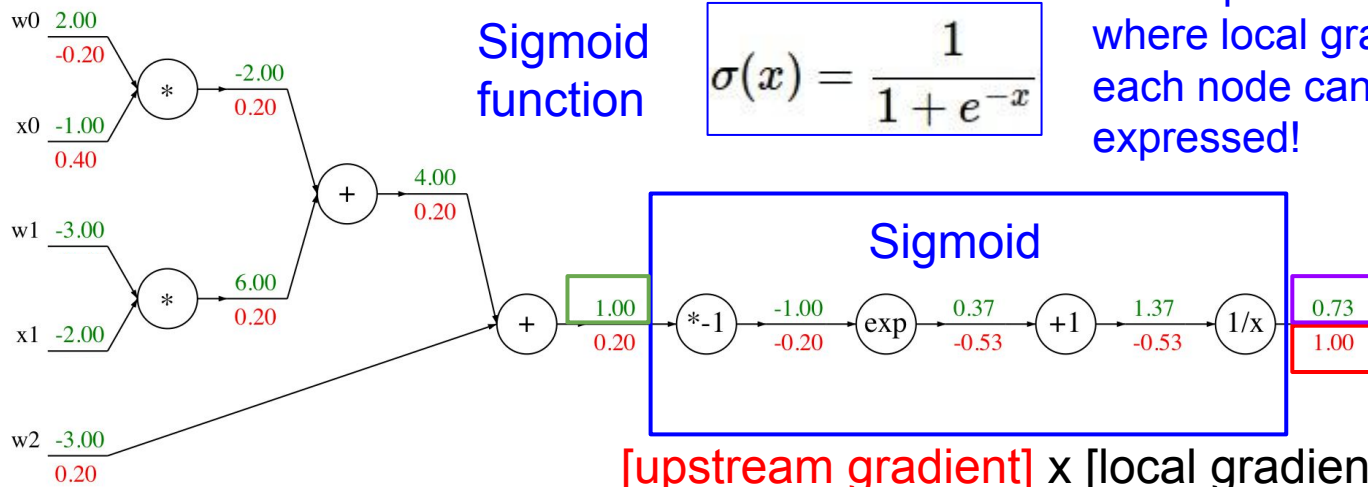
Sigmoid local gradient:

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

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!

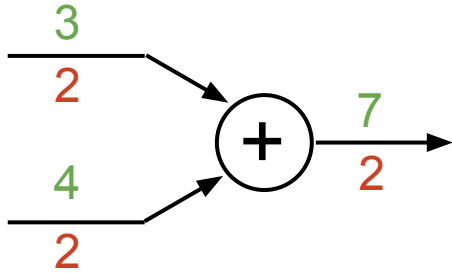


Sigmoid local gradient:

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

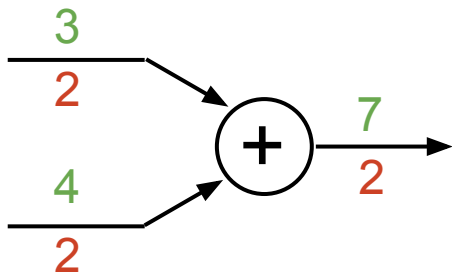
# Patterns in gradient flow

**add** gate: gradient distributor

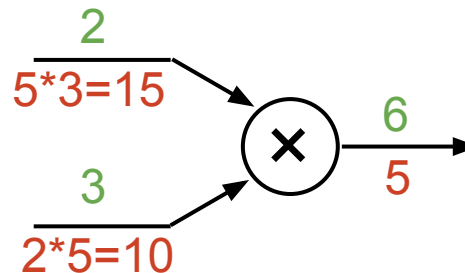


# Patterns in gradient flow

**add** gate: gradient distributor

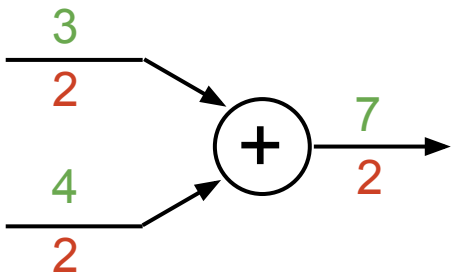


**mul** gate: “swap multiplier”

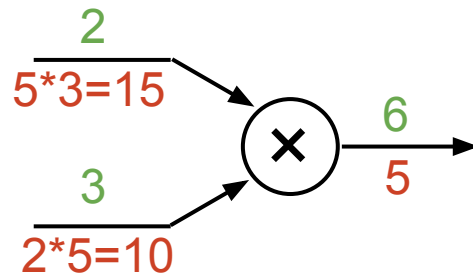


# Patterns in gradient flow

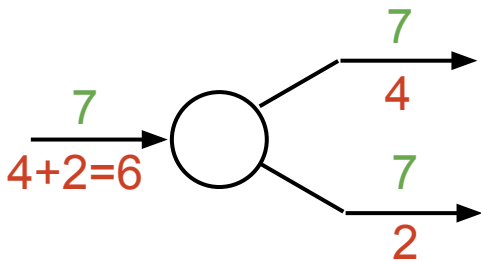
**add gate:** gradient distributor



**mul gate:** “swap multiplier”

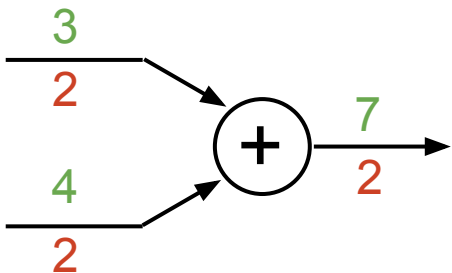


**copy gate:** gradient adder

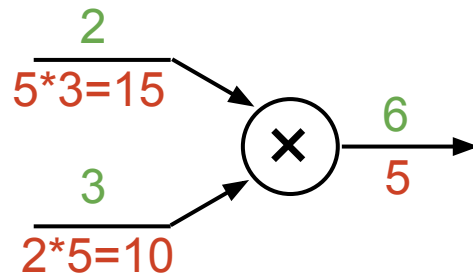


# Patterns in gradient flow

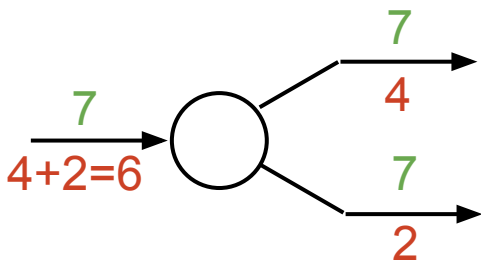
**add gate:** gradient distributor



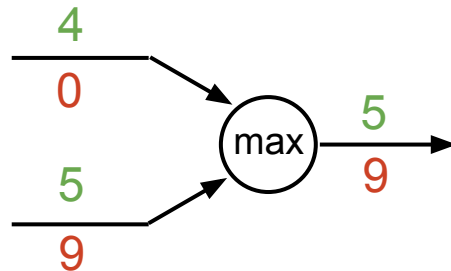
**mul gate:** “swap multiplier”



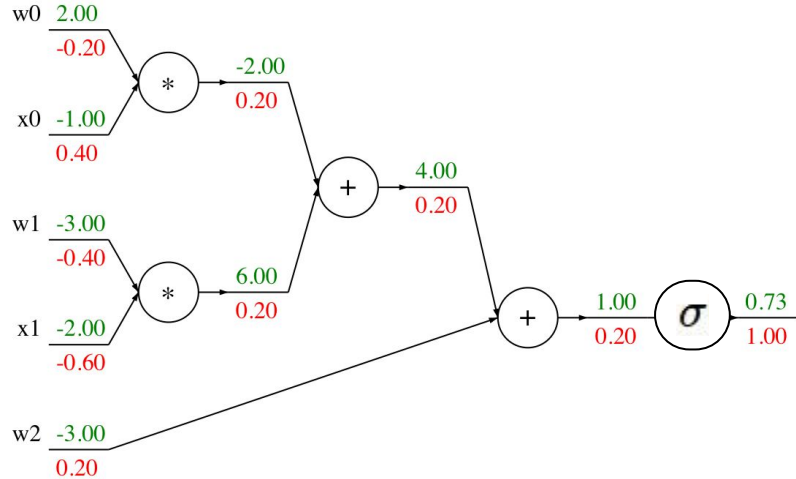
**copy gate:** gradient adder



**max gate:** gradient router



# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

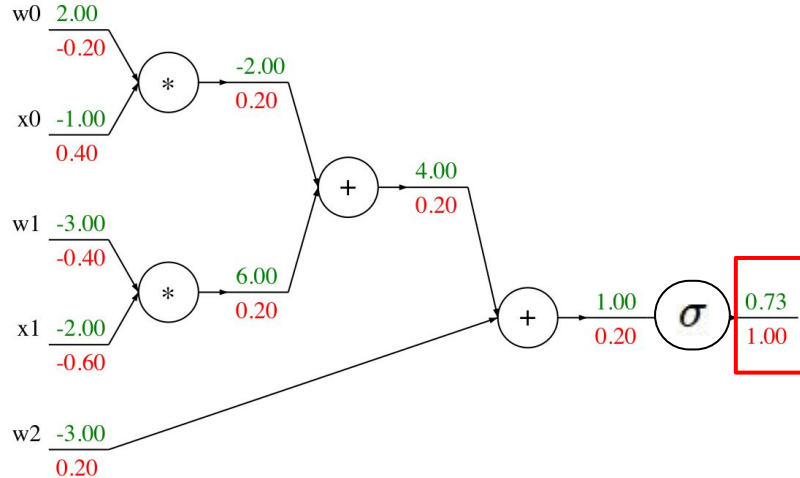
```
def f(w0, x0, w1, x1, w2):
```

```
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):
```

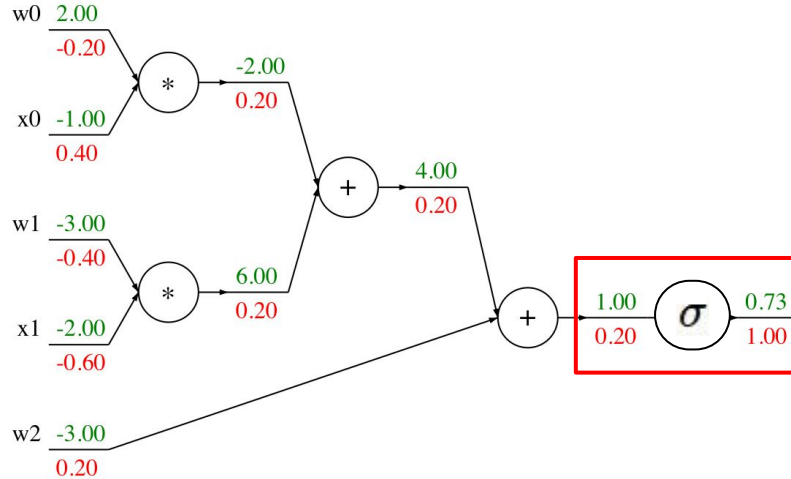
```
s0 = w0 * x0  
s1 = w1 * x1  
s2 = s0 + s1  
s3 = s2 + w2  
L = sigmoid(s3)
```

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
```

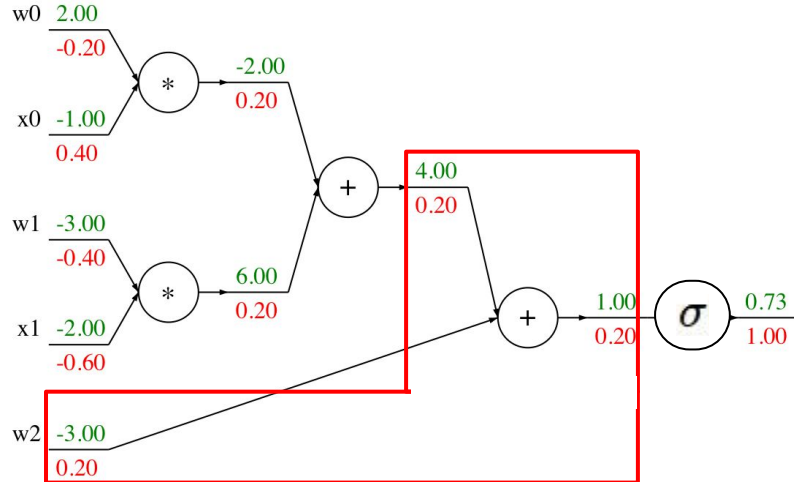
```
grad_w1 = grad_s1 * x1
```

```
grad_x1 = grad_s1 * w1
```

```
grad_w0 = grad_s0 * x0
```

```
grad_x0 = grad_s0 * w0
```

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

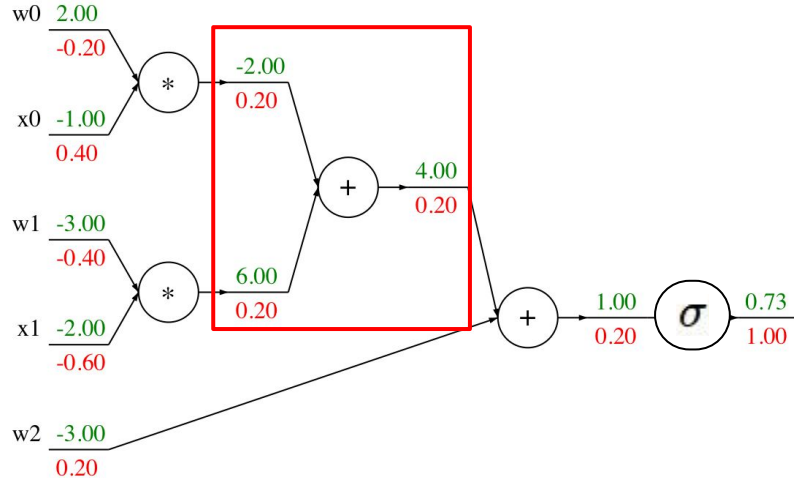
```
def f(w0, x0, w1, x1, w2):
```

```
    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)
```

```
    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
```

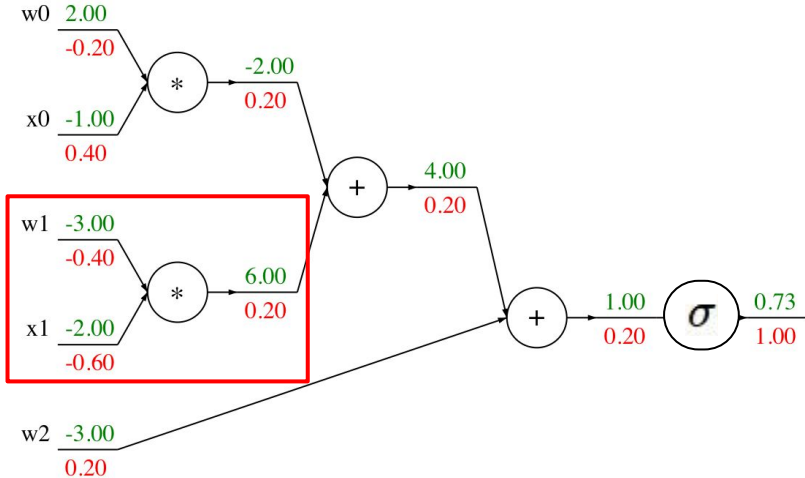
```
    grad_x1 = grad_s1 * w1
```

```
    grad_w0 = grad_s0 * x0
```

```
    grad_x0 = grad_s0 * w0
```

Add gate

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

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

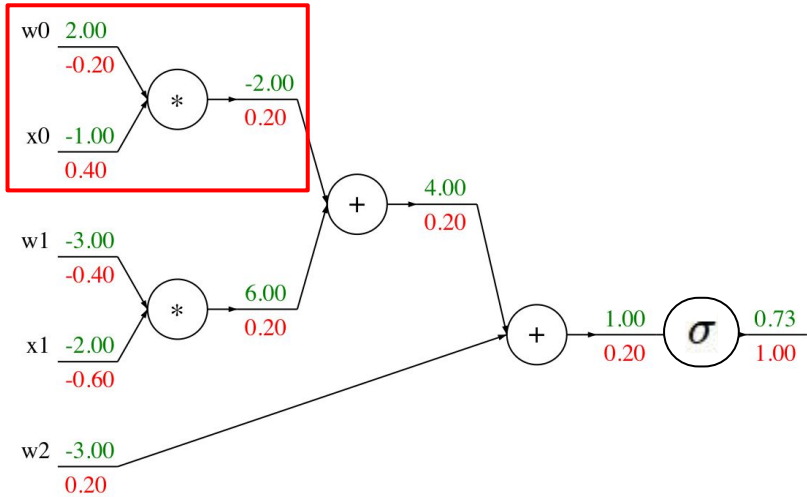
```
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

```
    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
```

Multiply gate

```
    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
```

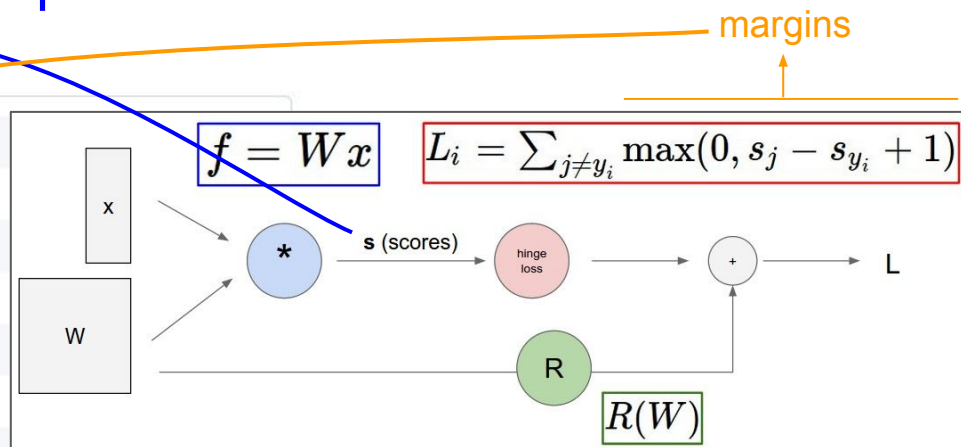
Multiply gate

# “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 = #...
```



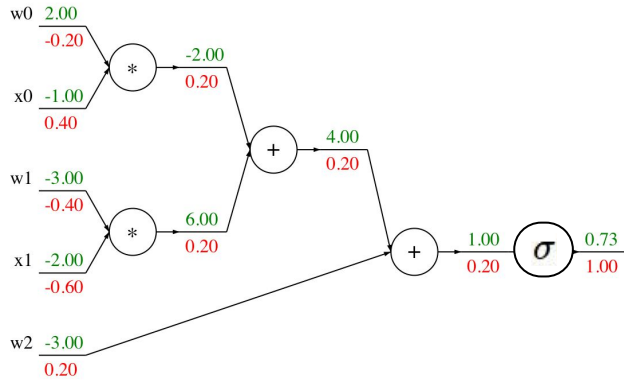
# “Flat” Backprop: Do this for assignment 1!

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*)

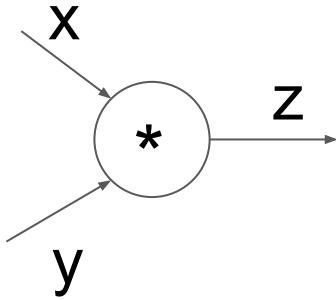


```
class ComputationalGraph(object):  
    #...  
    def forward(inputs):  
        # 1. [pass inputs to input gates...]  
        # 2. forward the computational graph:  
        for gate in self.graph.nodes_topologically_sorted():  
            gate.forward()  
        return loss # the final gate 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)

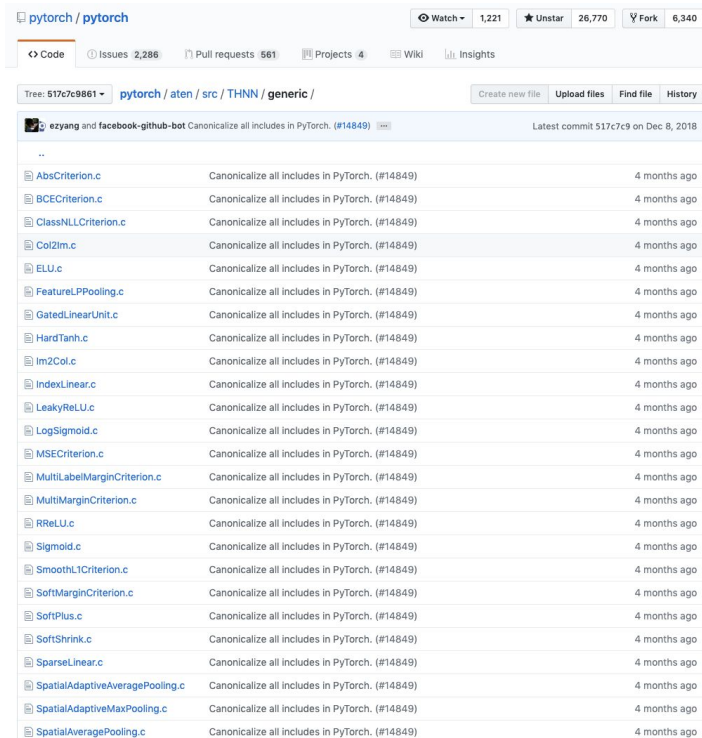
```
class Multiply(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x, y):
        ctx.save_for_backward(x, y)
        z = x * y
        return z
    @staticmethod
    def backward(ctx, grad_z):
        x, y = ctx.saved_tensors
        grad_x = y * grad_z # dz/dx * dL/dz
        grad_y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

Need to stash  
some values for  
use in backward

Upstream  
gradient

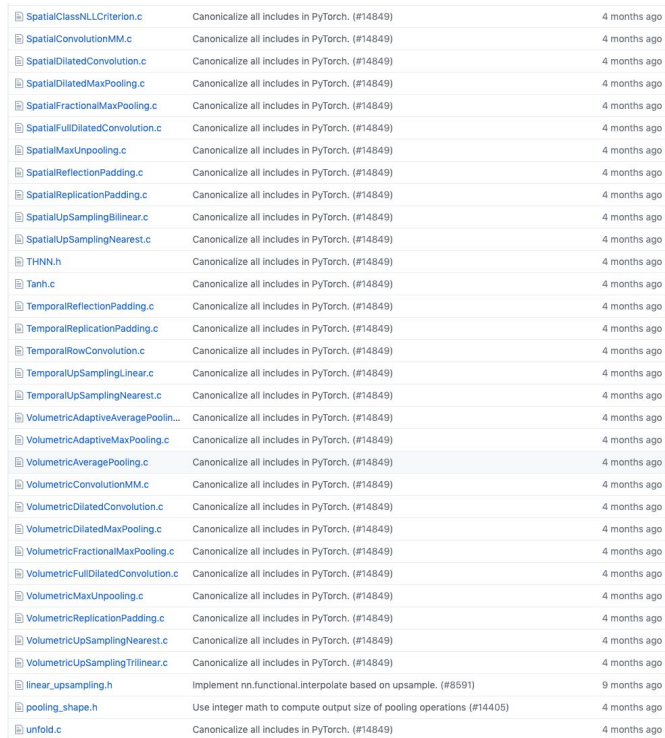
Multiply upstream  
and local gradients

# Example: PyTorch operators



The screenshot shows the GitHub repository for PyTorch, specifically the 'aten/src/THNN/generic/' directory. The repository has 1,221 watches, 26,770 stars, and 6,340 forks. The current commit is 517c7c9861, and the last commit was on Dec 8, 2018. The table lists various operators, each with a description and a commit hash.

Operator	Description	Commit Hash
AbsCriterion.c	Canonicalize all includes in PyTorch.	(#14849)
BCECriterion.c	Canonicalize all includes in PyTorch.	(#14849)
ClassNLLCriterion.c	Canonicalize all includes in PyTorch.	(#14849)
Col2Im.c	Canonicalize all includes in PyTorch.	(#14849)
ELU.c	Canonicalize all includes in PyTorch.	(#14849)
FeatureLPPooling.c	Canonicalize all includes in PyTorch.	(#14849)
GatedLinearUnit.c	Canonicalize all includes in PyTorch.	(#14849)
HardTanh.c	Canonicalize all includes in PyTorch.	(#14849)
Im2Col.c	Canonicalize all includes in PyTorch.	(#14849)
IndexLinear.c	Canonicalize all includes in PyTorch.	(#14849)
LeakyReLU.c	Canonicalize all includes in PyTorch.	(#14849)
LogSigmoid.c	Canonicalize all includes in PyTorch.	(#14849)
MSECriterion.c	Canonicalize all includes in PyTorch.	(#14849)
MultiLabelMarginCriterion.c	Canonicalize all includes in PyTorch.	(#14849)
MultiMarginCriterion.c	Canonicalize all includes in PyTorch.	(#14849)
RRReLU.c	Canonicalize all includes in PyTorch.	(#14849)
Sigmoid.c	Canonicalize all includes in PyTorch.	(#14849)
SmoothL1Criterion.c	Canonicalize all includes in PyTorch.	(#14849)
SoftMarginCriterion.c	Canonicalize all includes in PyTorch.	(#14849)
SoftPlus.c	Canonicalize all includes in PyTorch.	(#14849)
SoftShrink.c	Canonicalize all includes in PyTorch.	(#14849)
SparseLinear.c	Canonicalize all includes in PyTorch.	(#14849)
SpatialAdaptiveAveragePooling.c	Canonicalize all includes in PyTorch.	(#14849)
SpatialAdaptiveMaxPooling.c	Canonicalize all includes in PyTorch.	(#14849)
SpatialAveragePooling.c	Canonicalize all includes in PyTorch.	(#14849)



The screenshot shows the continuation of the PyTorch repository file browser, listing operators from 'SpatialClassNLLCriterion.c' to 'unfold.c'.

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)
VolumetricMaxUnpooling.c	Canonicalize all includes in PyTorch.	(#14849)
VolumetricReplicationPadding.c	Canonicalize all includes in PyTorch.	(#14849)
VolumetricUpsamplingNearest.c	Canonicalize all includes in PyTorch.	(#14849)
VolumetricUpsamplingTrilinear.c	Canonicalize all includes in PyTorch.	(#14849)
linear_upsampling.h	Implement nn.functional.interpolate based on upsample.	(#8591)
pooling_shape.h	Use integer math to compute output size of pooling operations	(#14405)
unfold.c	Canonicalize all includes in PyTorch.	(#14849)

# 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 }
26
27 #endif
```

[Source](#)

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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

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1 #ifndef TH_GENERIC_FILE
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22         scalar_t z = *output_data;
23         *gradInput_data = *gradOutput_data * (1. - z) * z;
24     );
25 }
```

Backward

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



```
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...

[Source](#)

# 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

So far: backprop with scalars

Next: 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

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Regular derivative:

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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

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Regular derivative:

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

## Vector to Vector

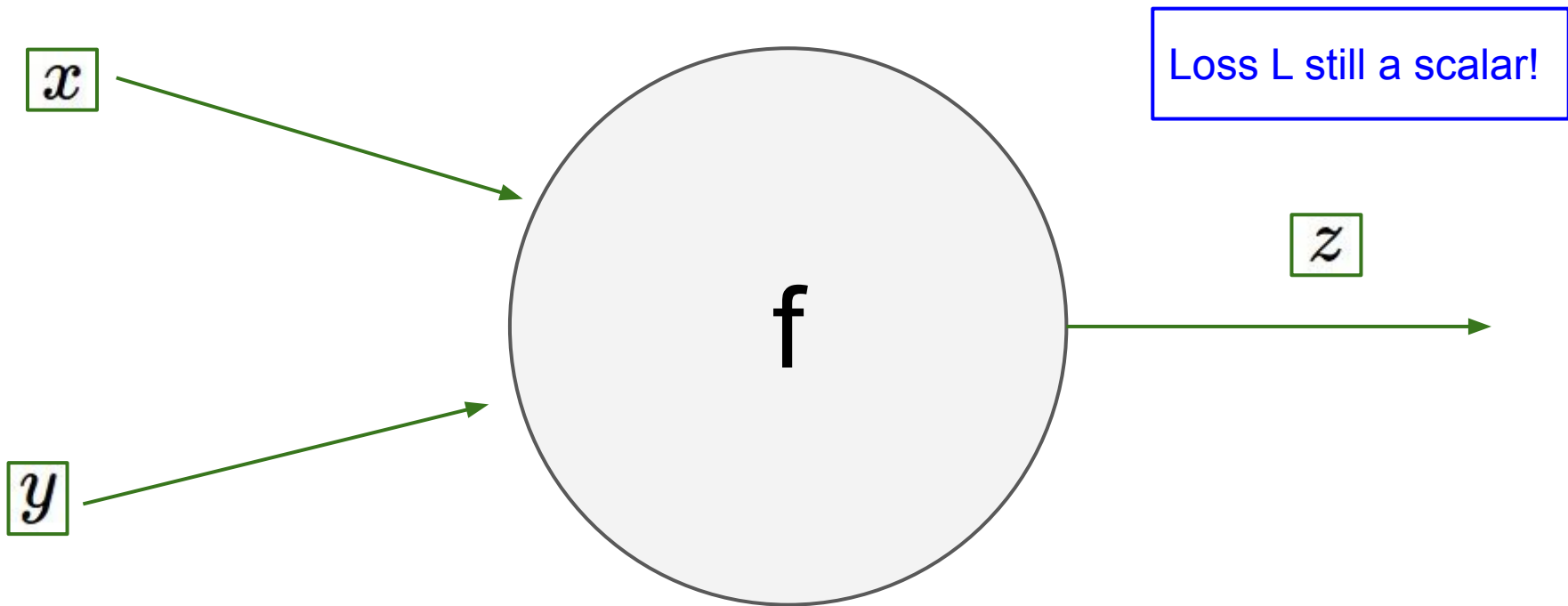
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

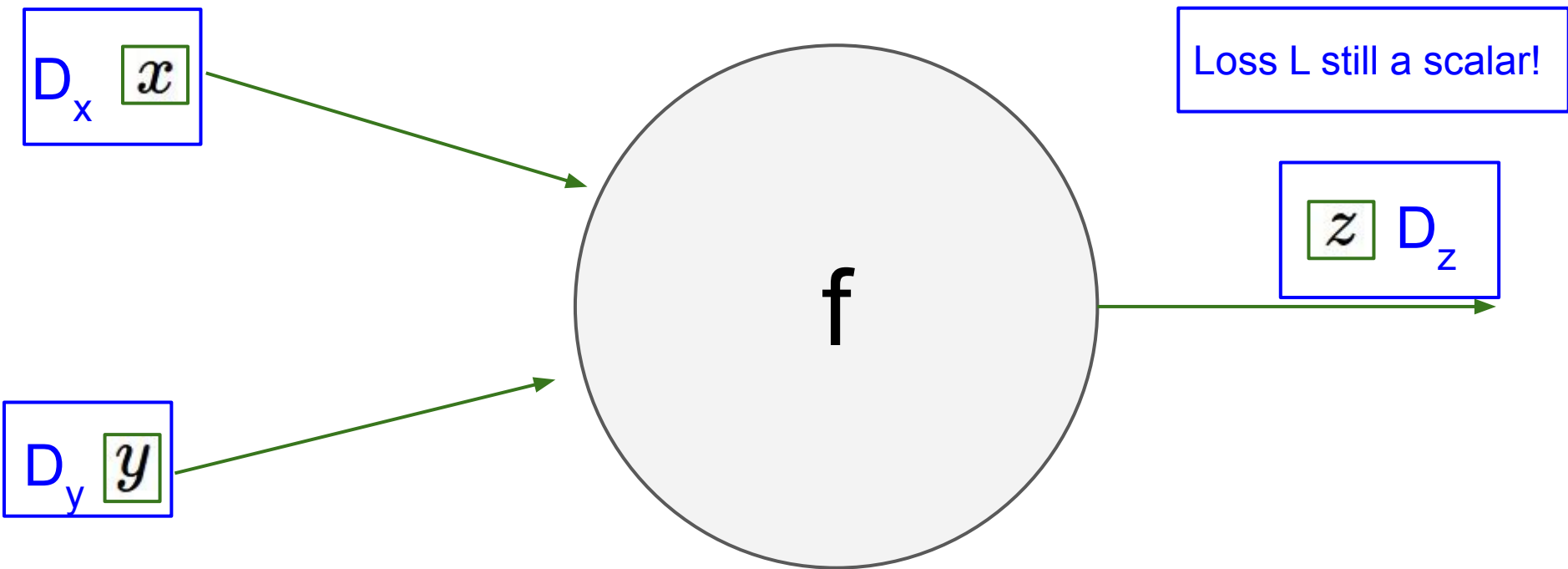
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left( \frac{\partial y}{\partial x} \right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

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

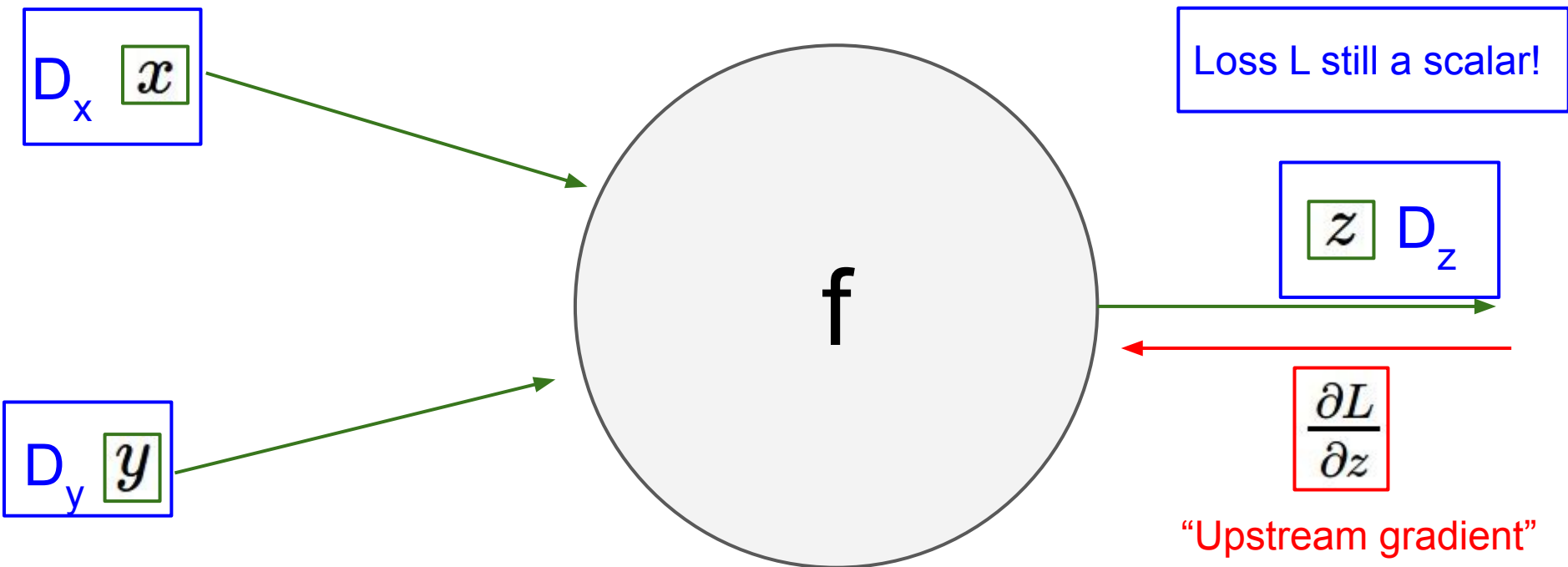
# Backprop with Vectors



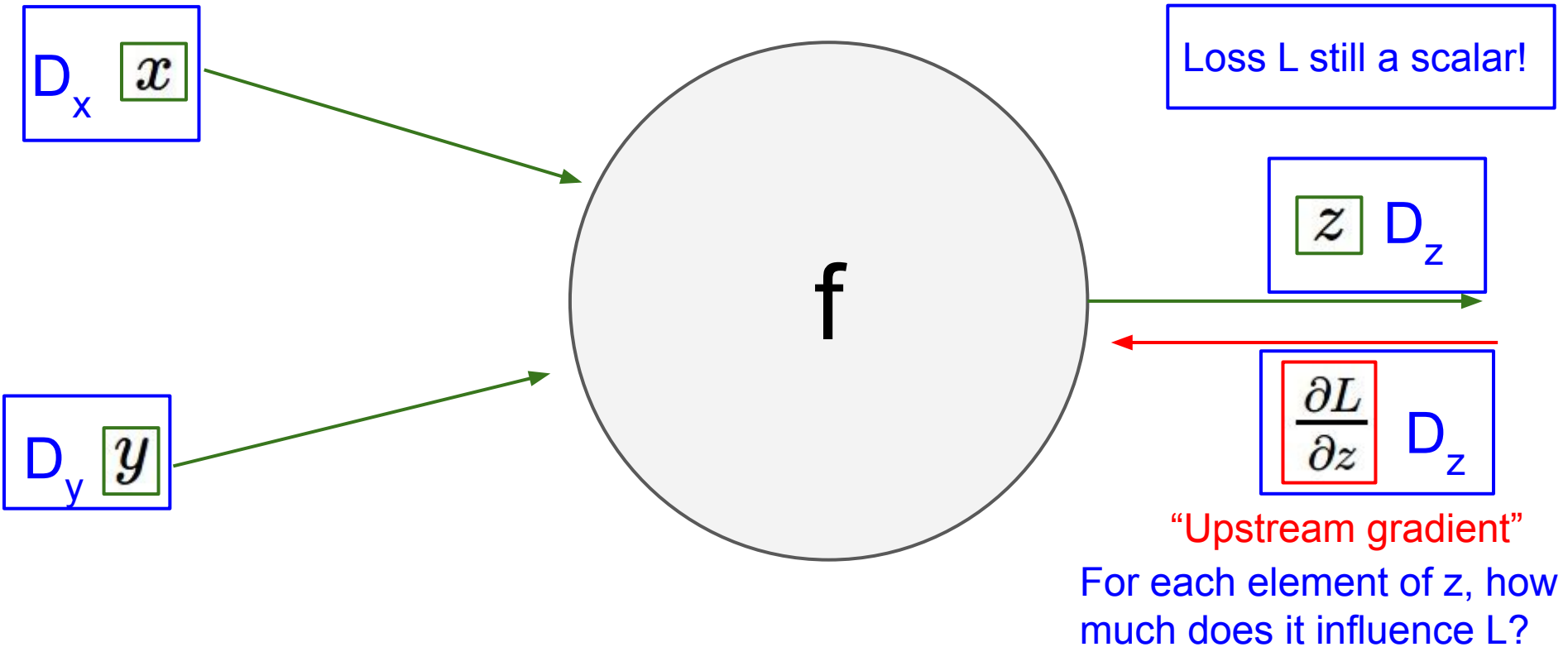
# Backprop with Vectors



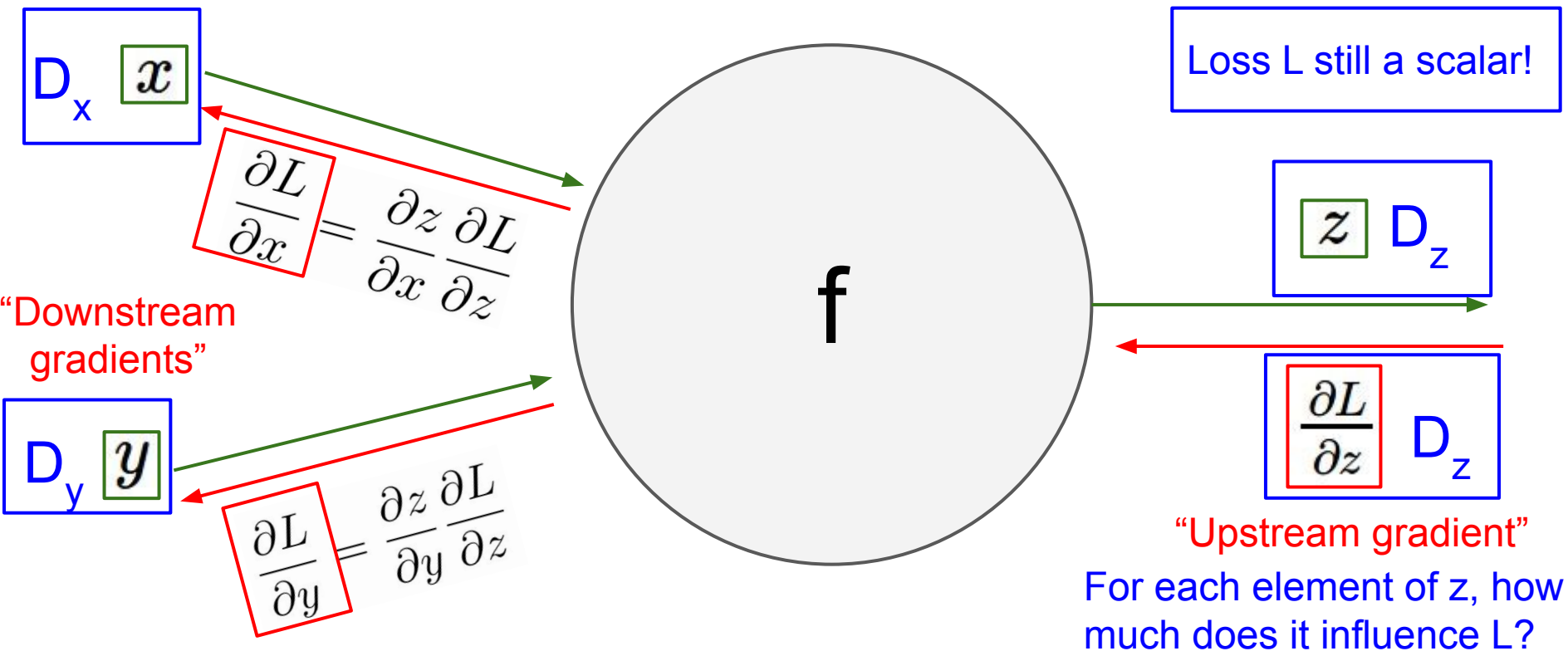
# Backprop with Vectors



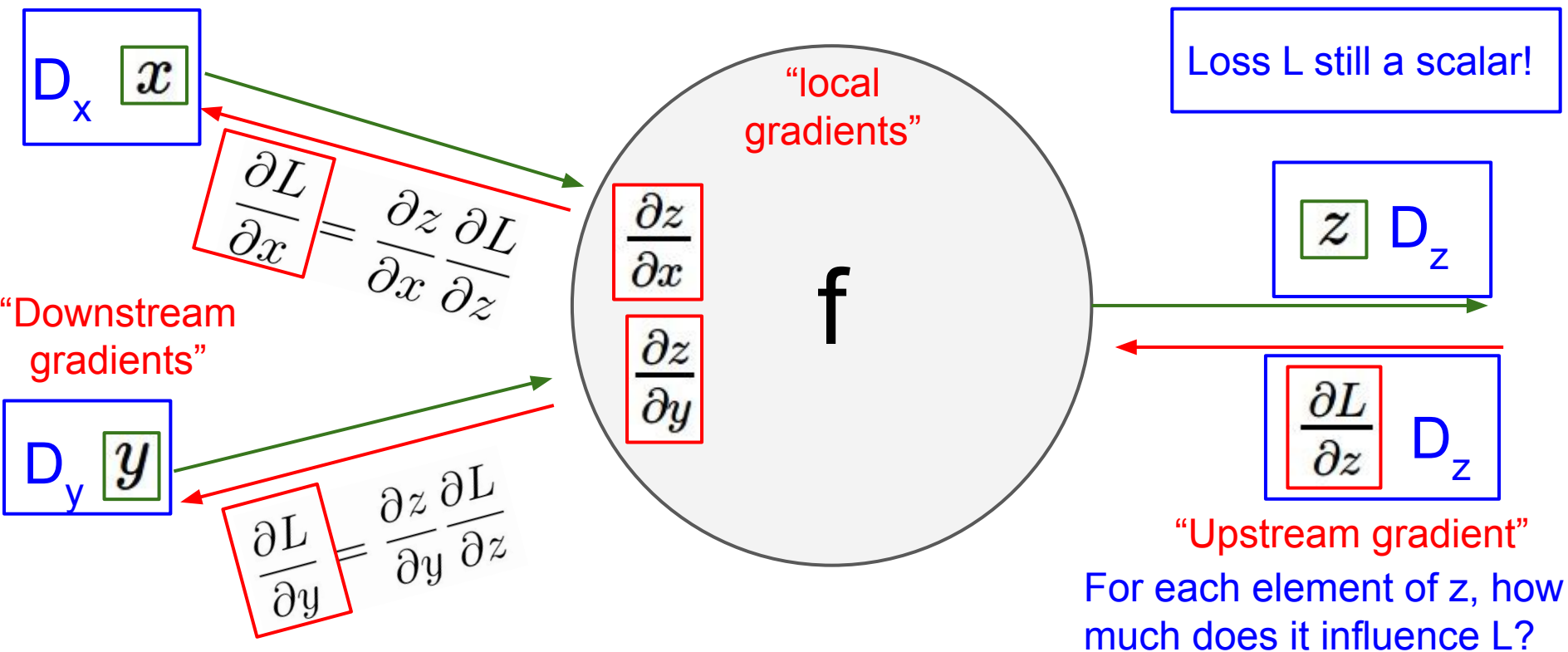
# Backprop with Vectors



# Backprop with Vectors

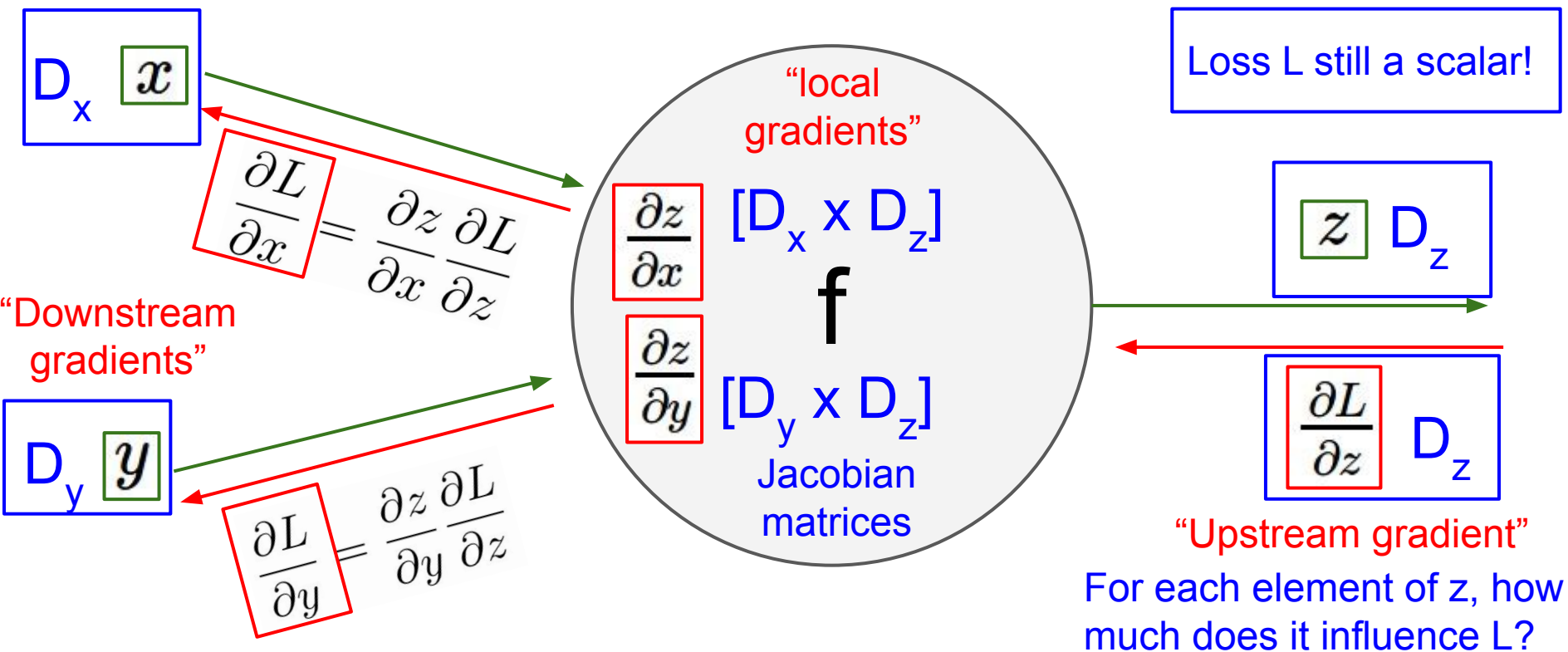


# Backprop with Vectors

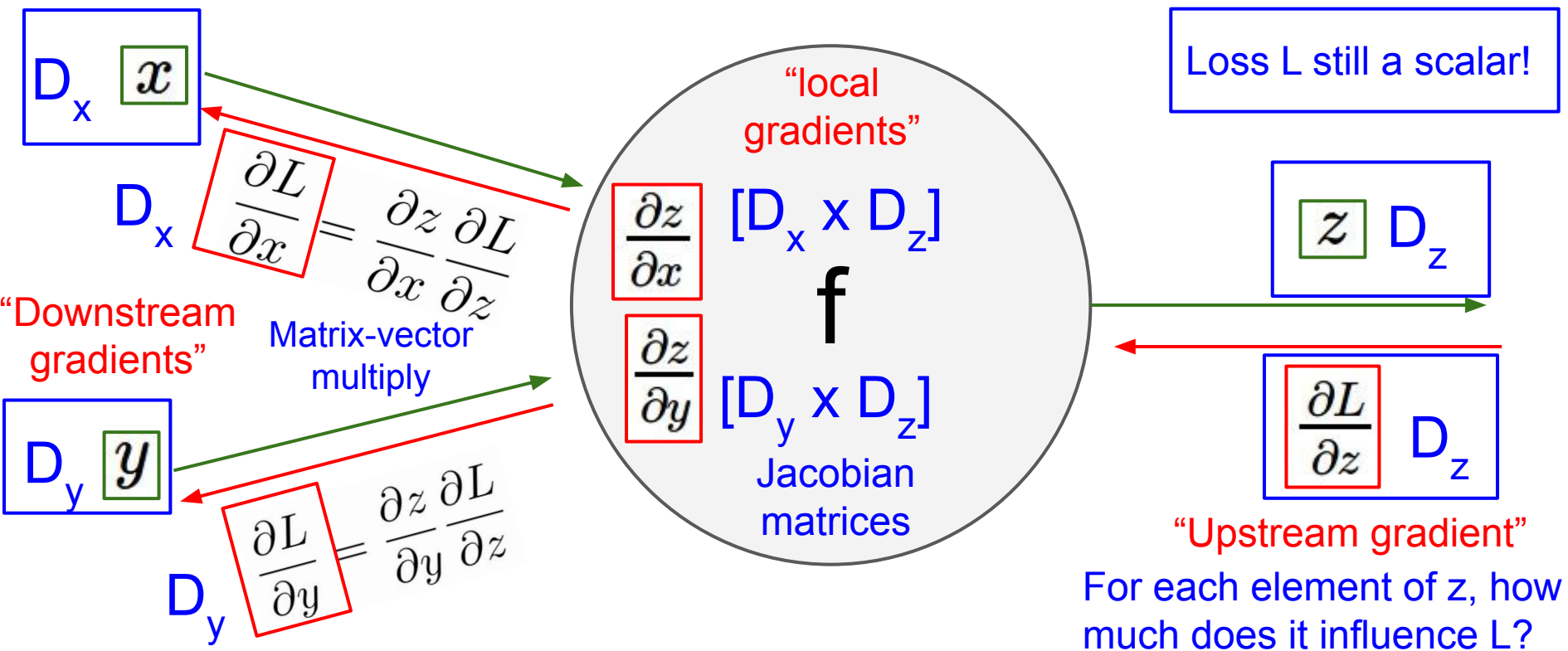




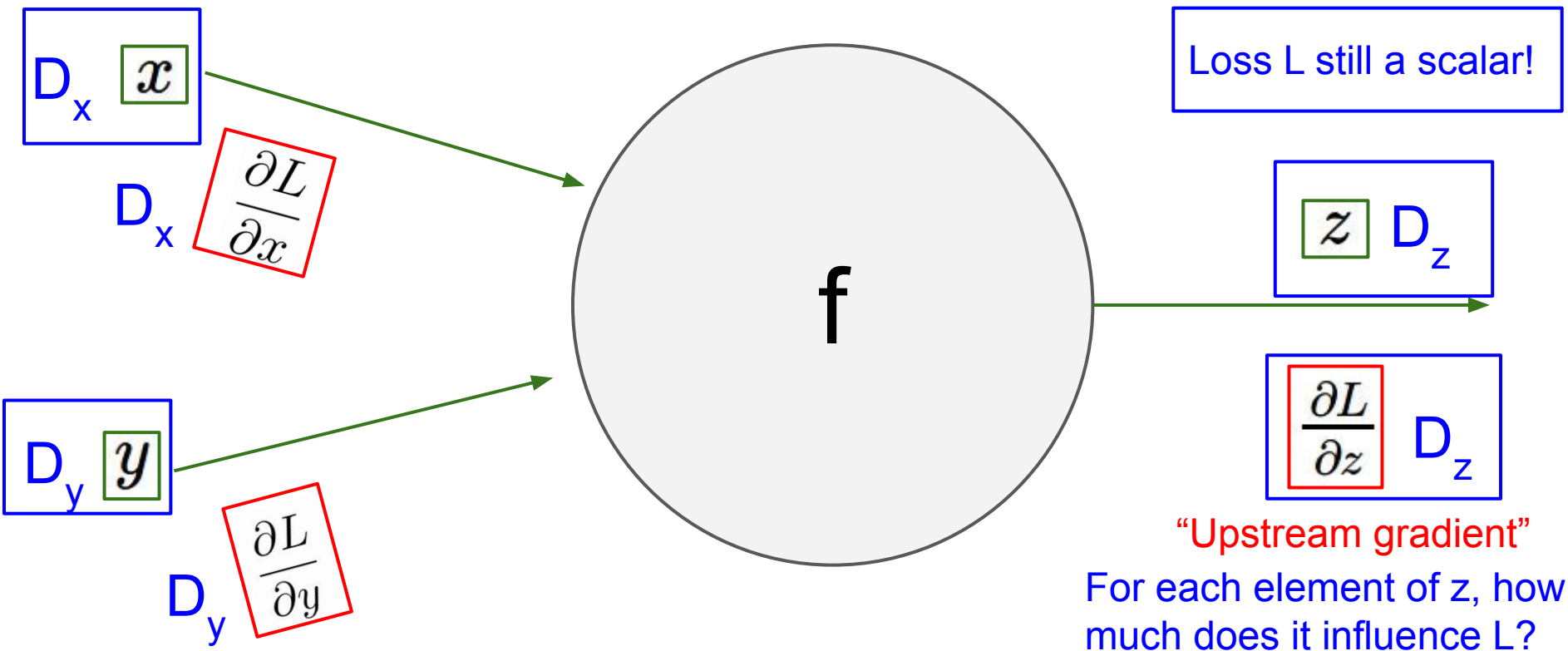
# Backprop with Vectors



# Backprop with Vectors



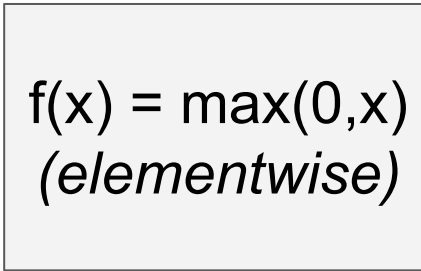
# Gradients of variables wrt loss have same dims as the original variable



# Backprop with Vectors

4D input x:

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



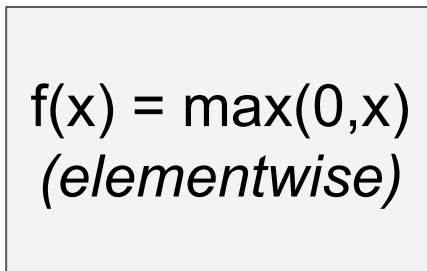
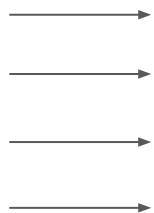
4D output z:

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

# Backprop with Vectors

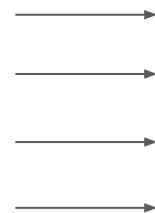
4D input  $x$ :

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



4D output  $z$ :

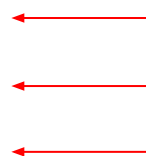
$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$



4D  $dL/dz$ :

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

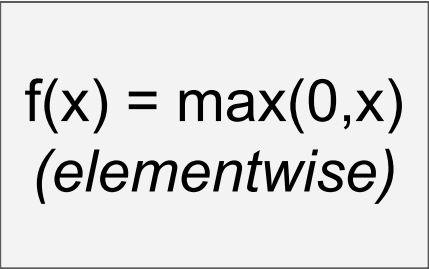
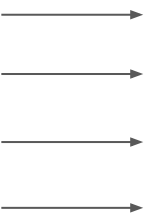
Upstream  
gradient



# Backprop with Vectors

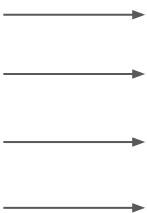
4D input x:

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



4D output z:

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



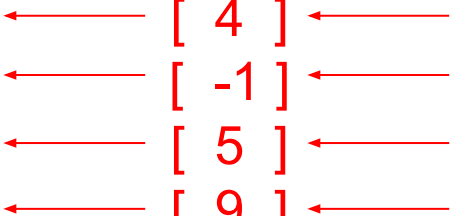
Jacobian  $dz/dx$

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

4D  $dL/dz$ :

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

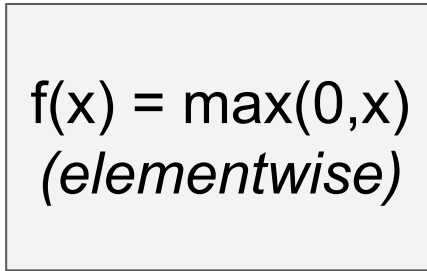
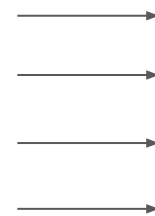
Upstream gradient



# Backprop with Vectors

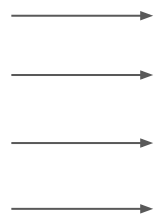
4D input  $x$ :

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



4D output  $z$ :

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



$[dz/dx] [dL/dz]$

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

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

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

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

4D  $dL/dz$ :

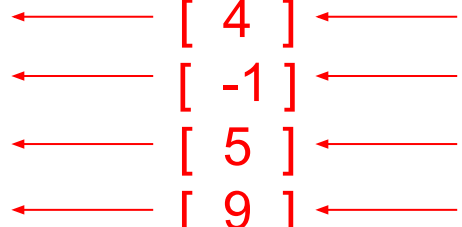
$\begin{bmatrix} 4 \end{bmatrix}$

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

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

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

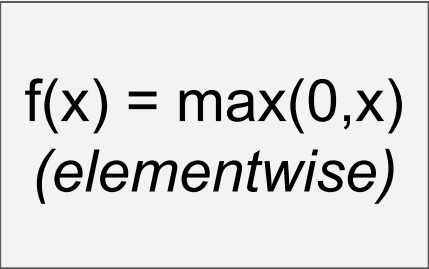
Upstream  
gradient



# Backprop with Vectors

4D input x:

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



4D output z:

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

4D dL/dx:

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

$[dz/dx] [dL/dz]$

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

4D dL/dz:

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

Upstream gradient



# Backprop with Vectors

4D input  $x$ :

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

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

(*elementwise*)

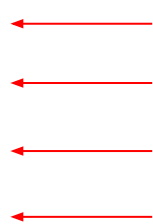
4D output  $z$ :

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

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

4D  $dL/dx$ :

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

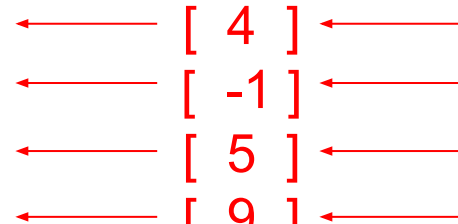


$[dz/dx] [dL/dz]$

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

4D  $dL/dz$ :

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



Upstream  
gradient

# Backprop with Vectors

4D input x:

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

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

4D output z:

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

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

4D  $dL/dx$ :

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

$[dz/dx] [dL/dz]$

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

4D  $dL/dz$ :

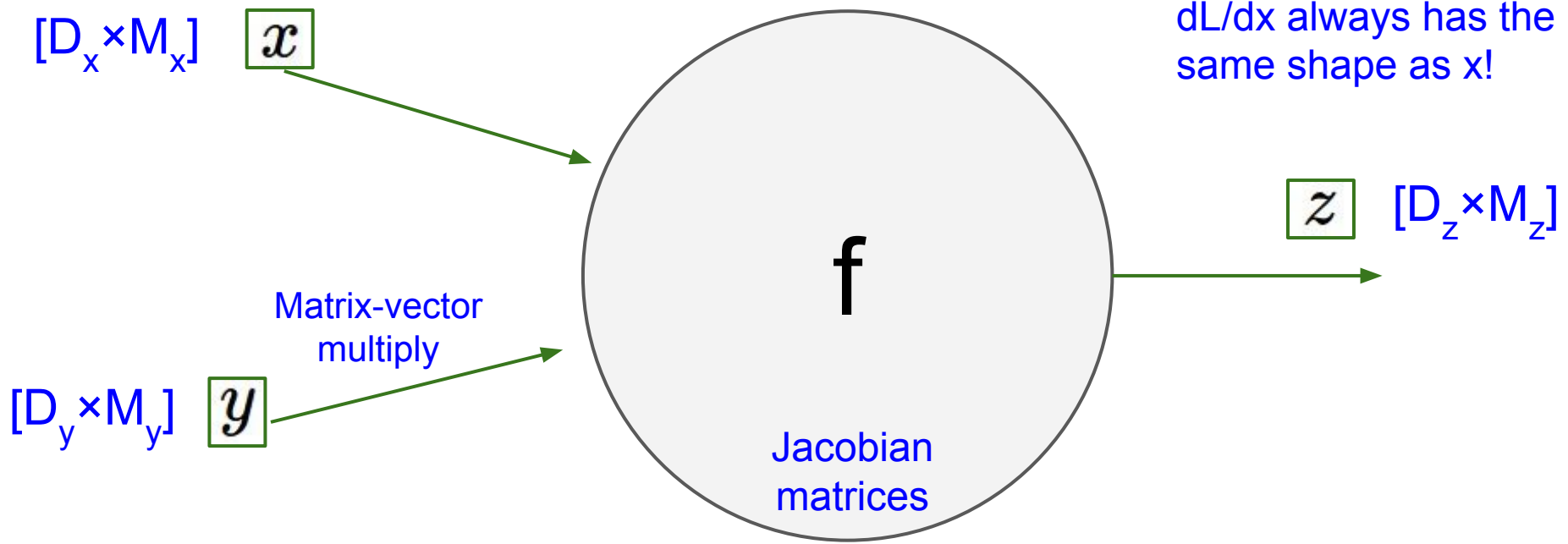
$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$

Upstream  
gradient

# Backprop with Matrices (or Tensors)

Loss L still a scalar!

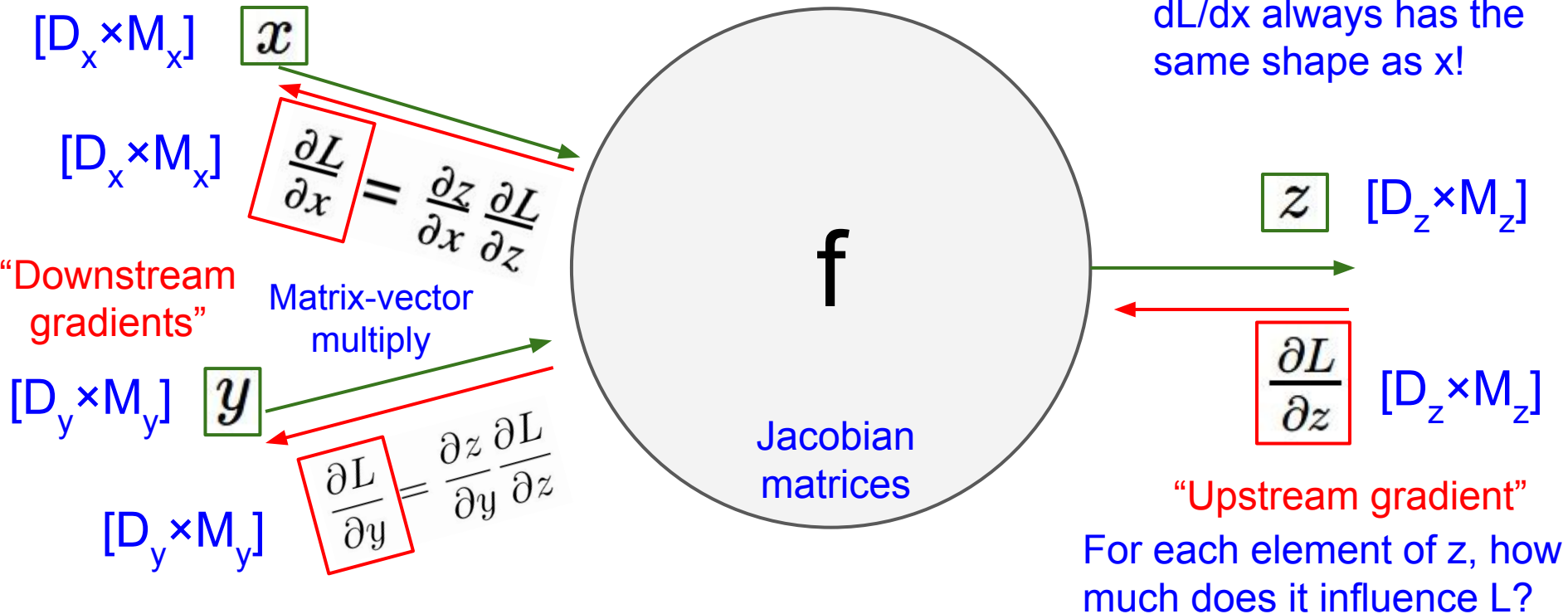
$dL/dx$  always has the same shape as  $x$ !



# Backprop with Matrices (or Tensors)

Loss L still a scalar!

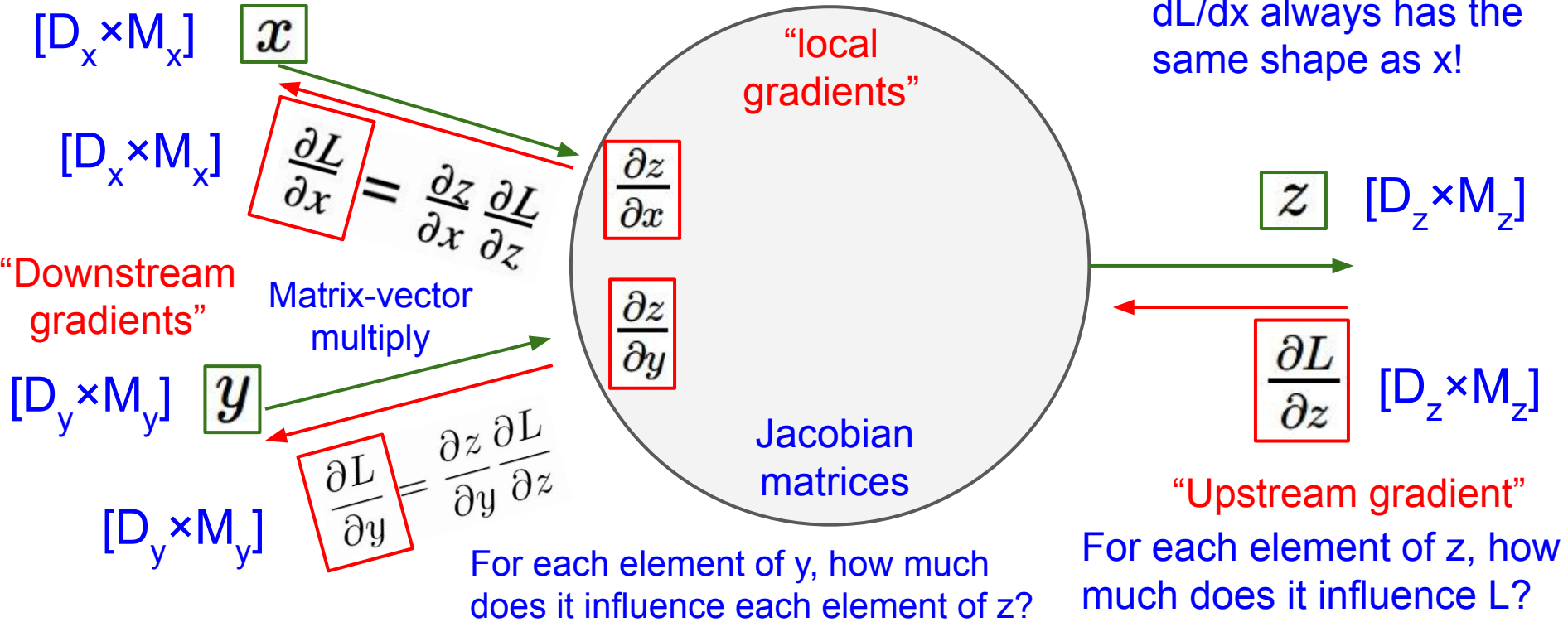
$dL/dx$  always has the same shape as  $x$ !



# Backprop with Matrices (or Tensors)

Loss L still a scalar!

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



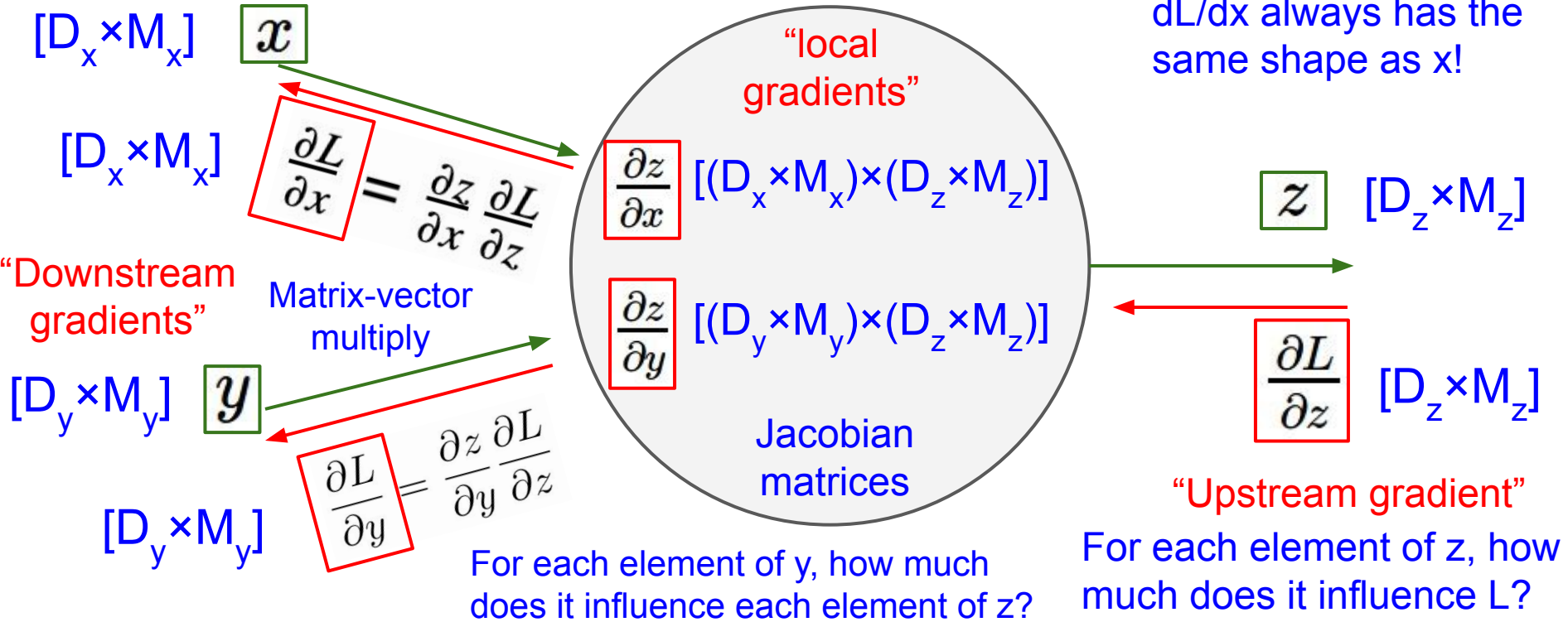
For each element of  $y$ , how much does it influence each element of  $z$ ?

For each element of  $z$ , how much does it influence  $L$ ?

# Backprop with Matrices (or Tensors)

Loss L still a scalar!

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



# Backprop with Matrices

x: [N×D]

[ 2 1 -3 ]

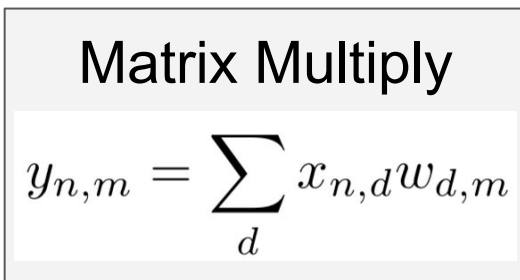
[ -3 4 2 ]

w: [D×M]

[ 3 2 1 -1 ]

[ 2 1 3 2 ]

[ 3 2 1 -2 ]



y: [N×M]

[13 9 -2 -6]

[ 5 2 17 1 ]

dL/dy: [N×M]

[ 2 3 -3 9 ]

[ -8 1 4 6 ]

Also see derivation by Prof. Justin Johnson:

<https://courses.cs.washington.edu/courses/cse493g1/23sp/resources/linear-backprop.pdf>

# Backprop with Matrices

$x: [N \times D]$

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

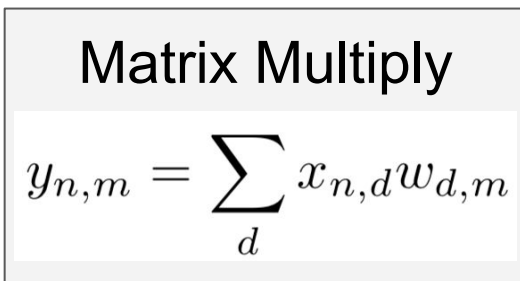
$\begin{bmatrix} -3 & 4 & 2 \end{bmatrix}$

$w: [D \times M]$

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

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

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



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

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



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

**Jacobians:**

$dy/dx: [(N \times D) \times (N \times M)]$

$dy/dw: [(D \times M) \times (N \times M)]$

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

x: [N×D]

[ 2 1 -3 ]

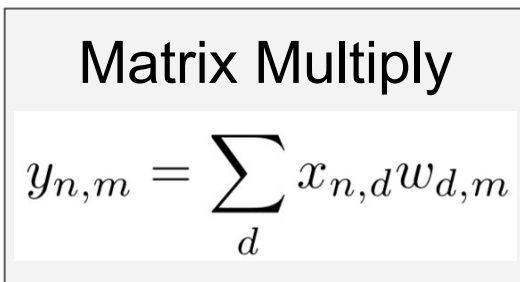
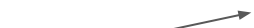
[ -3 4 2 ]

w: [D×M]

[ 3 2 1 -1 ]

[ 2 1 3 2 ]

[ 3 2 1 -2 ]



y: [N×M]  
[ 13 9 -2 -6 ]  
[ 5 2 17 1 ]

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



dL/dy: [N×M]  
[ 2 3 -3 9 ]  
[ -8 1 4 6 ]

# 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

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

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

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

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

y: [N×M]

[ 13 9 -2 -6 ]  
[ 5 2 17 1 ]

dL/dy: [N×M]

[ 2 3 -3 9 ]  
[ -8 1 4 6 ]

# 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**

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

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

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

**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  $y_{n,m}$ ?

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

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

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Matrix Multiply

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

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

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

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

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

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

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

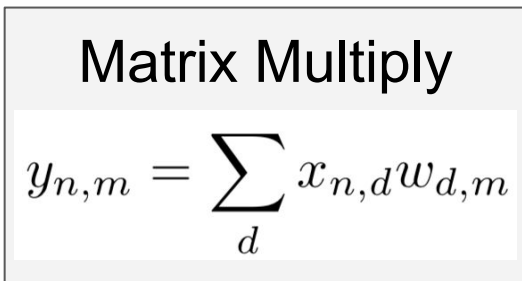
# Backprop with Matrices

x: [N×D]

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

w: [D×M]

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



y: [N×M]

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

dL/dy: [N×M]

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

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

[N×D] [N×M] [M×D]

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

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

# Backprop with Matrices

x: [N×D]

[ 2 1 -3 ]  
[ -3 4 2 ]

w: [D×M]

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[ 2 1 3 2 ]  
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Matrix Multiply

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

y: [N×M]

[ 13 9 -2 -6 ]  
[ 5 2 17 1 ]

dL/dy: [N×M]

[ 2 3 -3 9 ]  
[ -8 1 4 6 ]

By similar logic:

[N×D] [N×M] [M×D]

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

[D×M] [D×N] [N×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!

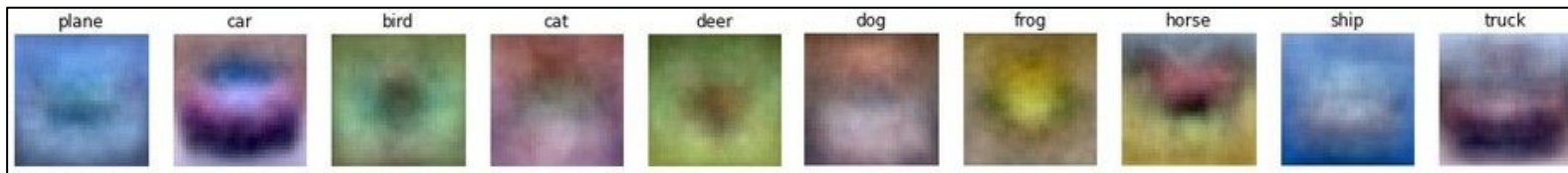
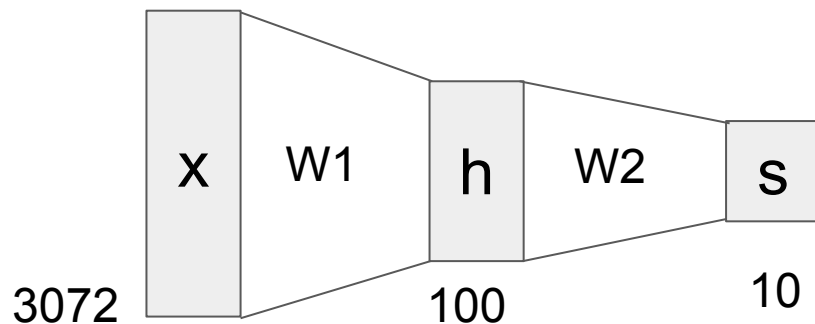
# Wrapping up: Neural Networks

Linear score function:

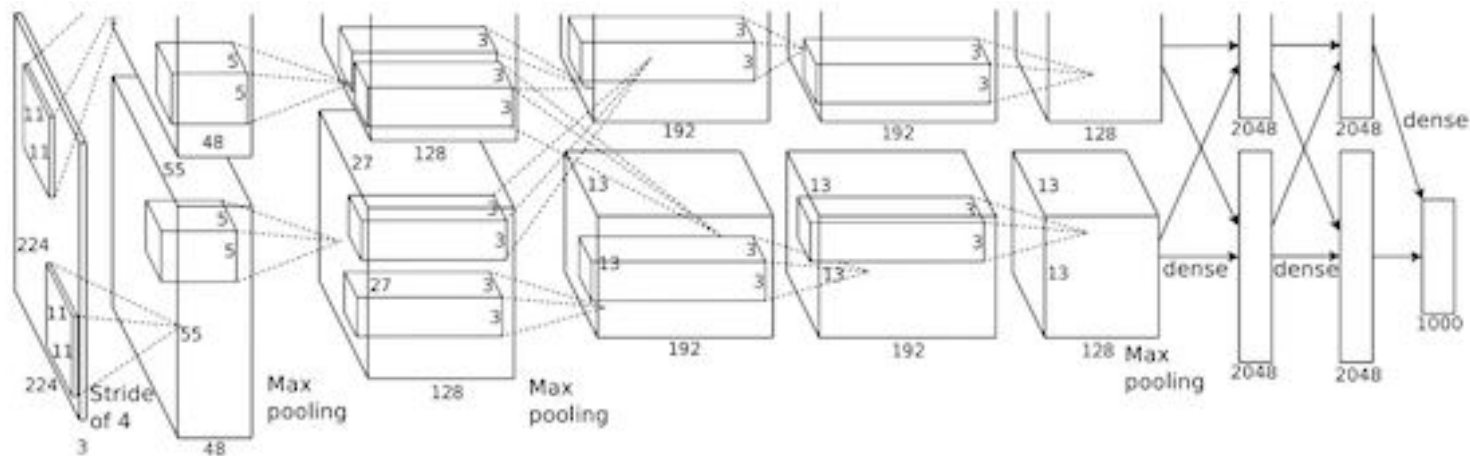
$$f = Wx$$

2-layer Neural Network

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



# Next Time: Convolutional neural networks



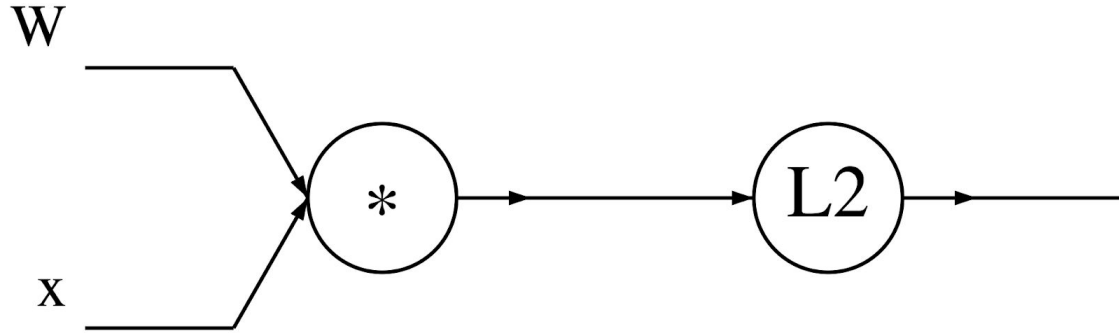


A vectorized example:  $f(x, W) = \|W \cdot x\|^2 = \sum_{i=1}^n (W \cdot x)_i^2$

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

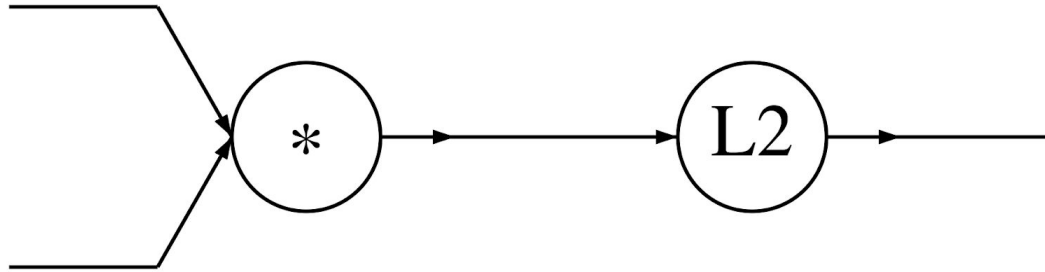
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$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} W$$

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

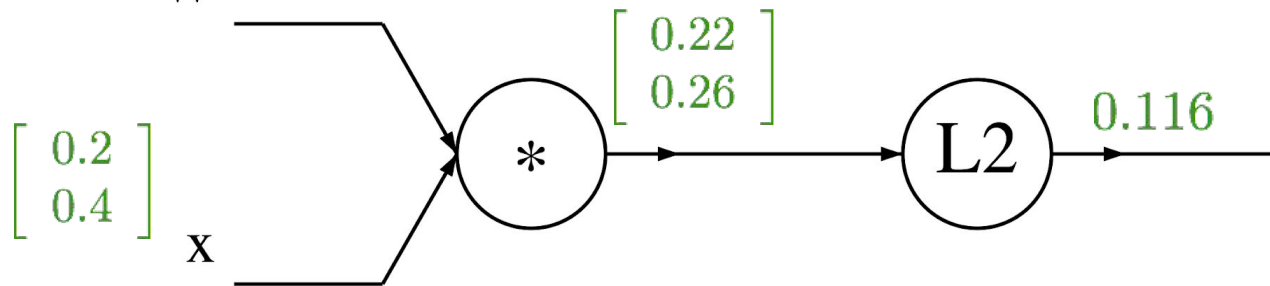


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

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

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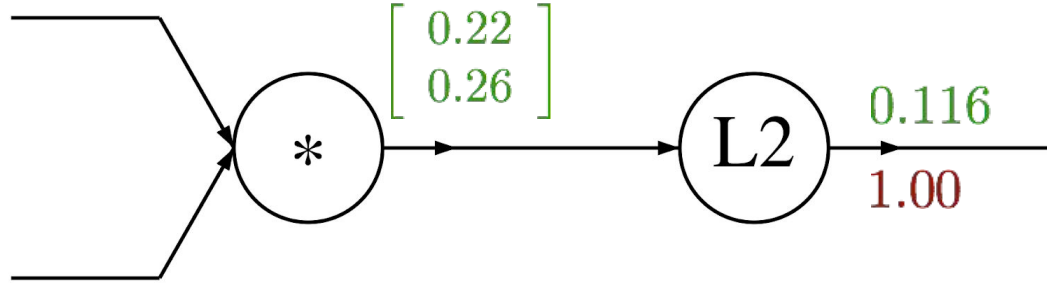
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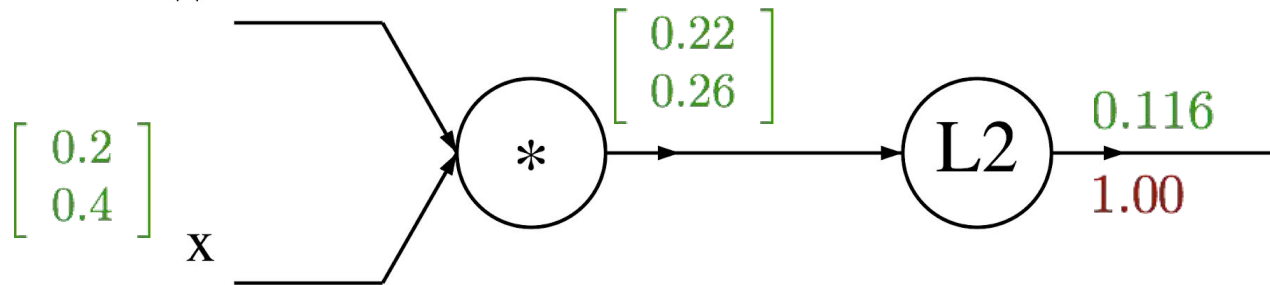


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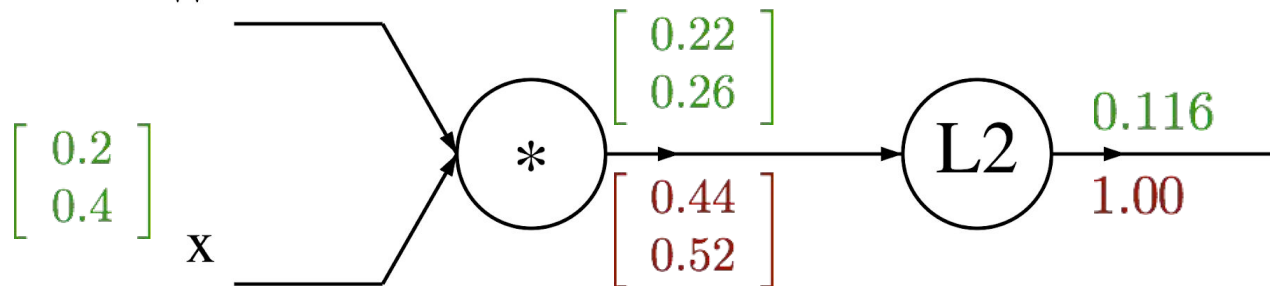
$$f(q) = \|q\|^2 = q_1^2 + \dots + q_n^2$$

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

$$\nabla_q f = 2q$$

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

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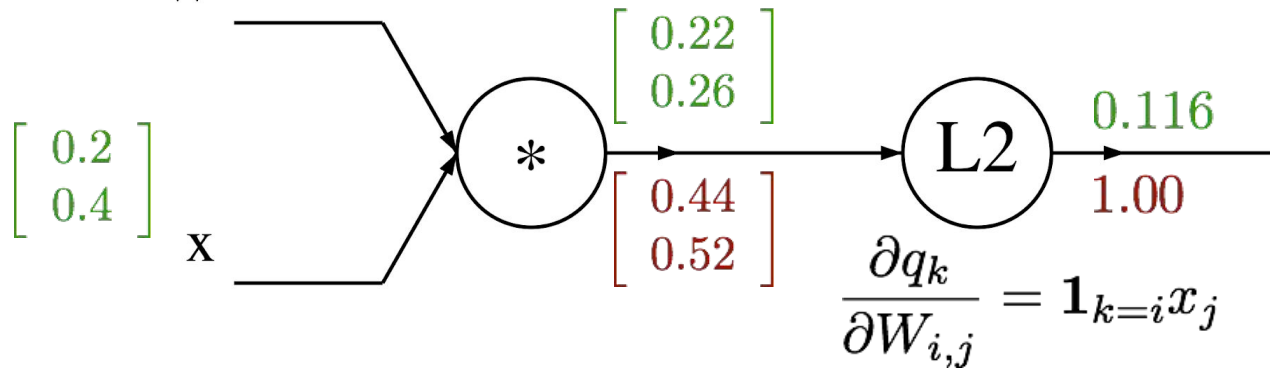
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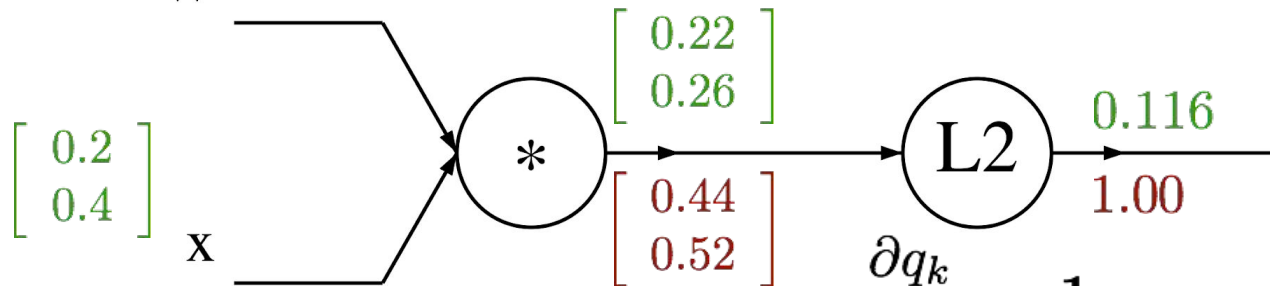
$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

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

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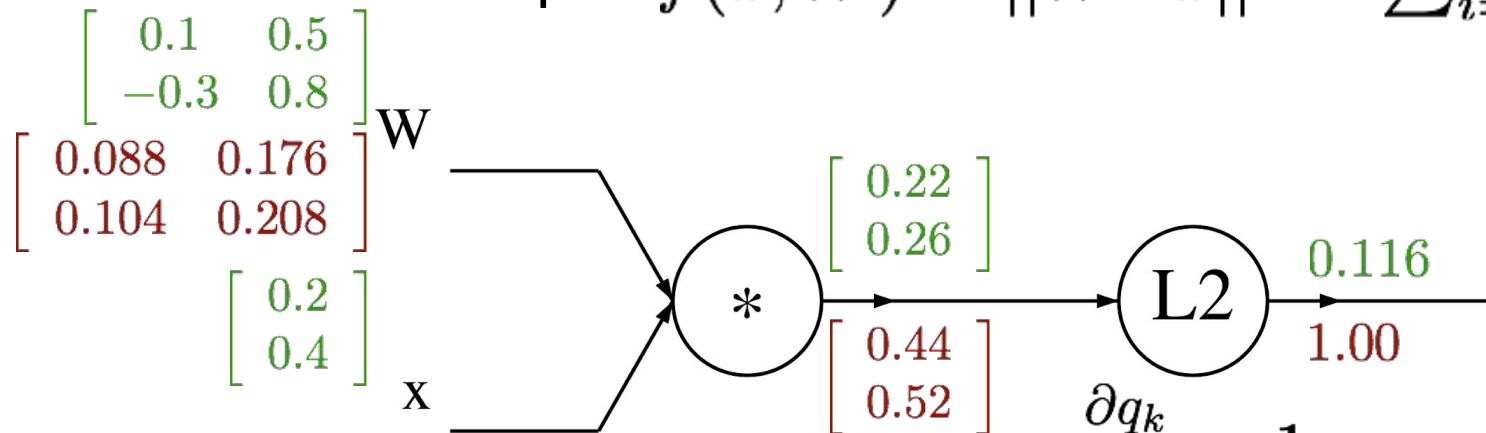
$$= \sum_k (2q_k) (\mathbf{1}_{k=i} x_j)$$

$$= 2q_i x_j$$

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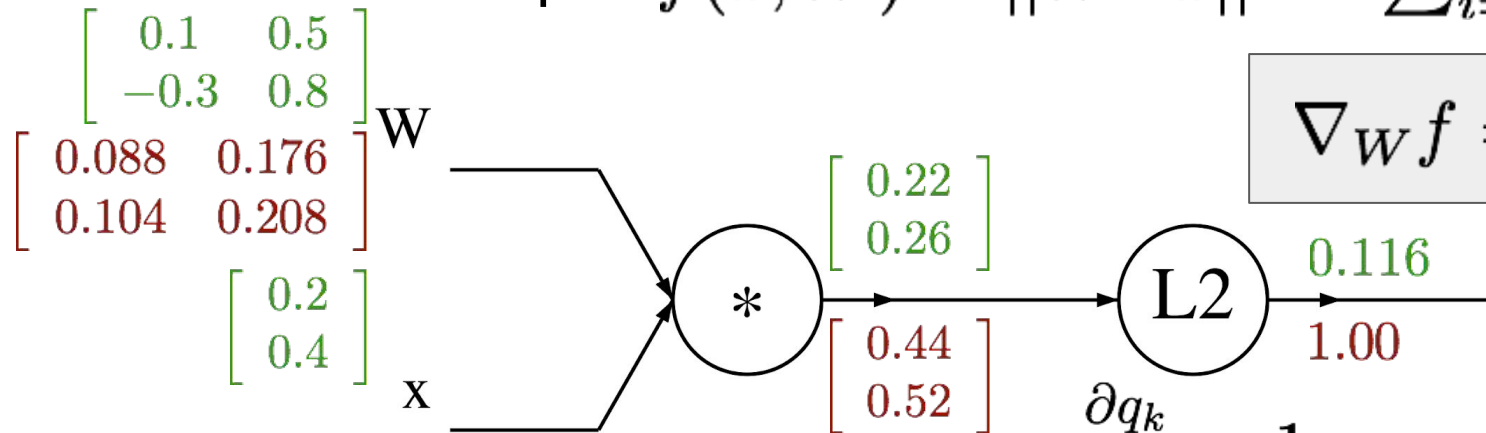


$$\begin{aligned} \frac{\partial q_k}{\partial W_{i,j}} &= \mathbf{1}_{k=i} x_j \\ \frac{\partial f}{\partial W_{i,j}} &= \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}} \\ &= \sum_k (2q_k) (\mathbf{1}_{k=i} x_j) \\ &= 2q_i x_j \end{aligned}$$

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$$\nabla_W f = 2q \cdot x^T$$

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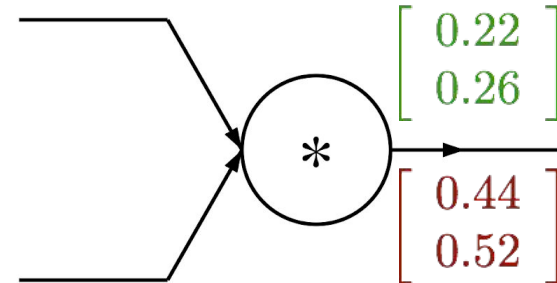
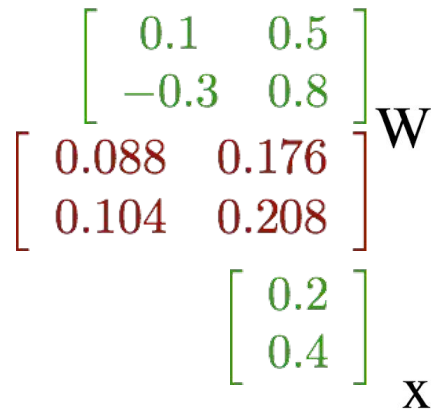
$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i}x_j$$

$$\frac{\partial f}{\partial W_{i,j}} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}}$$

$$= \sum_k (2q_k)(\mathbf{1}_{k=i}x_j)$$

$$= 2q_i x_j$$

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



$$\nabla_W f = 2q \cdot x^T$$

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

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

$$\frac{\partial f}{\partial W_{i,j}} = \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}}$$

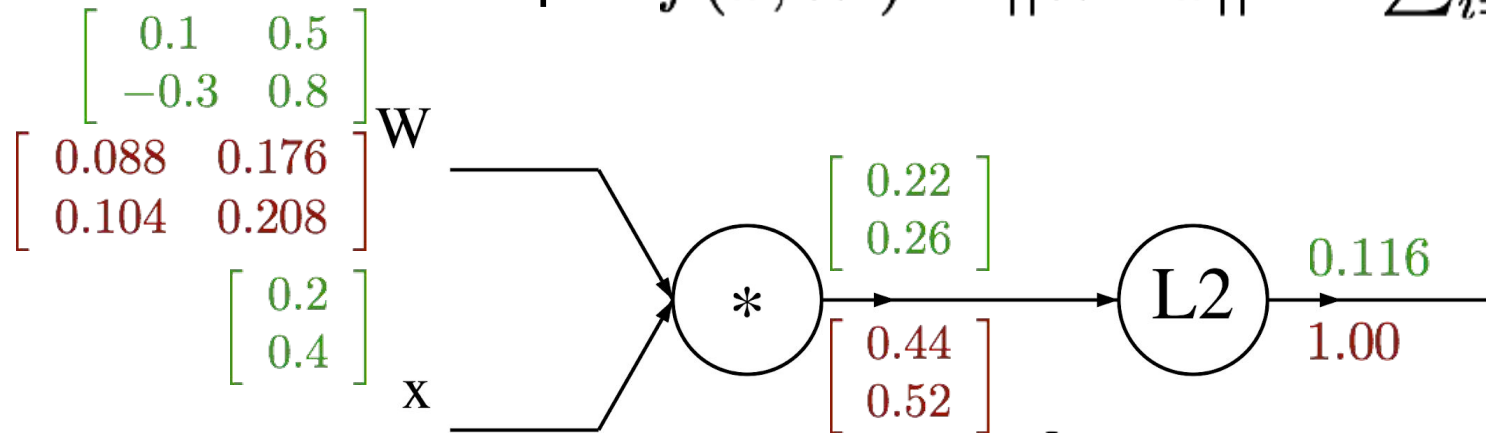
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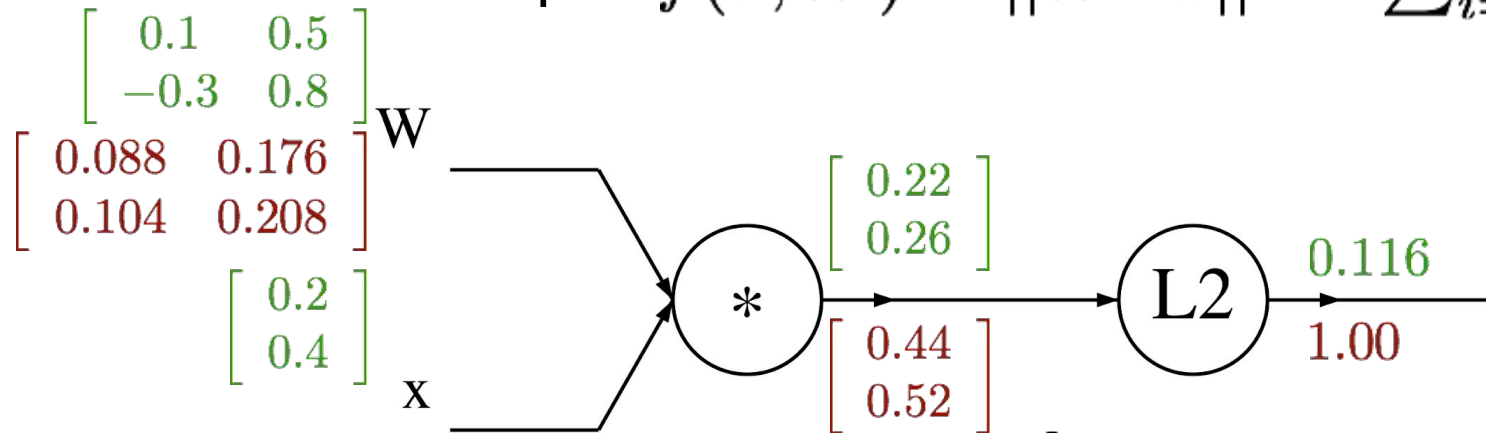


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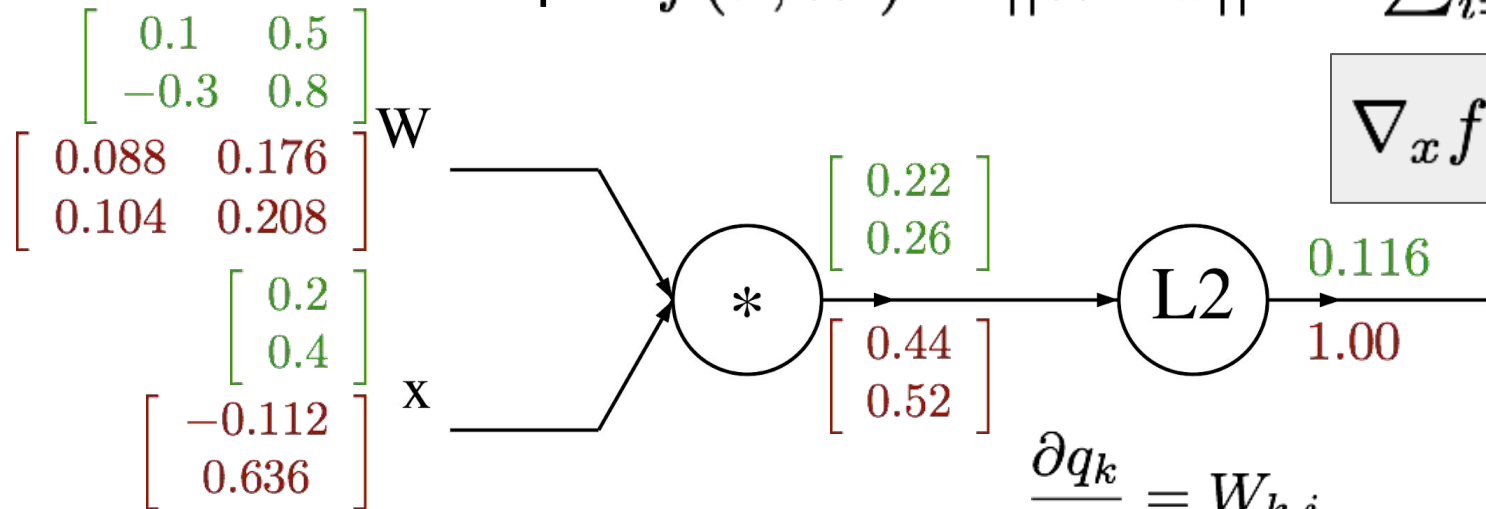
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$$\frac{\partial q_k}{\partial x_i} = W_{k,i}$$

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

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

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



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

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

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

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



# In discussion section: A matrix example...

$$z_1 = XW_1$$

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

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

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

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

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

