

Lecture 4: Neural Networks and Backpropagation

Administrative: Assignment 1

Assignment 1 due Wednesday April 22, 11:59pm

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

Administrative: Project Proposal

Project proposal due 4/27

Administrative: Discussion Section

Discussion section tomorrow:

Backpropagation

Administrative: Midterm Updates

University has updated guidance on administering exams in spring quarter. In order to comply with the current policies, we have changed the exam format as the following to be consistent with exams in previous offerings of cs 231n:

Date: released on Tuesday 5/12 (open for 24 hours to choose 1hr 40 mins time frame)

Format: Timestamped with Gradescope

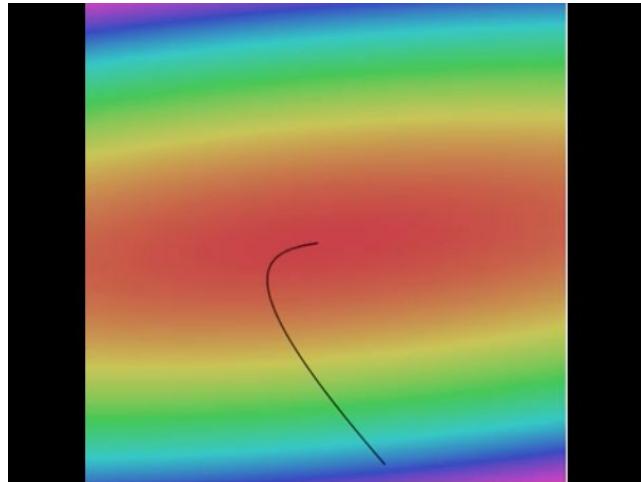
Where we are...

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

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

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

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

Where we are...

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

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How to find the best W ?

$$\boxed{\nabla_W L}$$

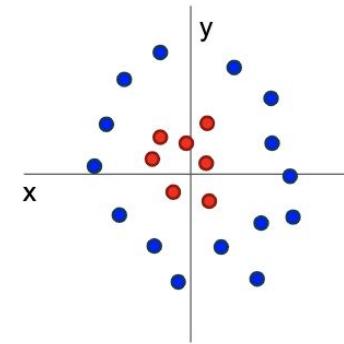
Problem: Linear Classifiers are not very powerful

Visual Viewpoint



Linear classifiers learn
one template per class

Geometric Viewpoint



Linear classifiers
can only draw linear
decision boundaries

Pixel Features

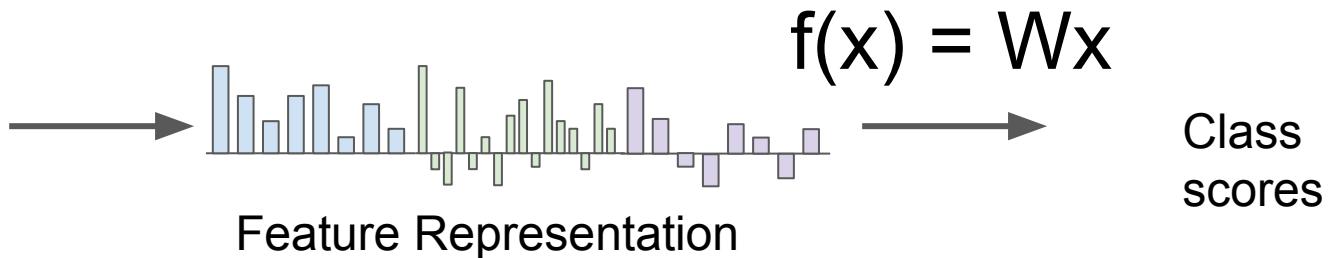


$$f(x) = Wx$$

Class
scores

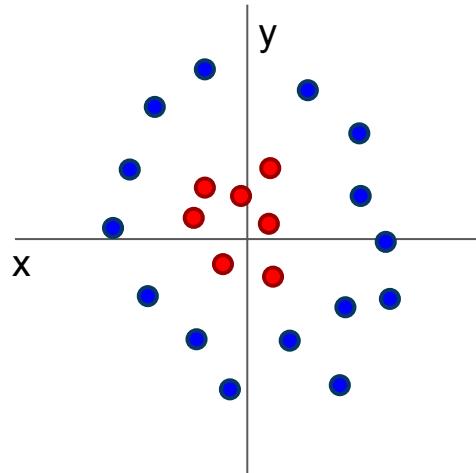


Image Features



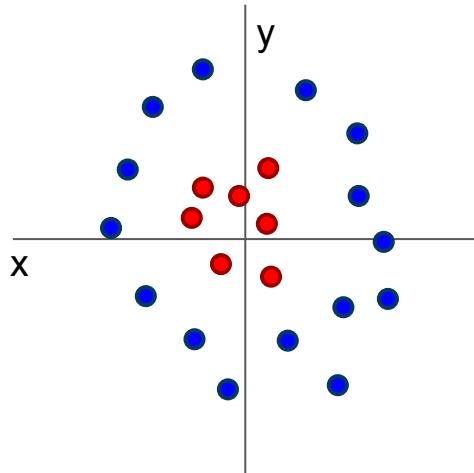
feed feature representation instead of raw pixels

Image Features: Motivation



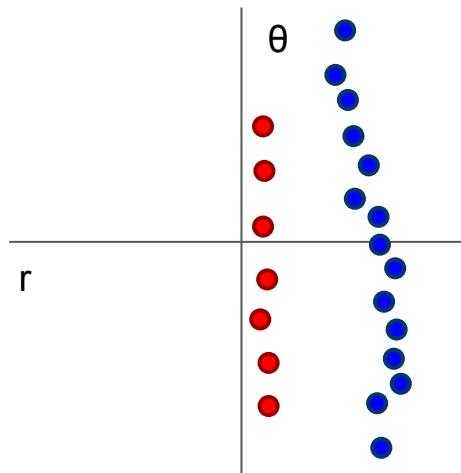
Cannot separate red
and blue points with
linear classifier

Image Features: Motivation



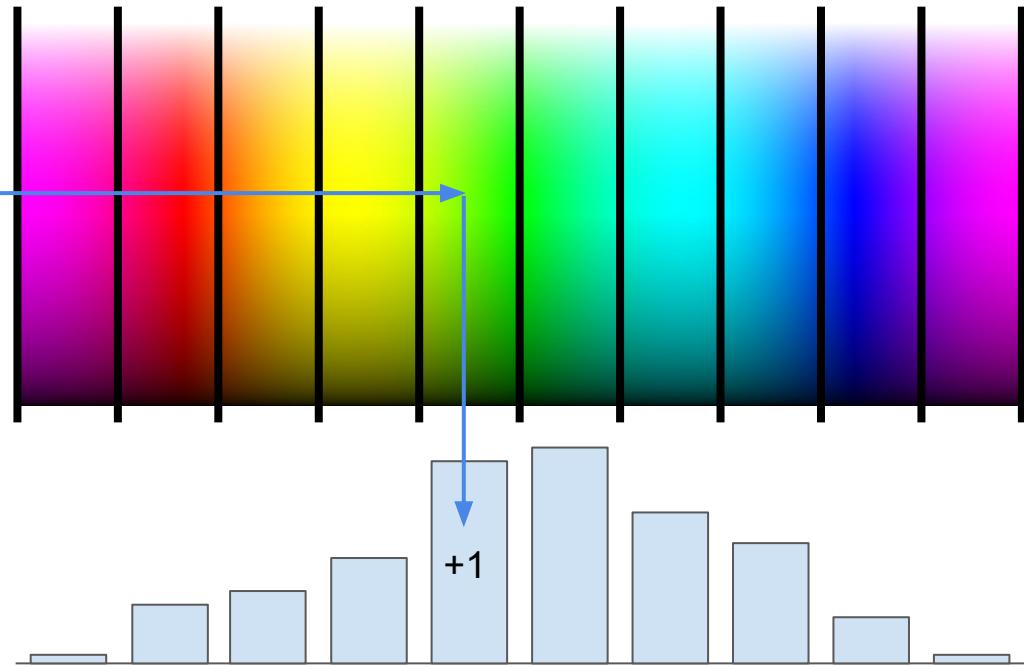
Cannot separate red
and blue points with
linear classifier

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



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

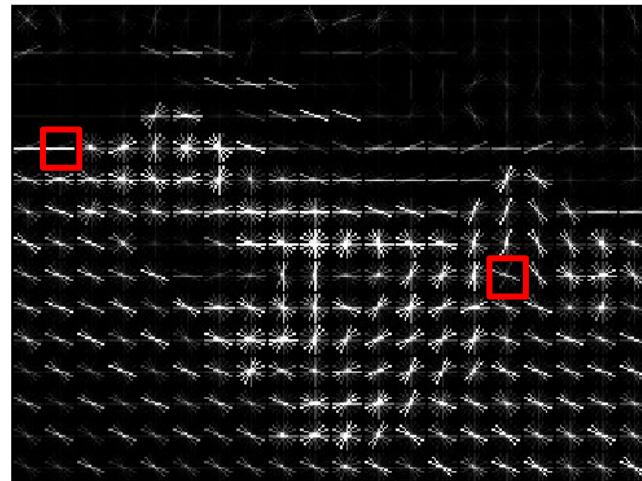
Example: Color Histogram



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
 $30*40*9 = 10,800$ numbers

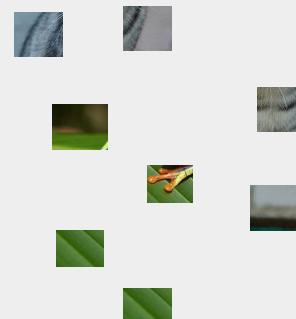
Lowe, "Object recognition from local scale-invariant features", ICCV 1999
Dalal and Triggs, "Histograms of oriented gradients for human detection," CVPR 2005

Example: Bag of Words

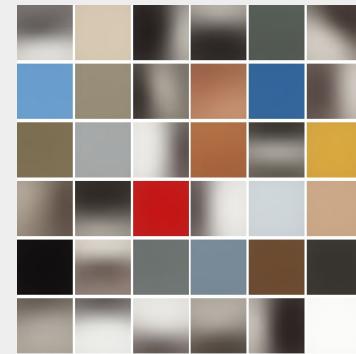
Step 1: Build codebook



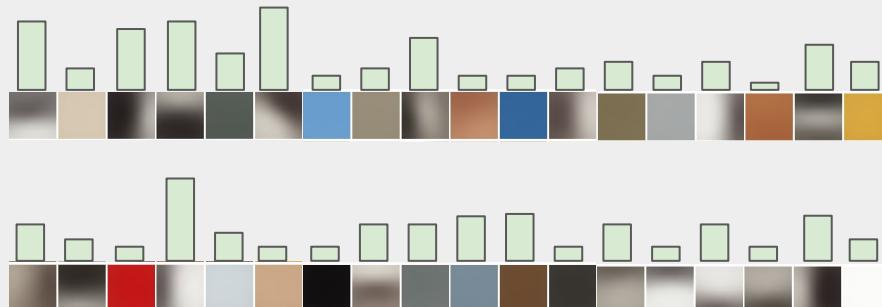
Extract random patches



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

Image Features

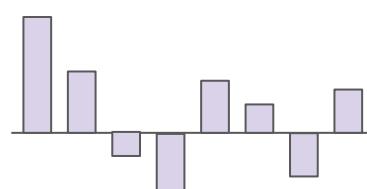
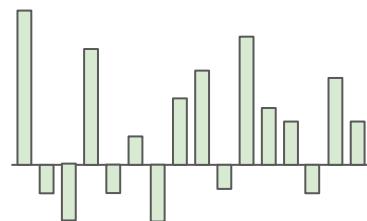
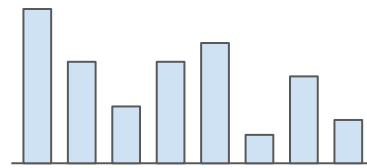


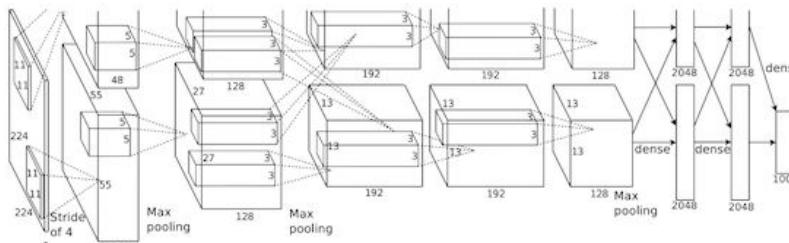
Image features vs ConvNets



f

training

10 numbers giving scores for classes

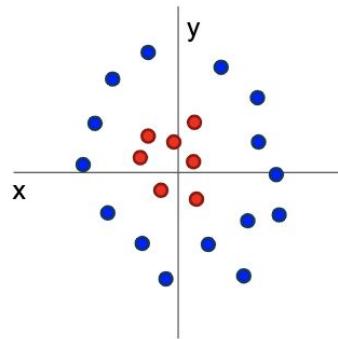


Krizhevsky, Sutskever, and Hinton, "Imagenet classification with deep convolutional neural networks", NIPS 2012.
Figure copyright Krizhevsky, Sutskever, and Hinton, 2012.
Reproduced with permission.

training

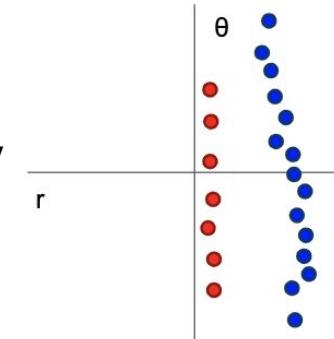
10 numbers giving scores for classes

One Solution: Feature Transformation

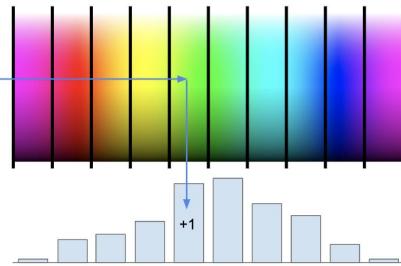


$$f(x, y) = (r(x, y), \theta(x, y))$$

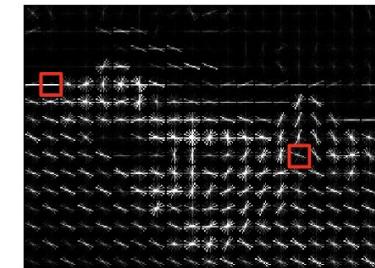
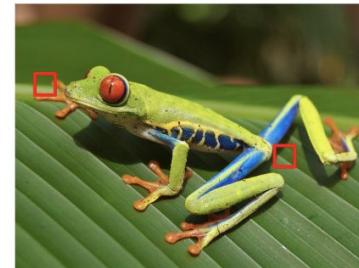
Transform data with a cleverly chosen **feature transform** f , then apply linear classifier



Color Histogram



Histogram of Oriented Gradients (HoG)



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

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

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

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

Neural networks: without the brain stuff

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“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

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

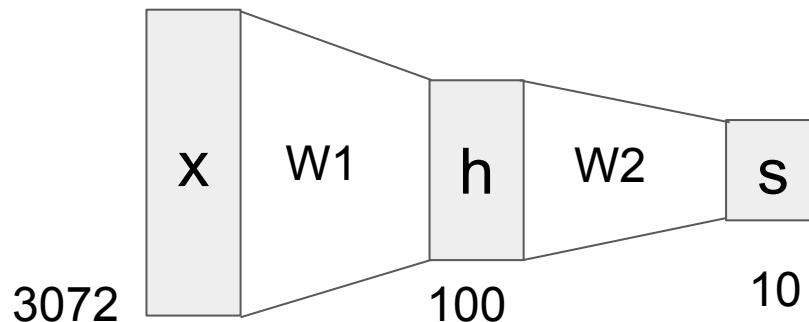
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

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

Neural networks: without the brain stuff

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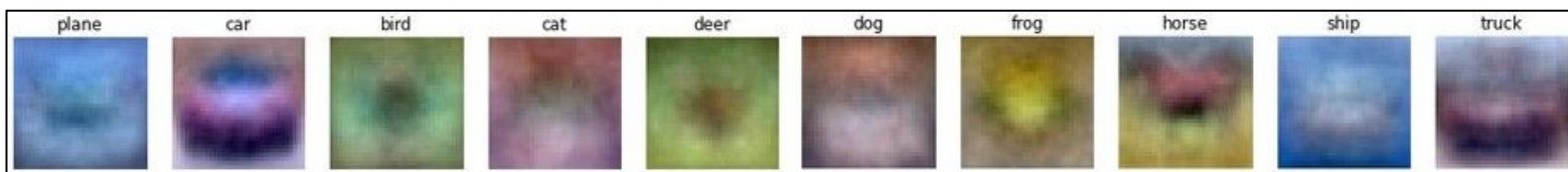
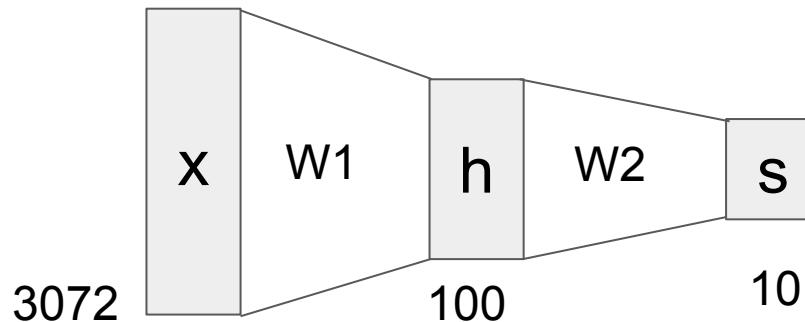


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Neural networks: without the brain stuff

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

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



Learn 100 templates instead of 10.

Share templates between classes

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

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

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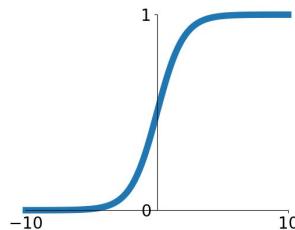
$$f = W_2 W_1 x \quad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

A: We end up with a linear classifier again!

Activation functions

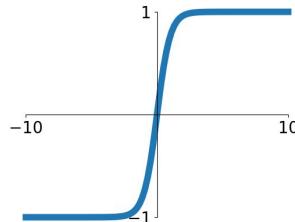
Sigmoid

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



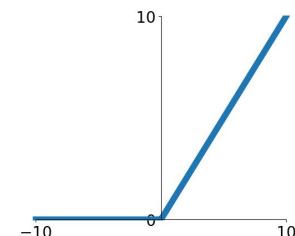
tanh

$$\tanh(x)$$



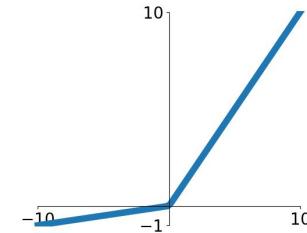
ReLU

$$\max(0, x)$$



Leaky ReLU

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

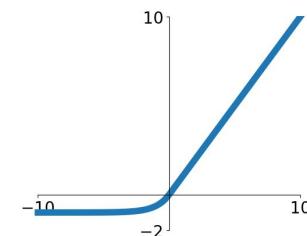


Maxout

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

ELU

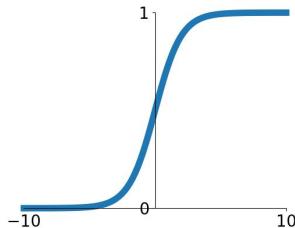
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Activation functions

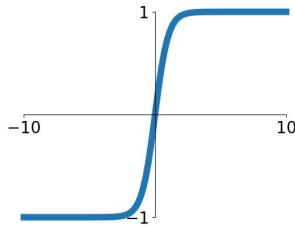
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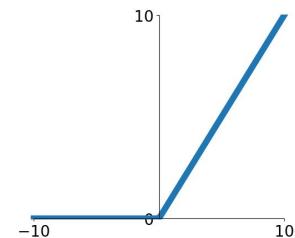
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ReLU

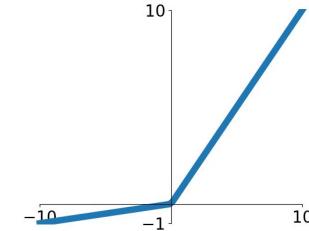
$$\max(0, x)$$



ReLU is a good default choice for most problems

Leaky ReLU

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

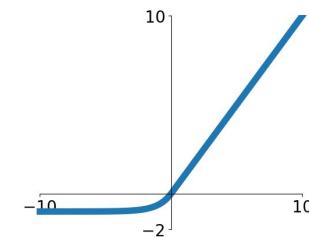


Maxout

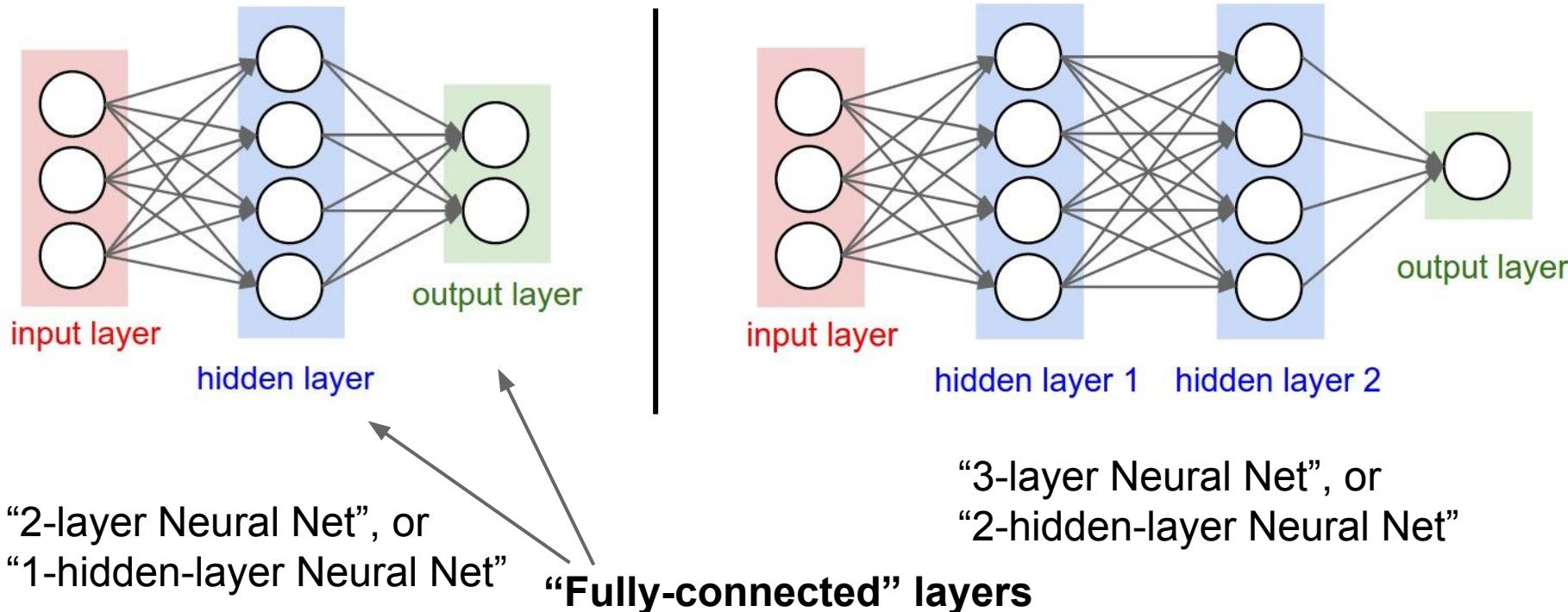
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

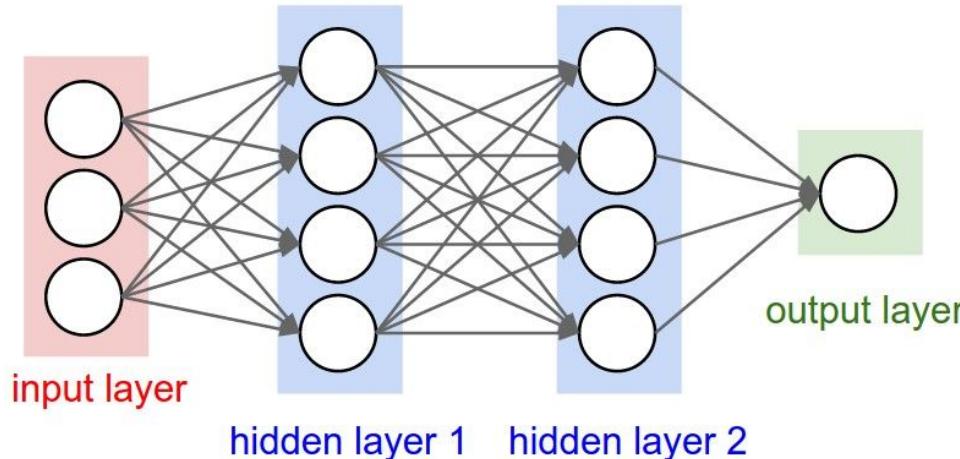
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Neural networks: Architectures



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
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Define the network

Forward pass

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Define the network

Forward pass

Calculate the analytical gradients

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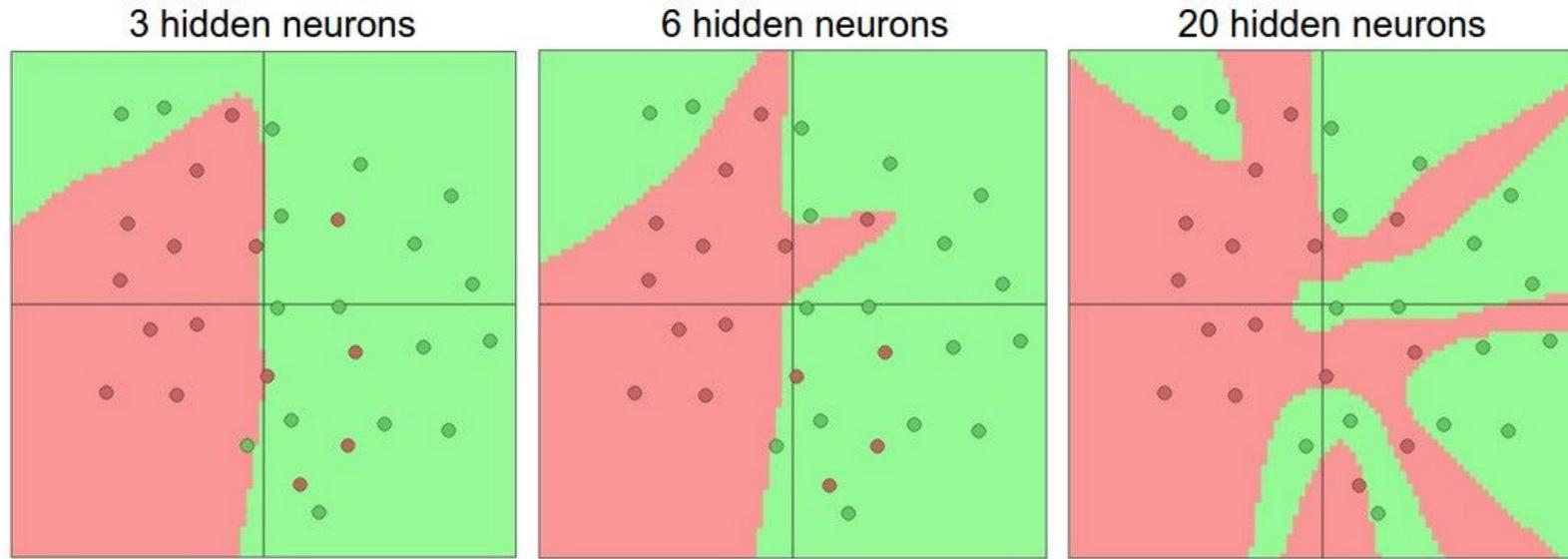
Define the network

Forward pass

Calculate the analytical gradients

Gradient descent

Setting the number of layers and their sizes



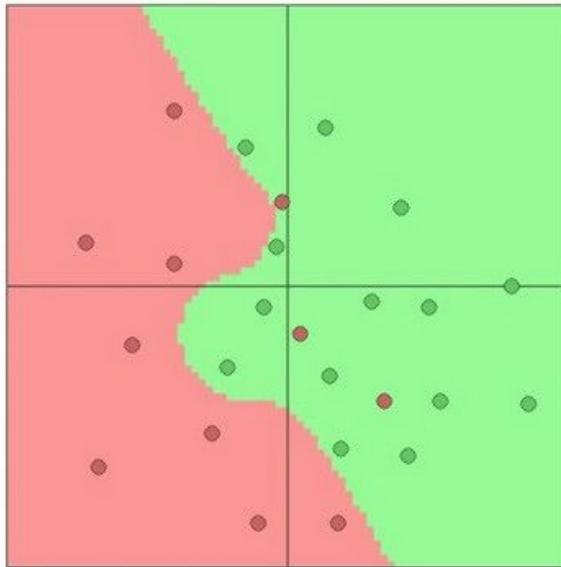
more neurons = more capacity

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

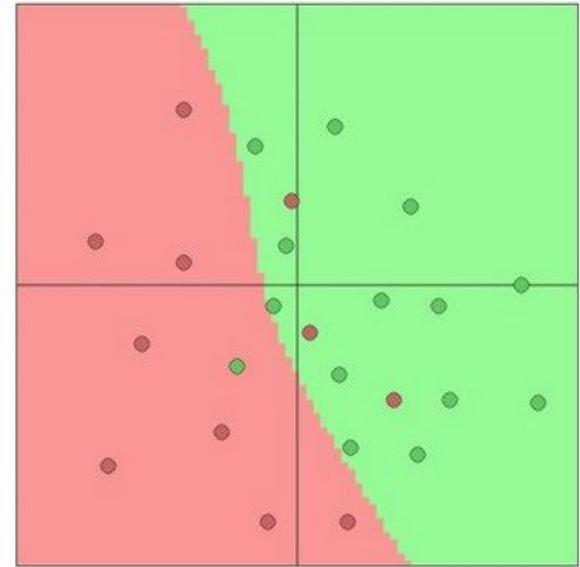
$\lambda = 0.001$



$\lambda = 0.01$



$\lambda = 0.1$



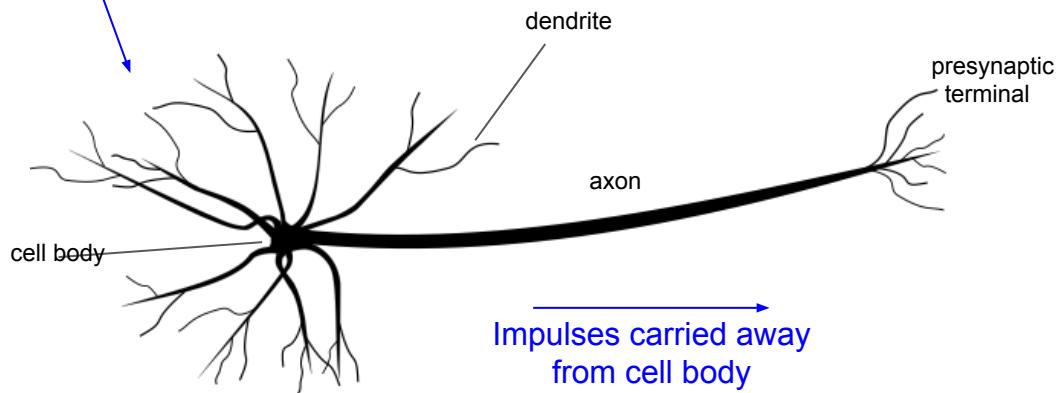
(Web demo with ConvNetJS:
[http://cs.stanford.edu/people/karpathy/convnetjs/demo
/classify2d.html](http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html))

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



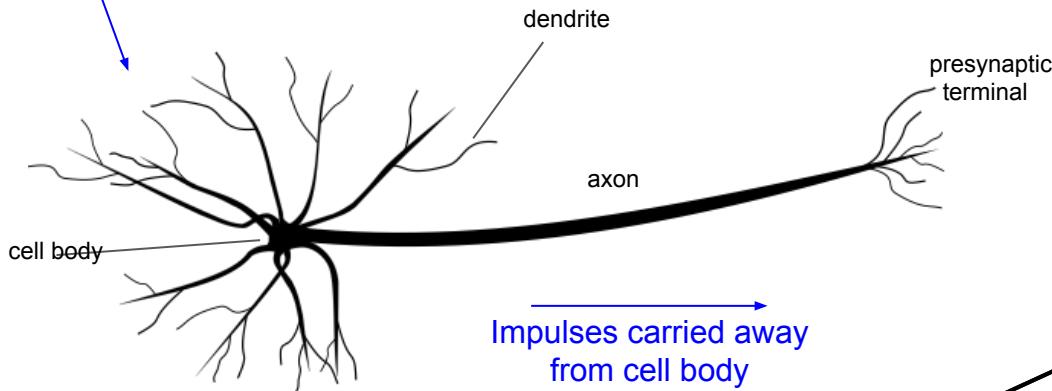
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Impulses carried toward cell body



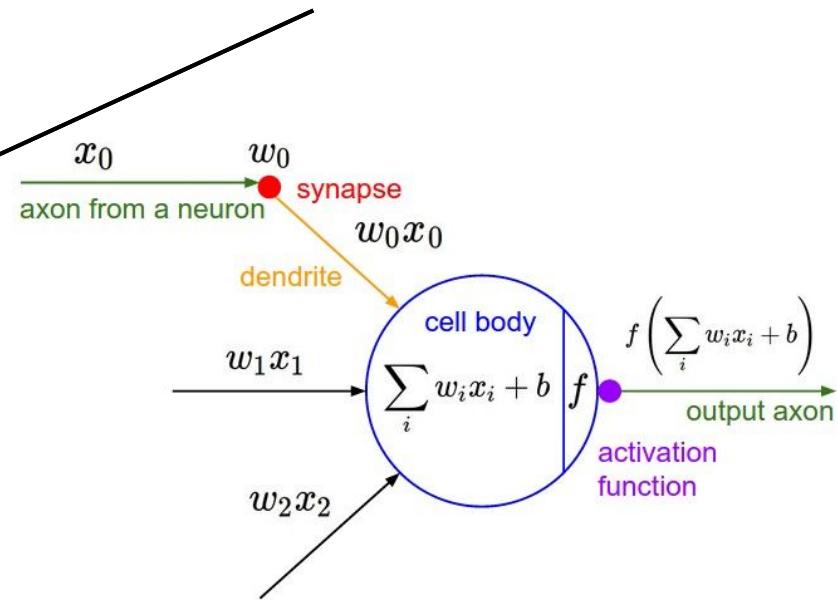
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Impulses carried toward cell body

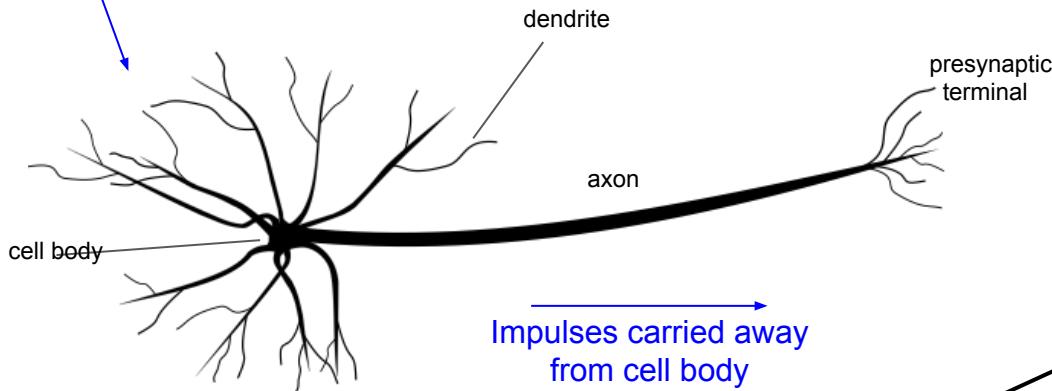


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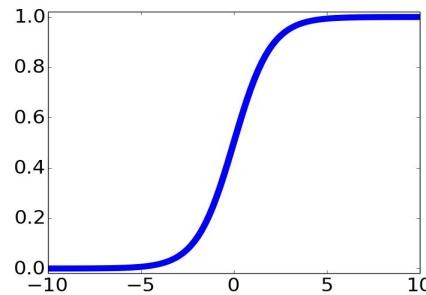
Impulses carried away
from cell body



Impulses carried toward cell body



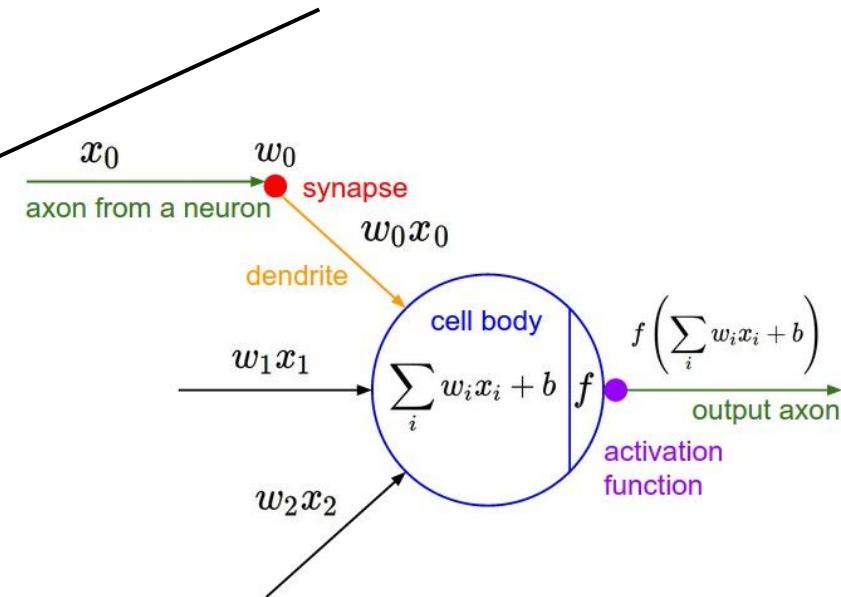
This image by Felipe Perucho
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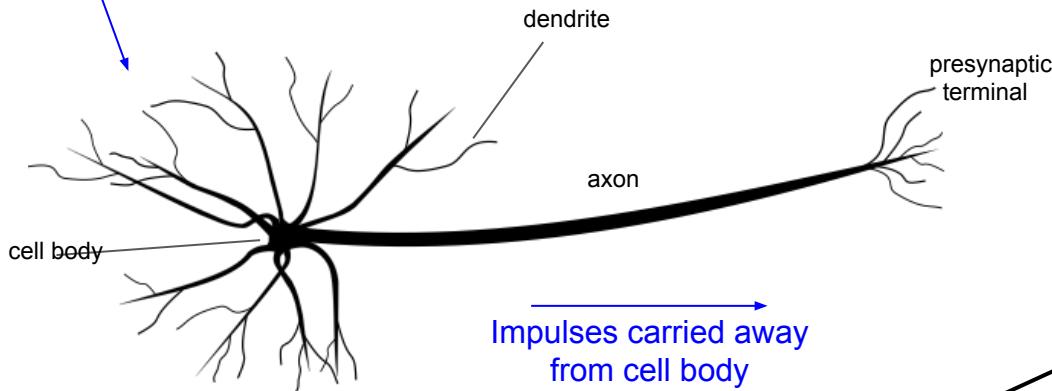
sigmoid activation function

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

Impulses carried away from cell body

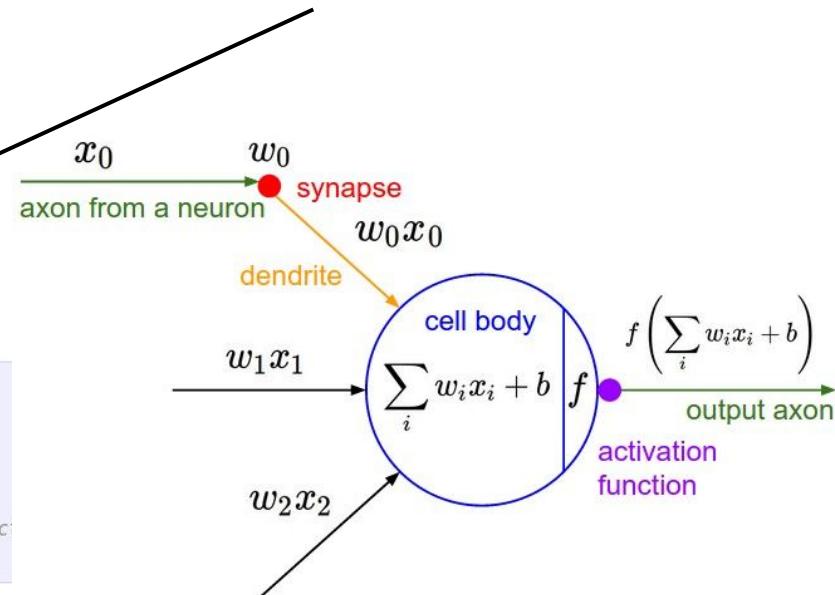


Impulses carried toward cell body

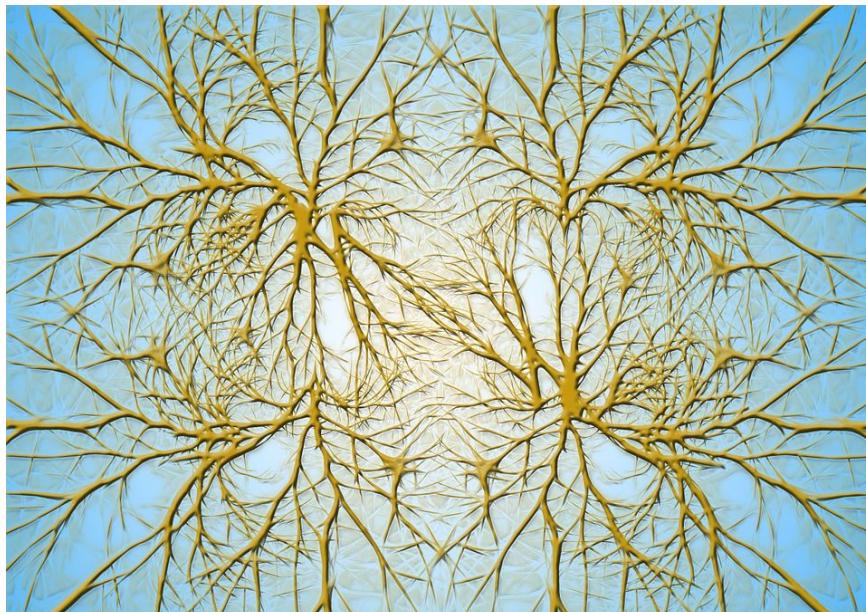


This image by Felipe Perucho
is licensed under CC-BY 3.0

```
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 function  
        return firing_rate
```

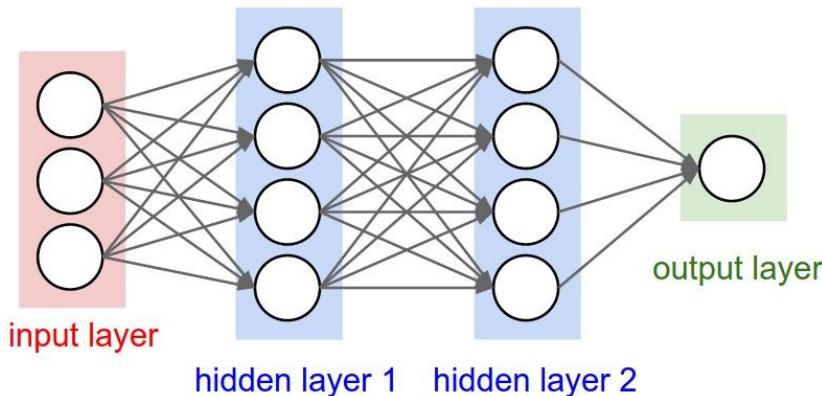


Biological Neurons: Complex connectivity patterns

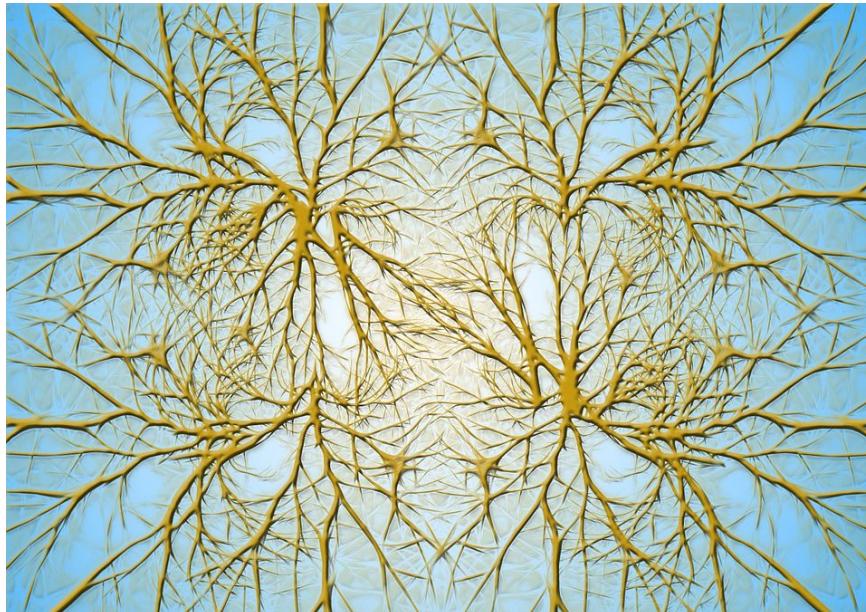


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Neurons in a neural network:
Organized into regular layers for
computational efficiency

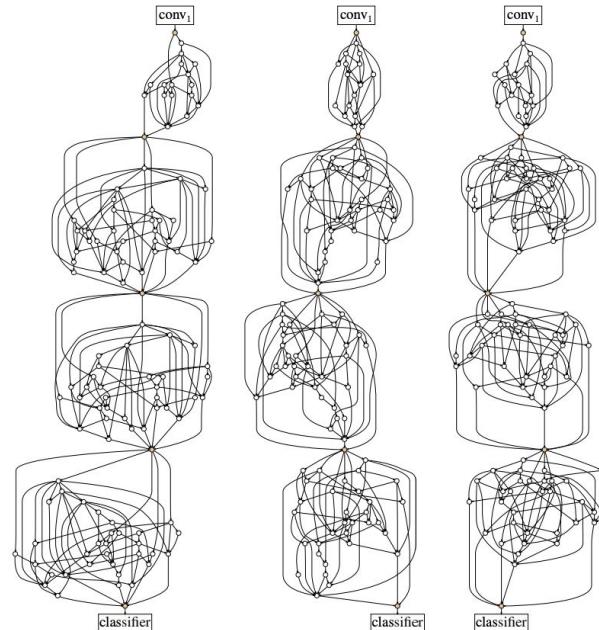


Biological Neurons: Complex connectivity patterns



[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 Häusser]

how to compute the analytic gradient for arbitrarily complex functions, using a framework that I'm going to call computational graphs.

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

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

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

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

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

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

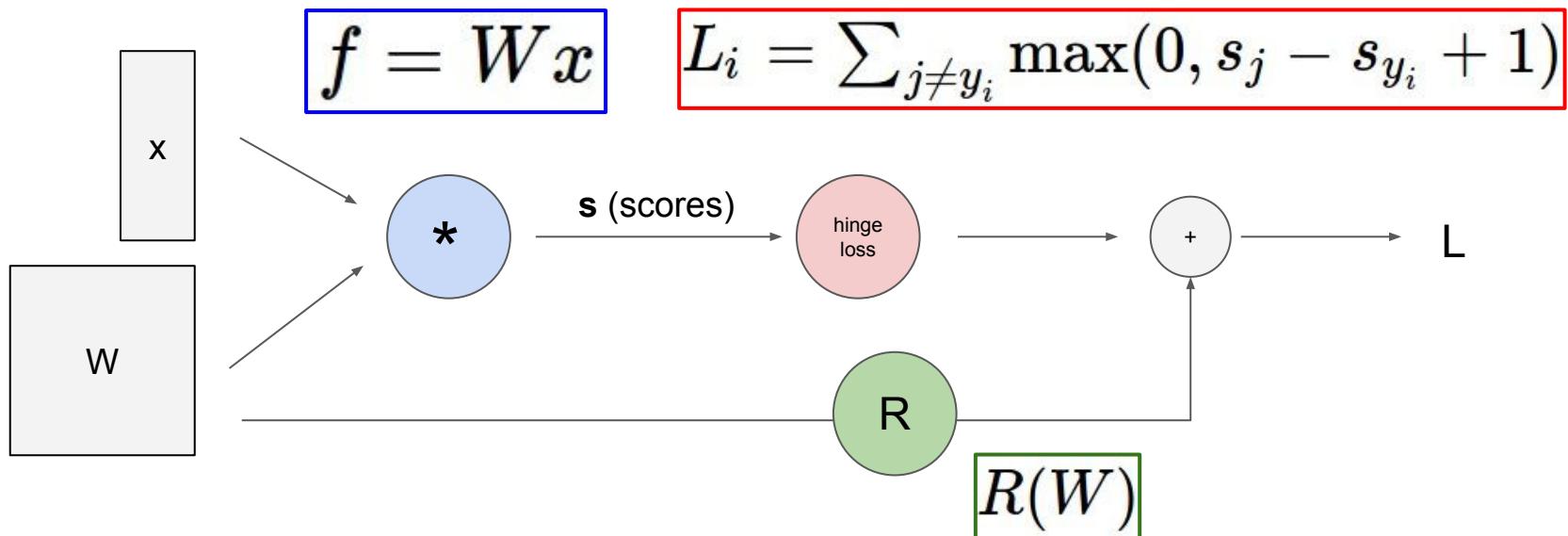
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

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



The advantage is that once we can express a function using a computational graph, then we can use a technique called 'backpropagation' which is going to recursively use the chain rule in order to compute the gradient with respect to every variable in the computational graph.

Convolutional network (AlexNet)

input image

weights

loss

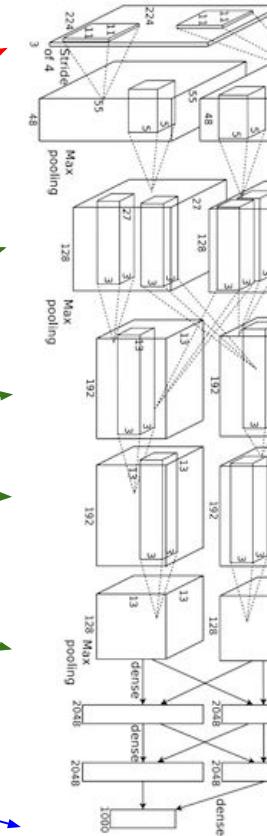


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

Neural Turing Machine

input image

loss

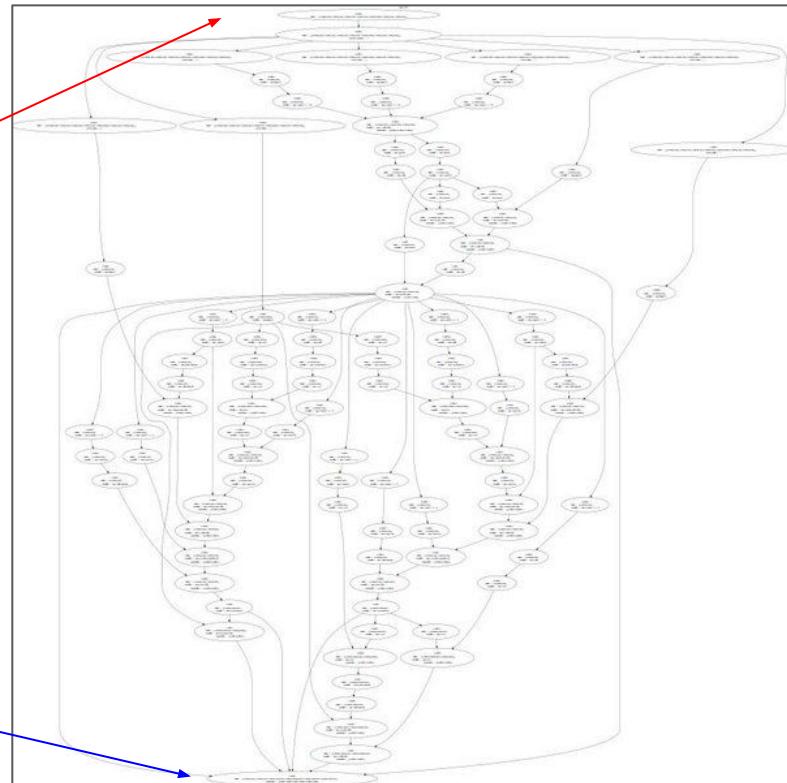


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

Neural Turing Machine

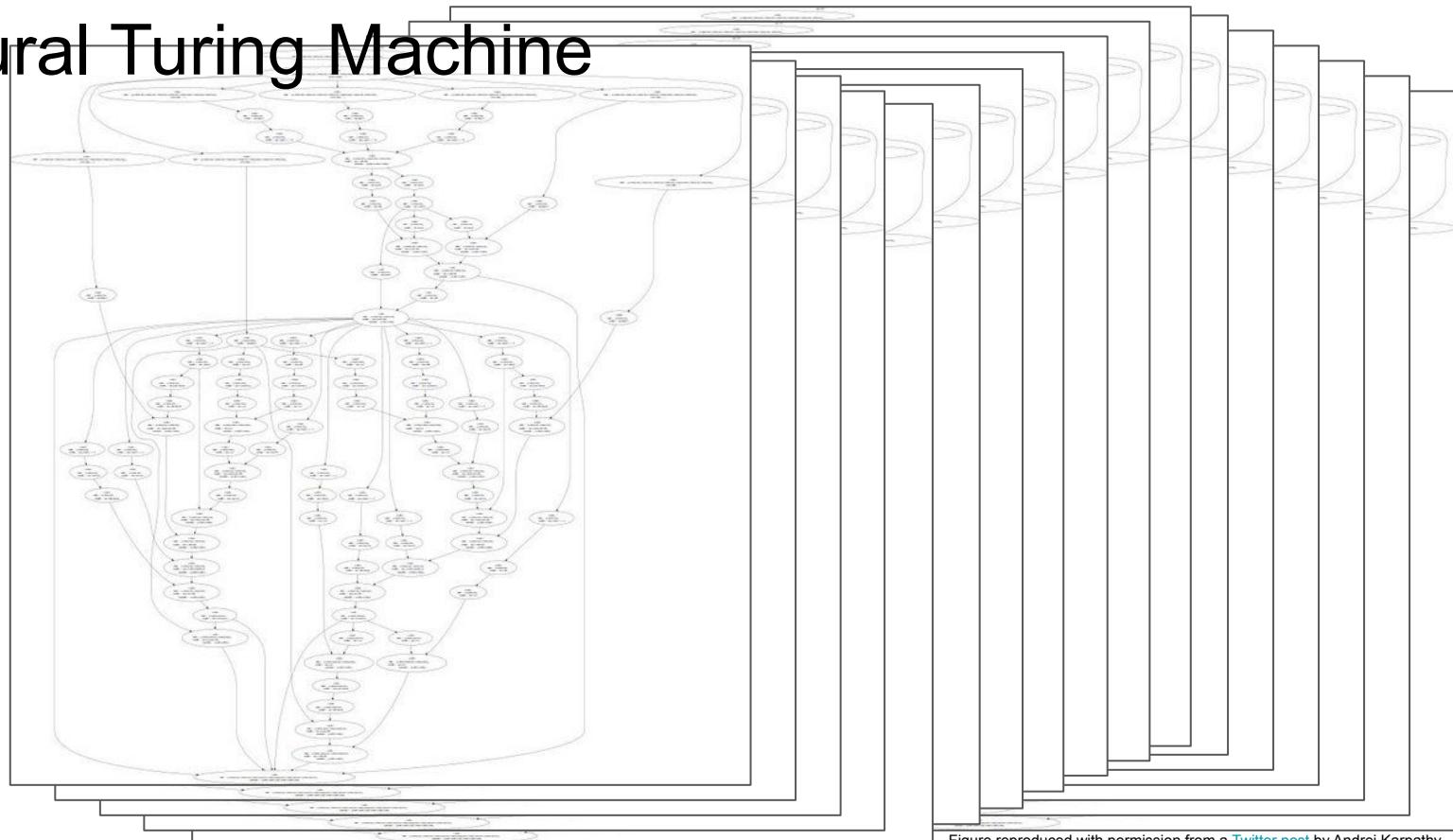


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

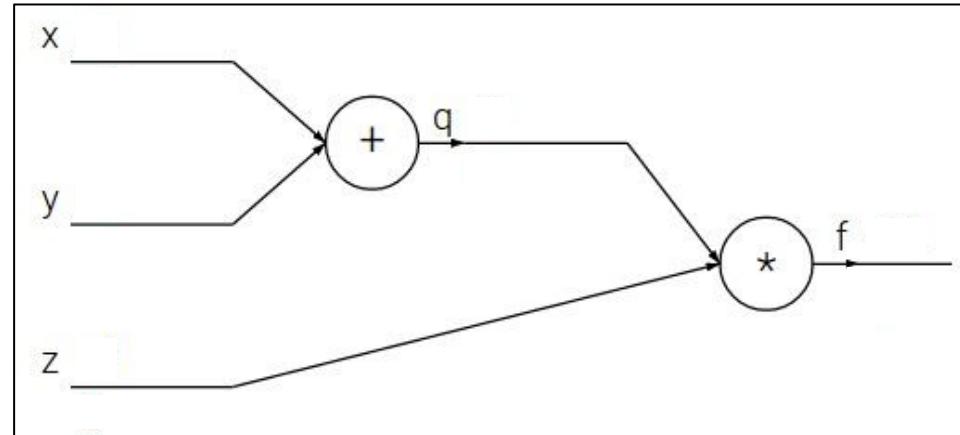
Solution: Backpropagation

Backpropagation: a simple example

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

Backpropagation: a simple example

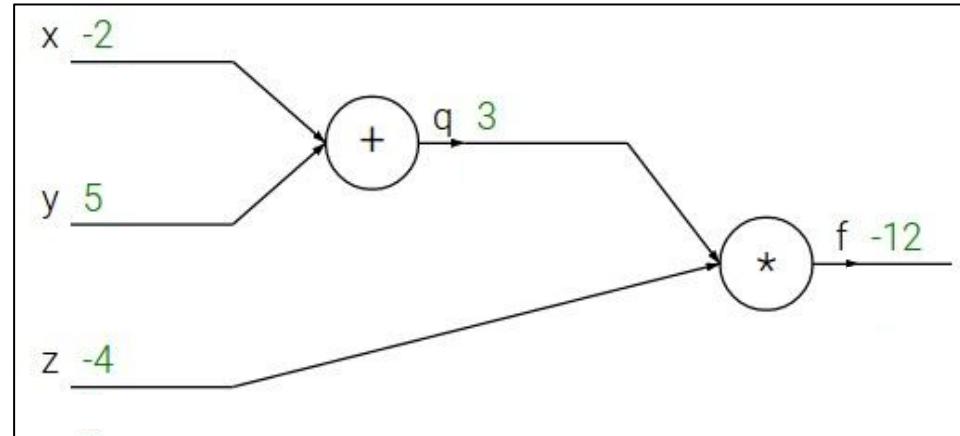
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Backpropagation: a simple example

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

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

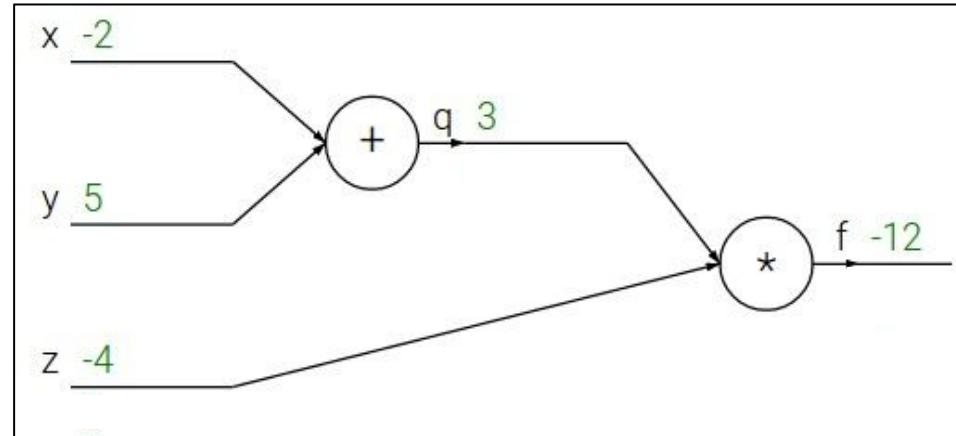


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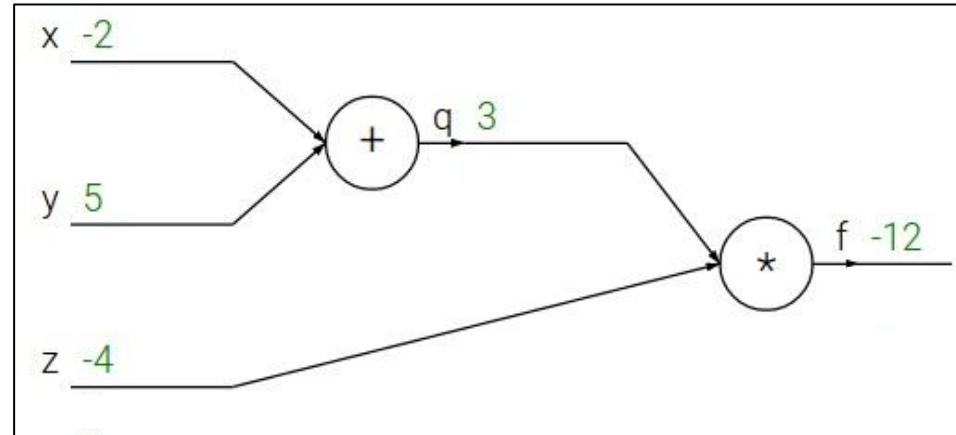
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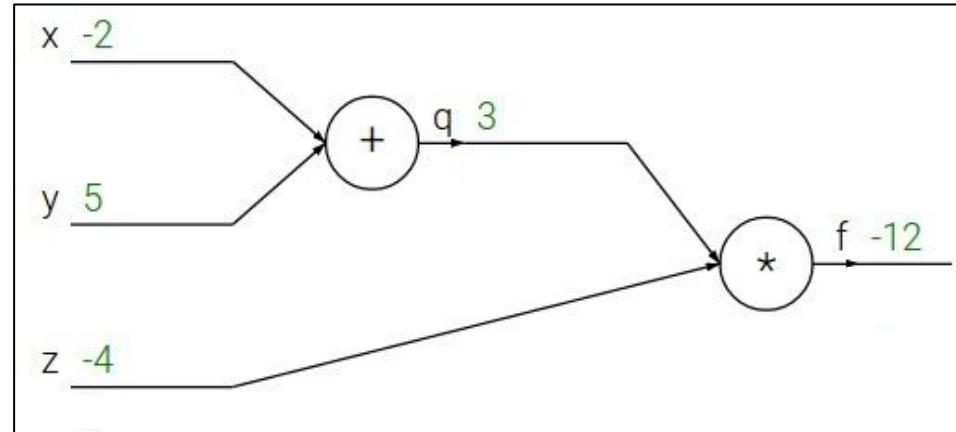
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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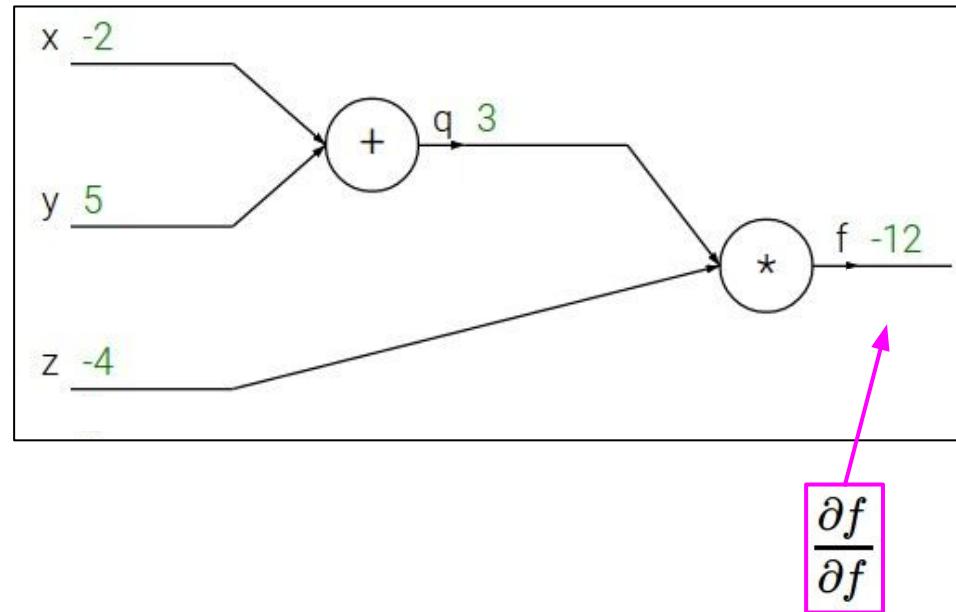
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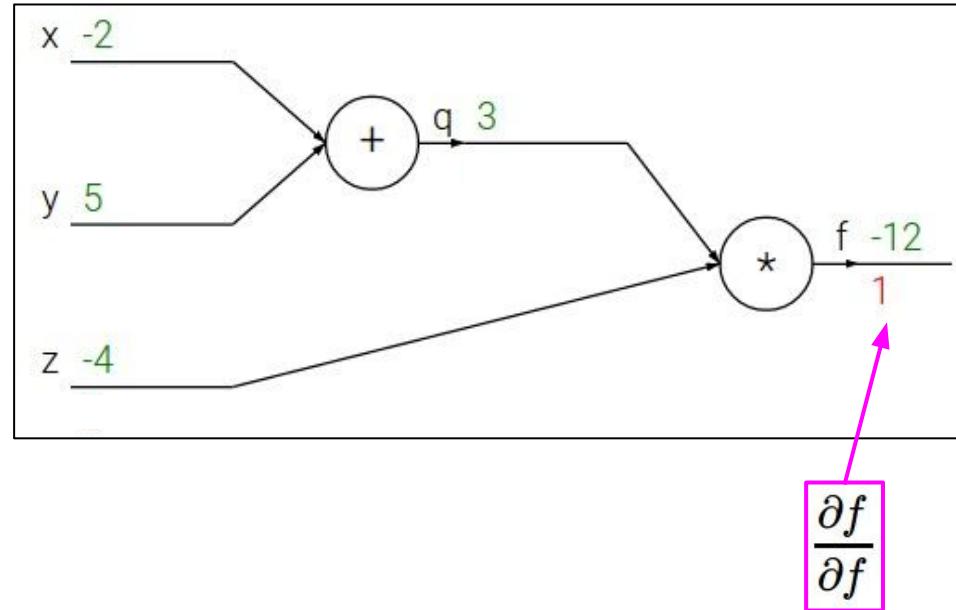
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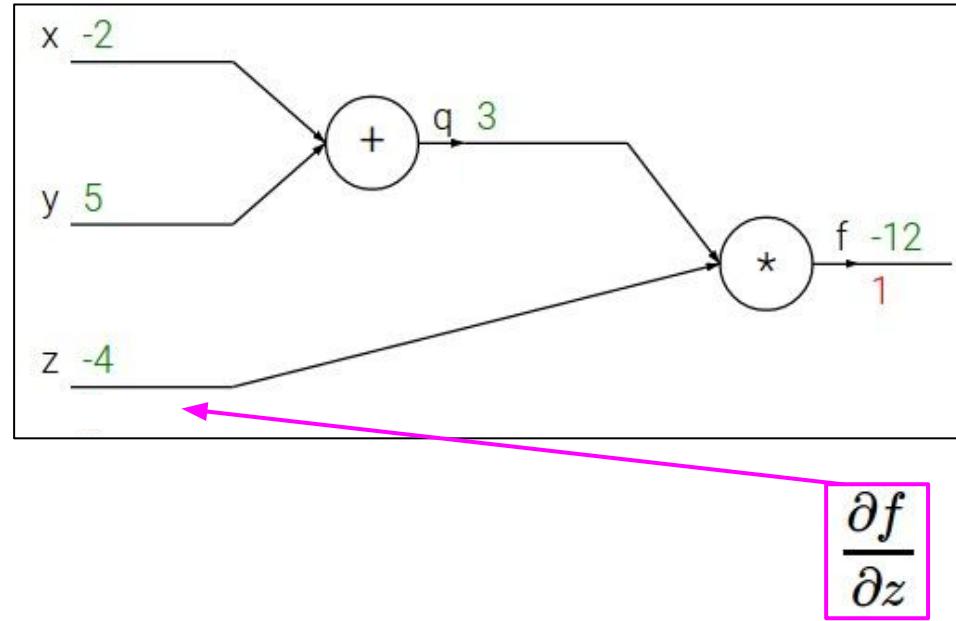
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$$\frac{\partial f}{\partial z}$$

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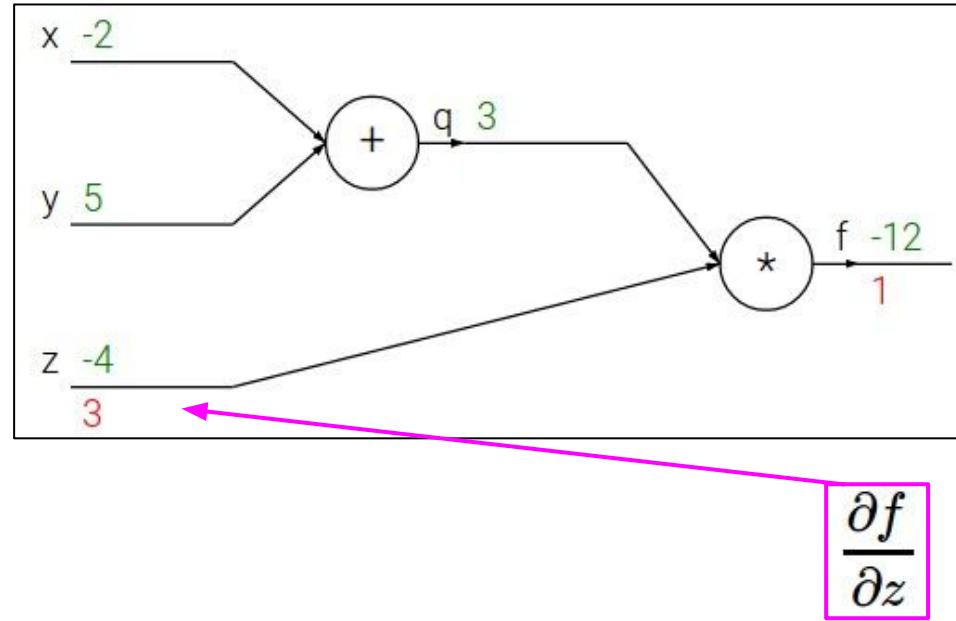
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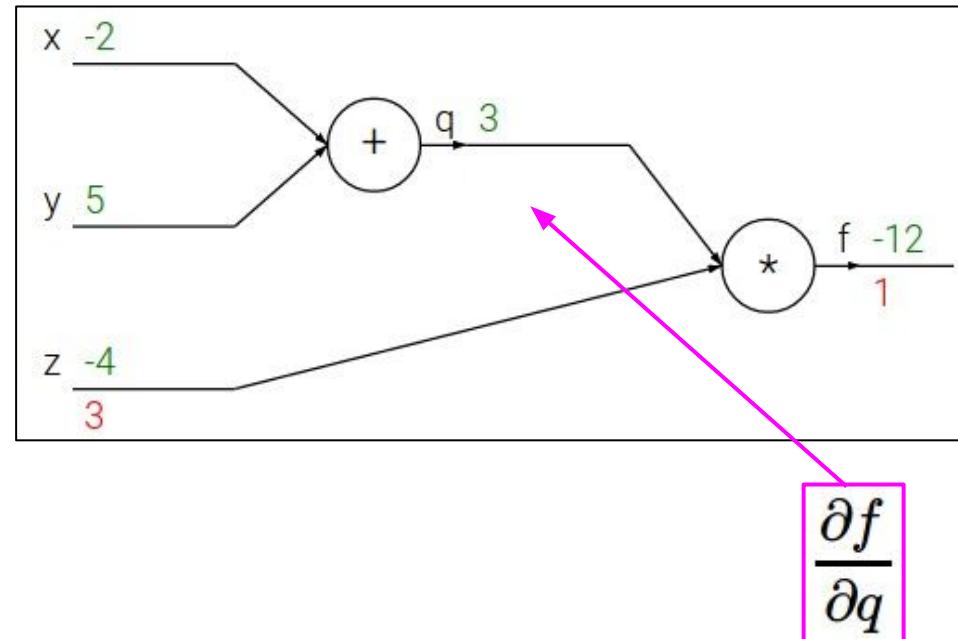
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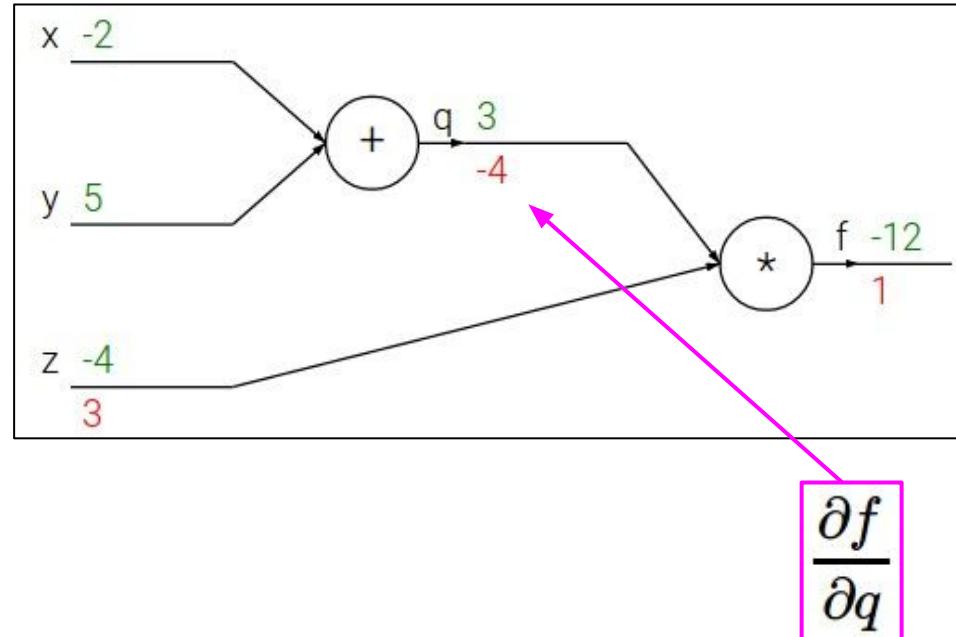
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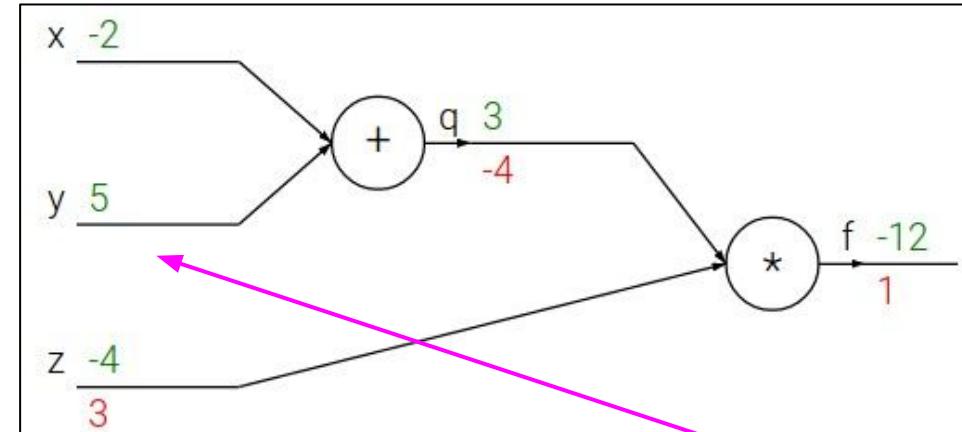
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Chain rule:

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

Upstream
gradient

Local
gradient

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

Backpropagation: a simple example

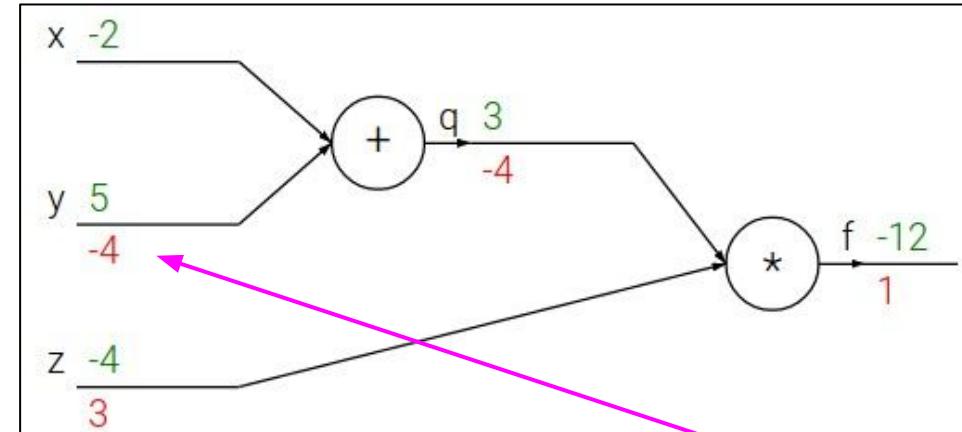
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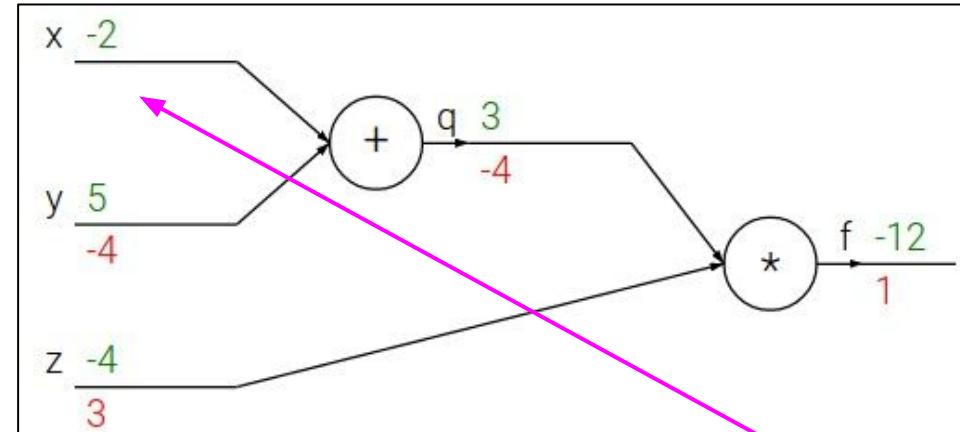
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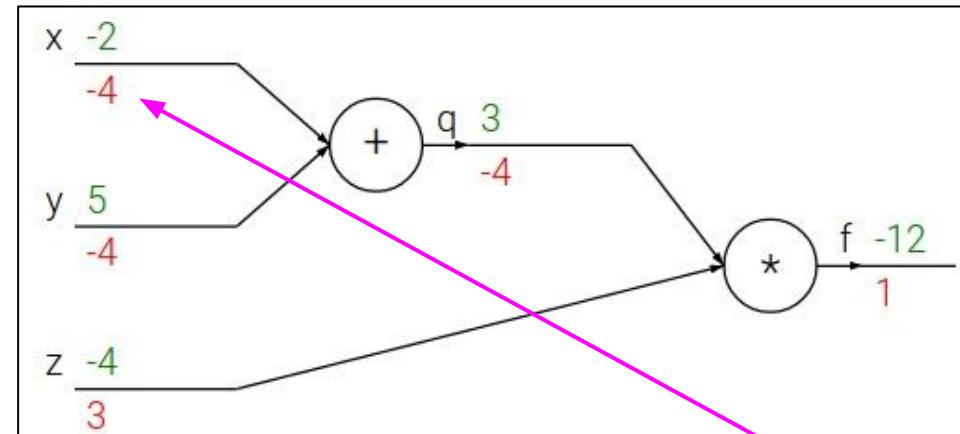
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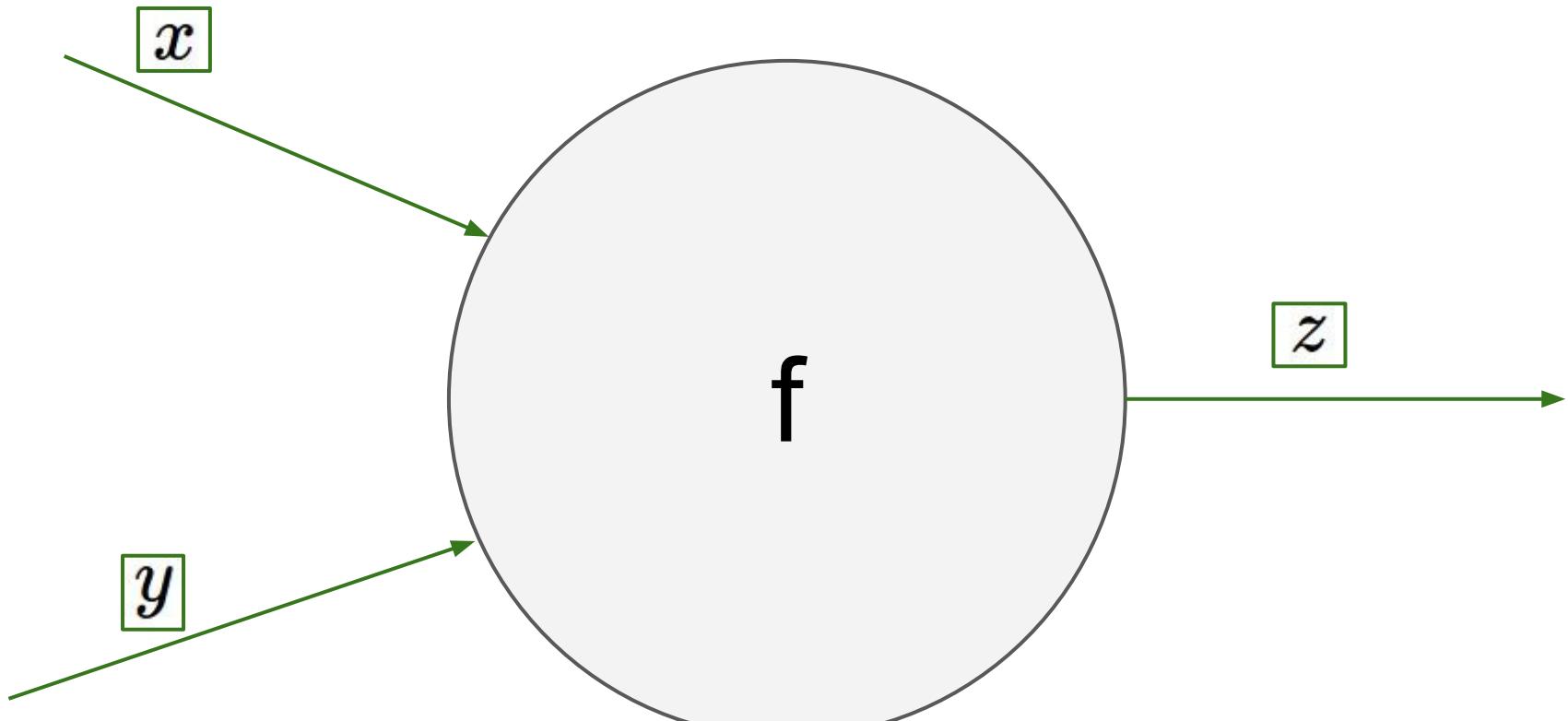


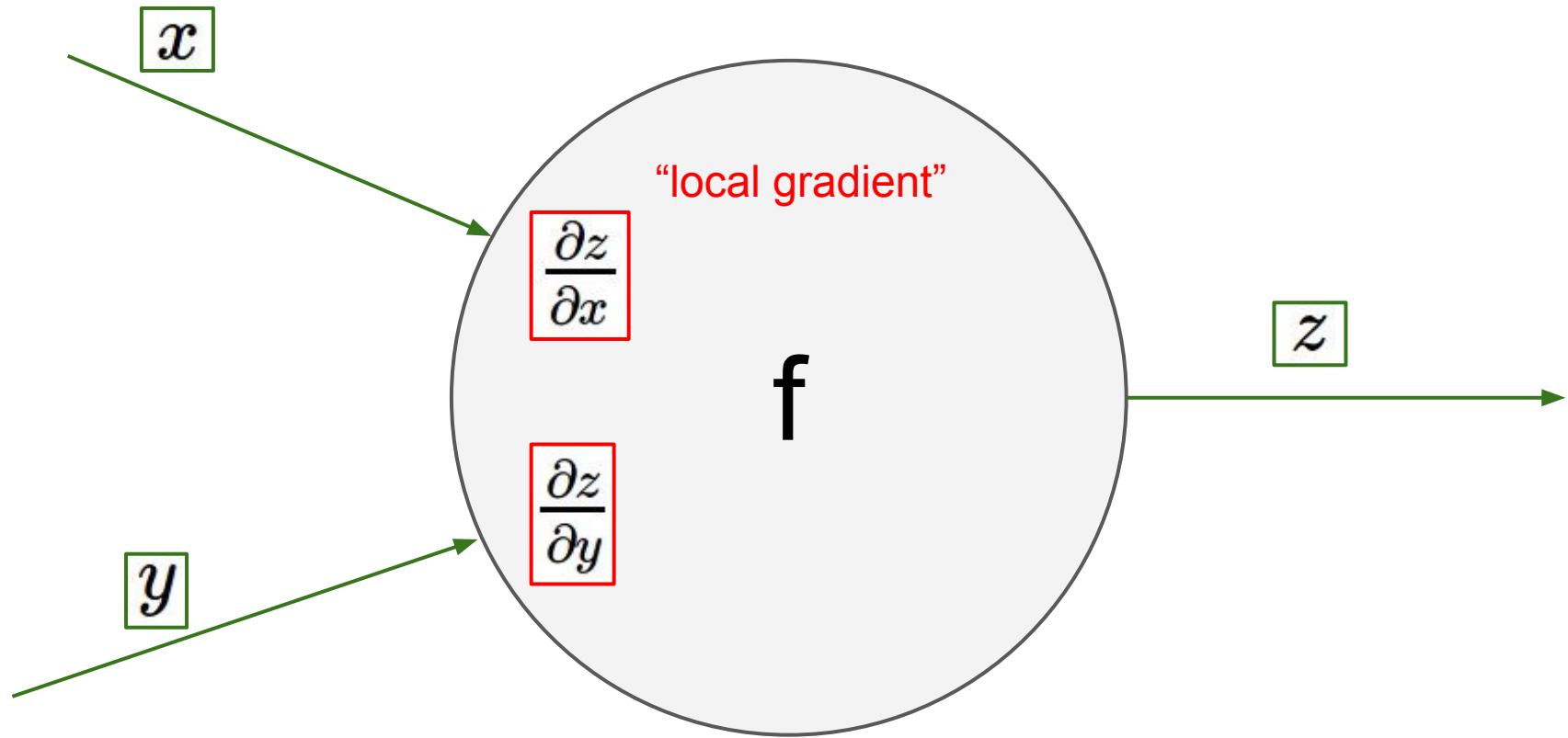
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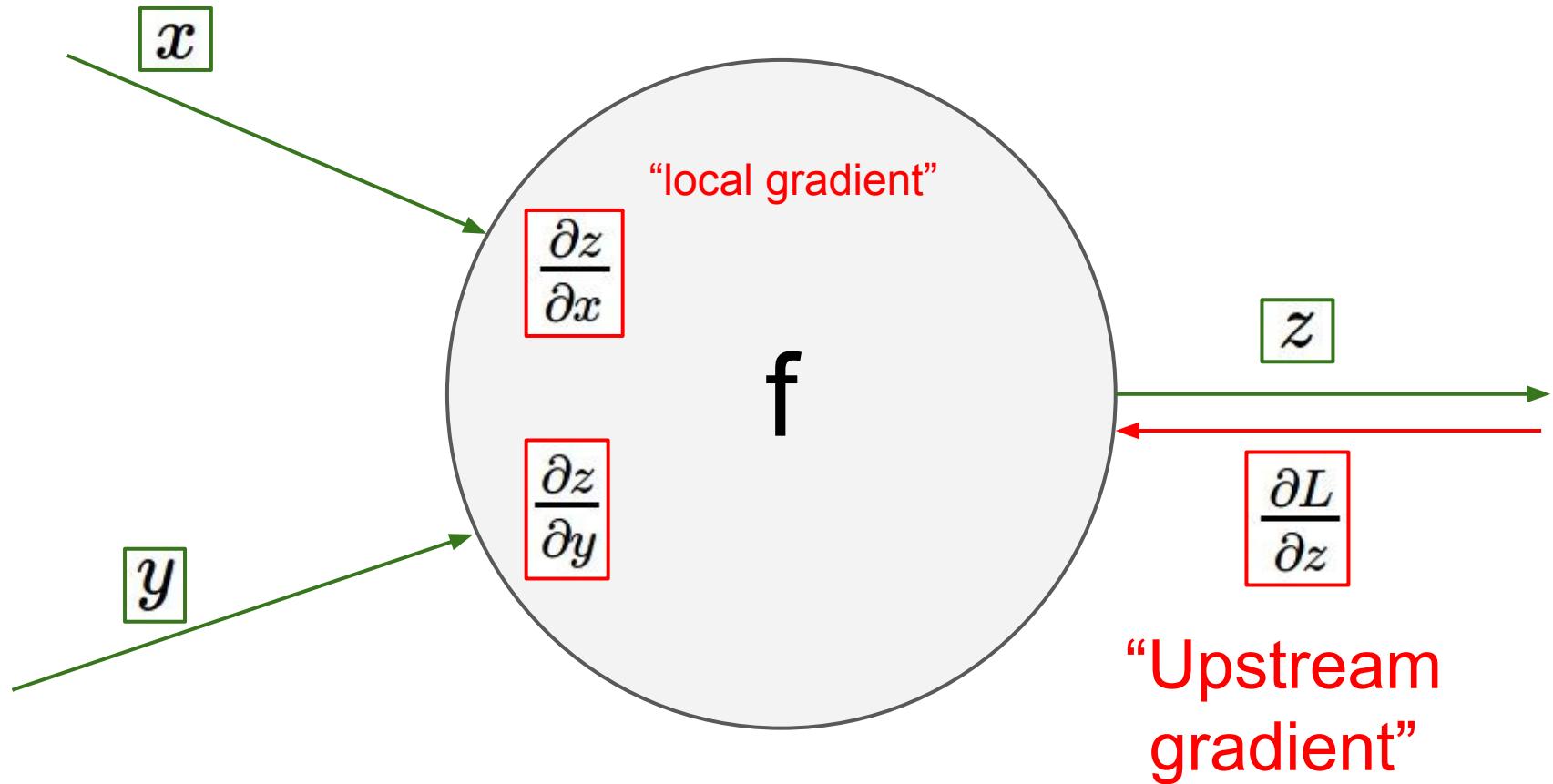
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

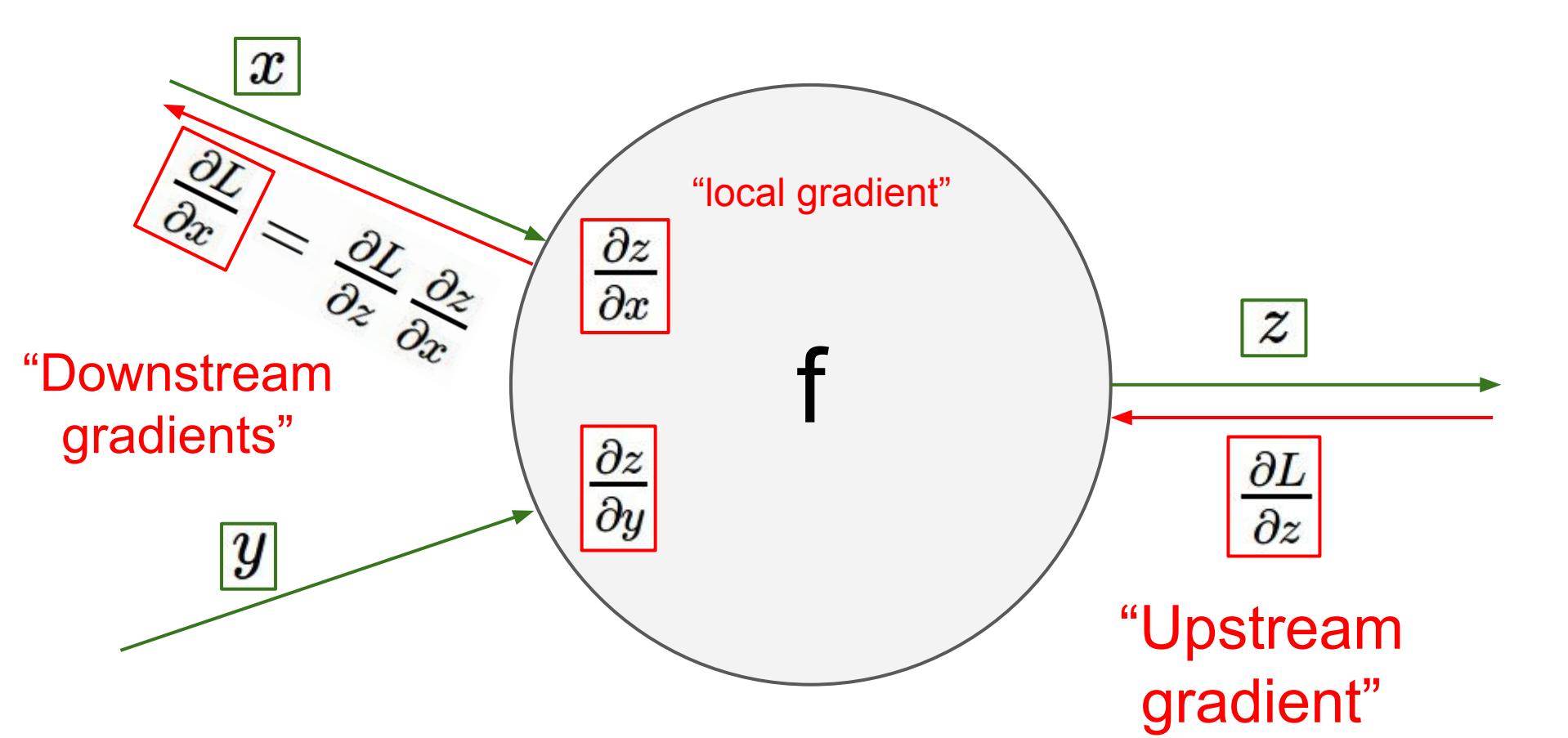
Upstream
gradient

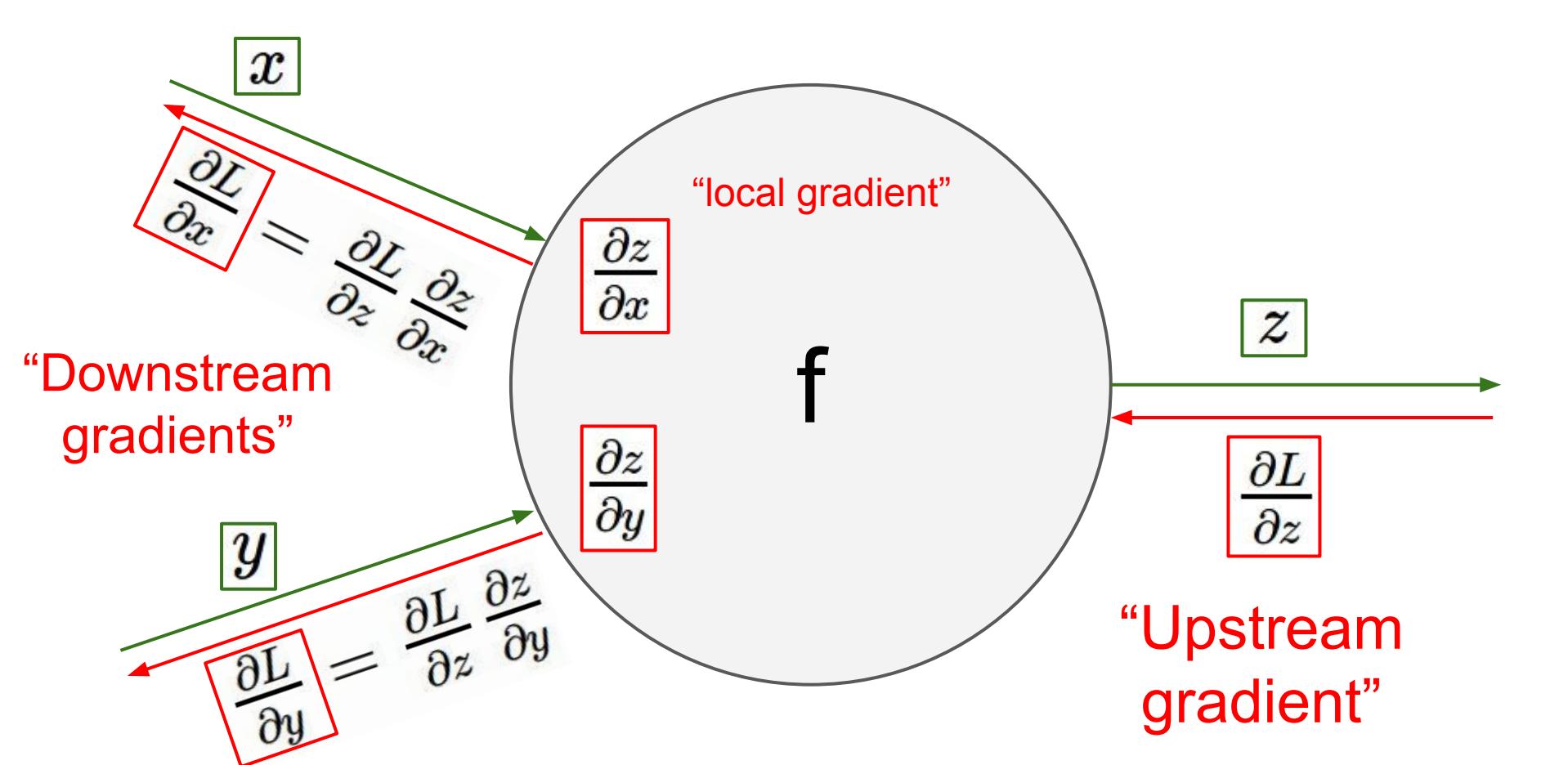
Local
gradient

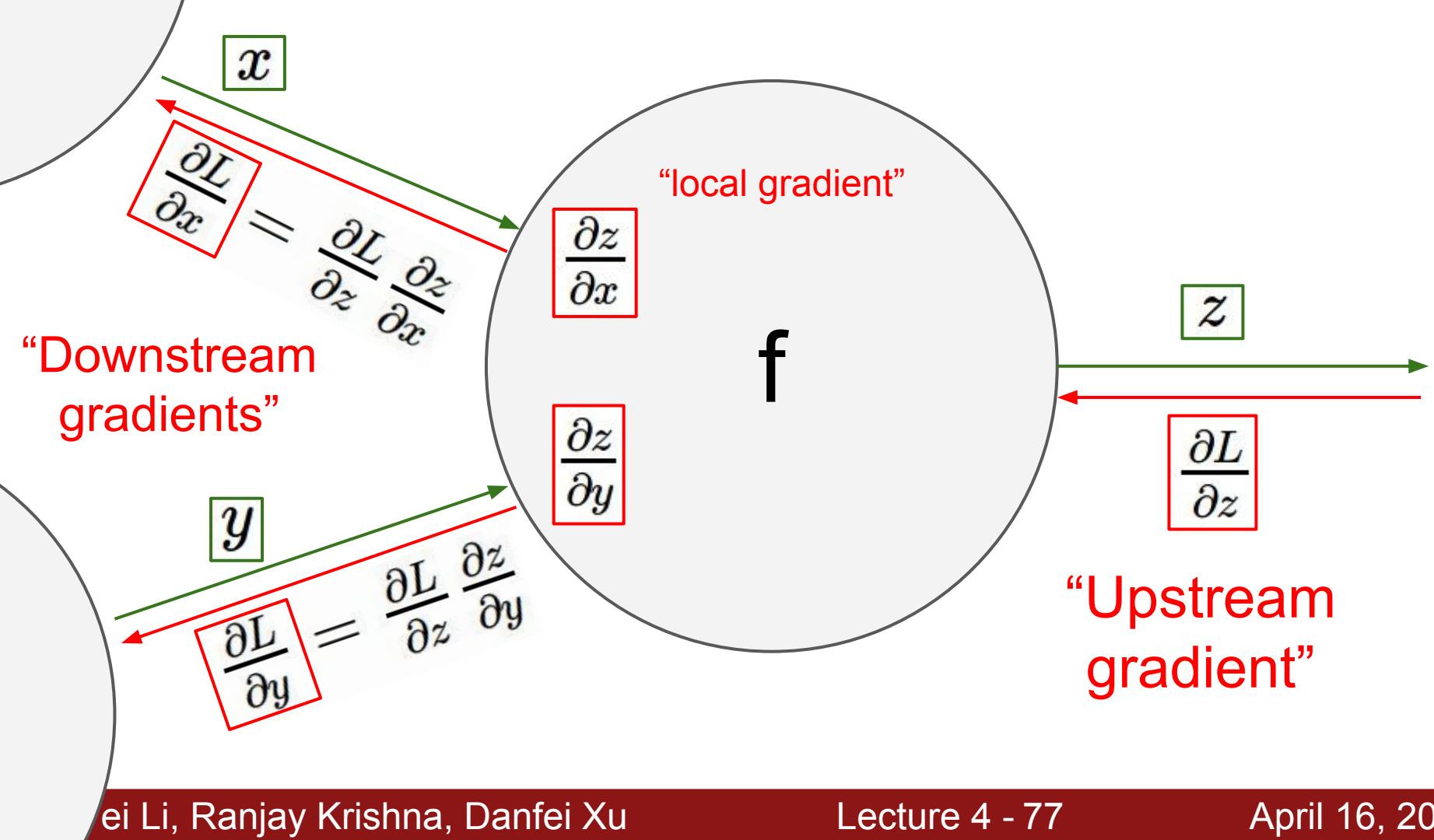






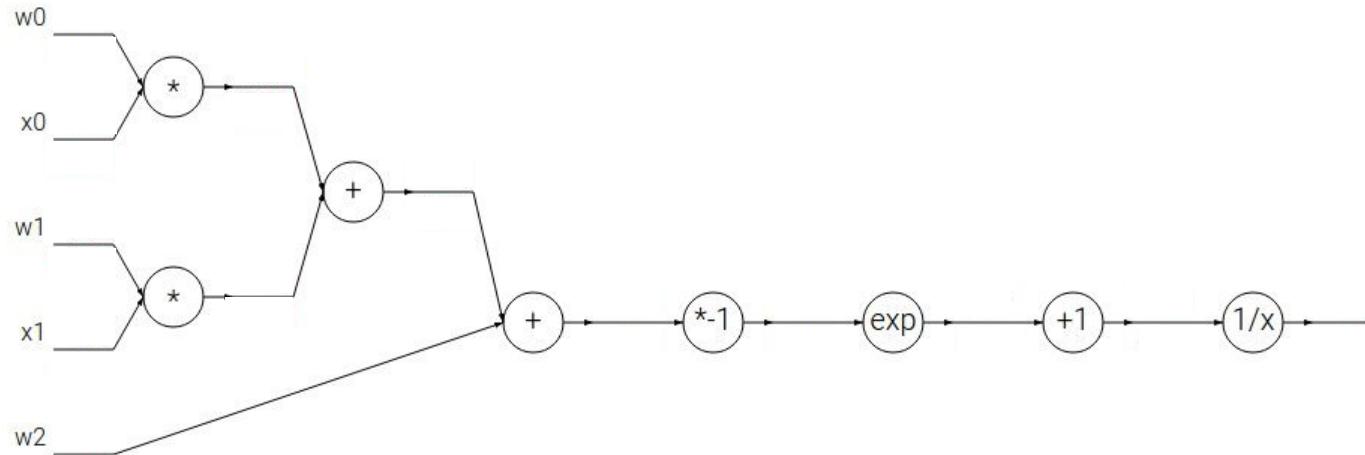






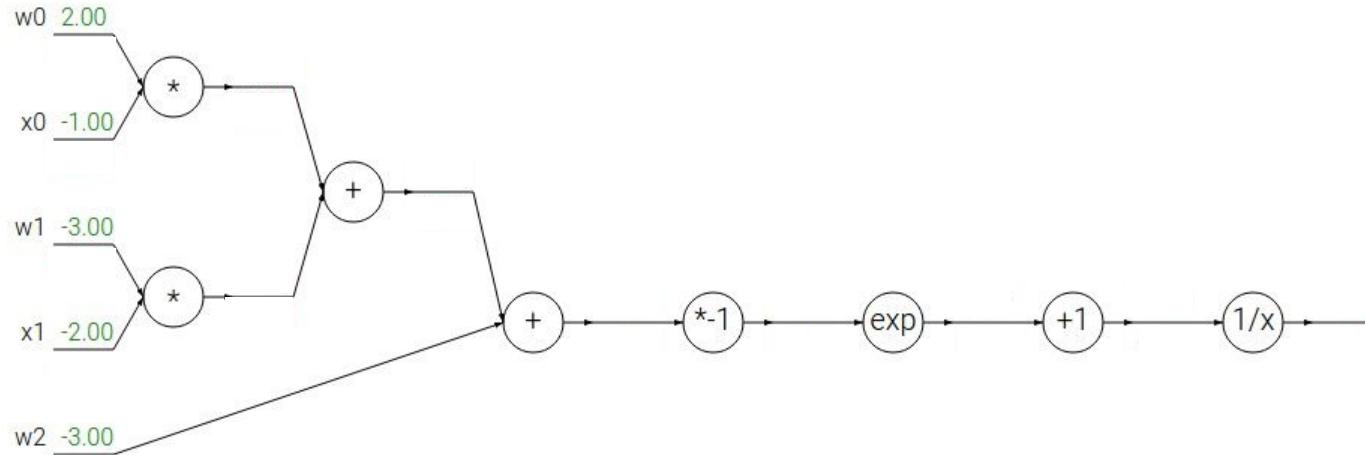
Another example:

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



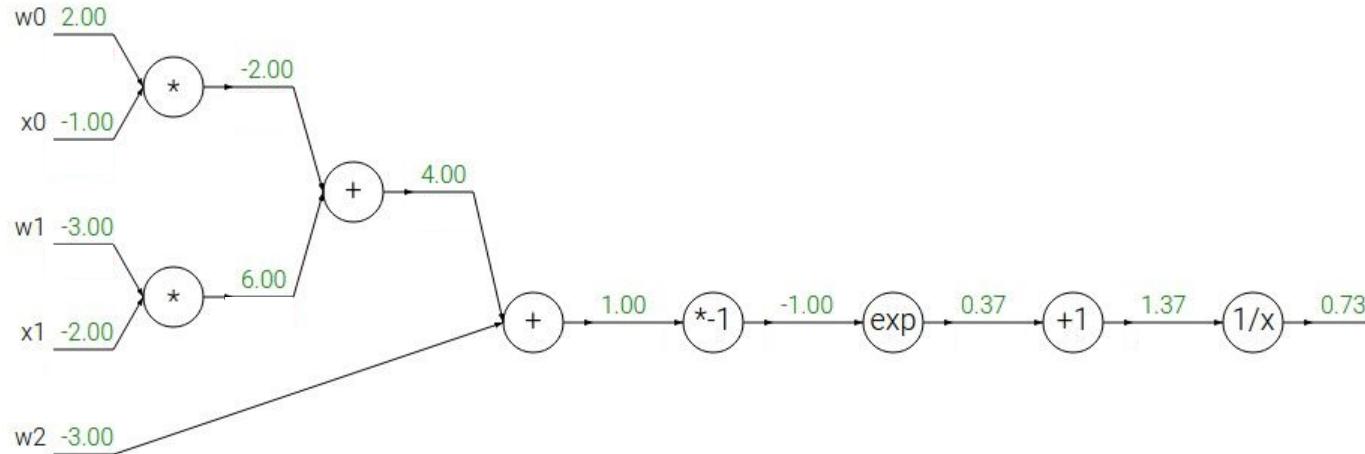
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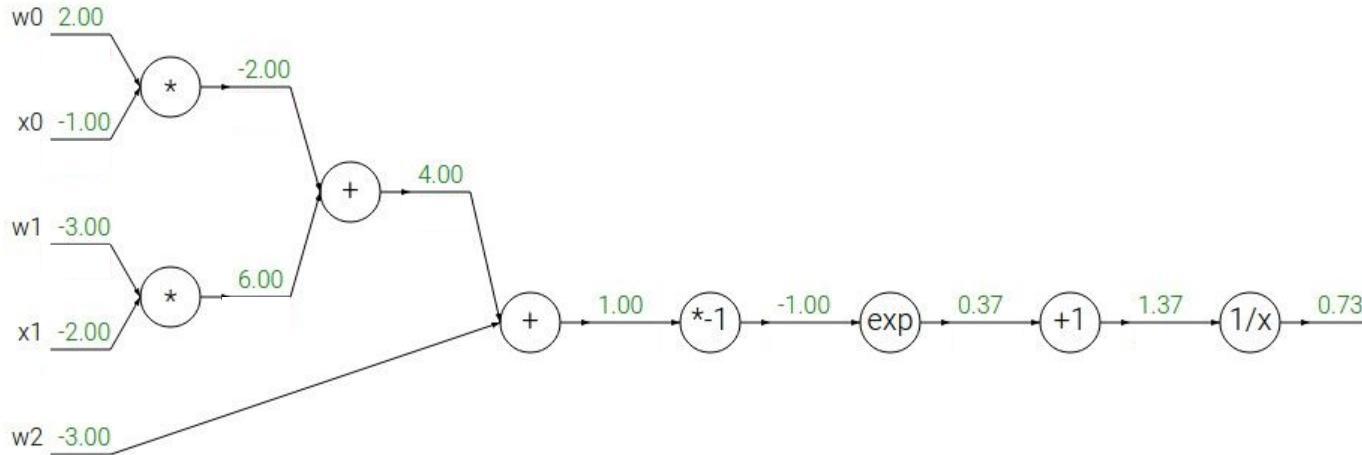
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Another example:

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



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

\rightarrow

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

$$f_a(x) = ax$$

\rightarrow

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

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

\rightarrow

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

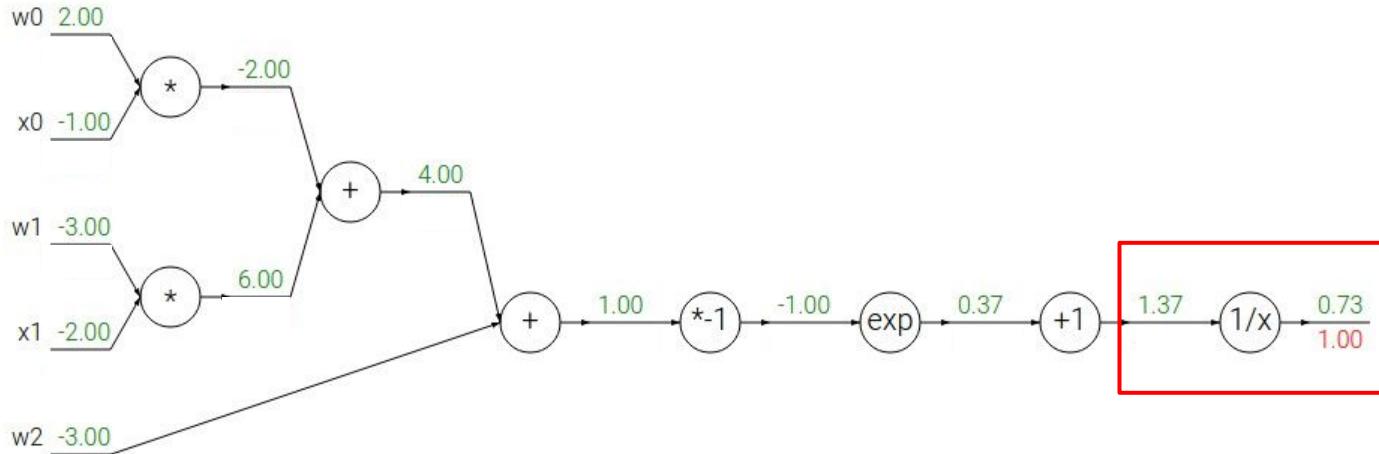
$$f_c(x) = c + x$$

\rightarrow

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

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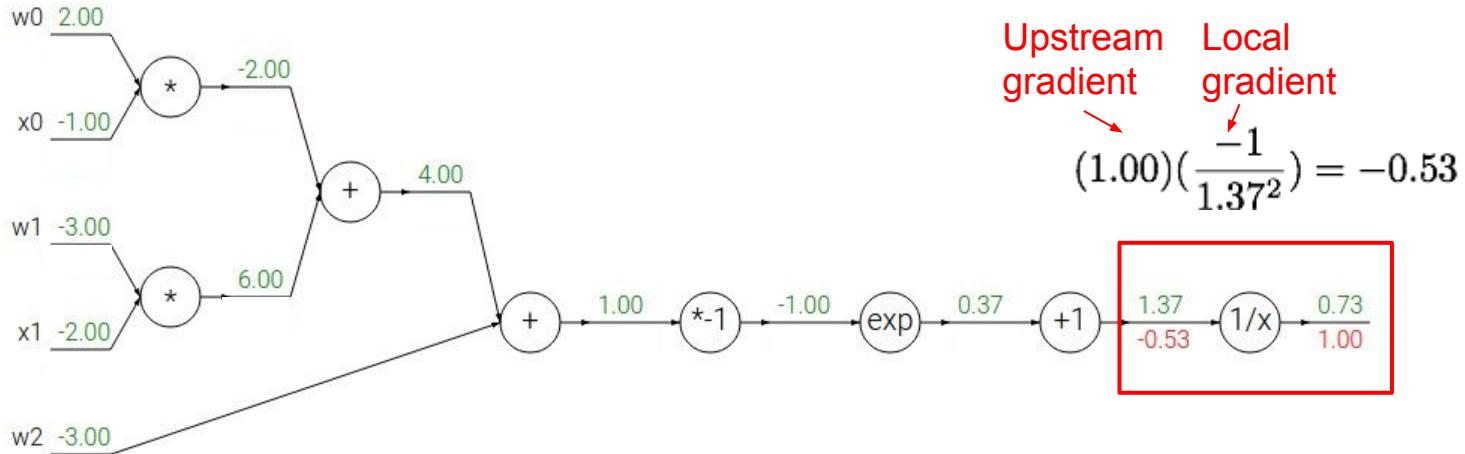
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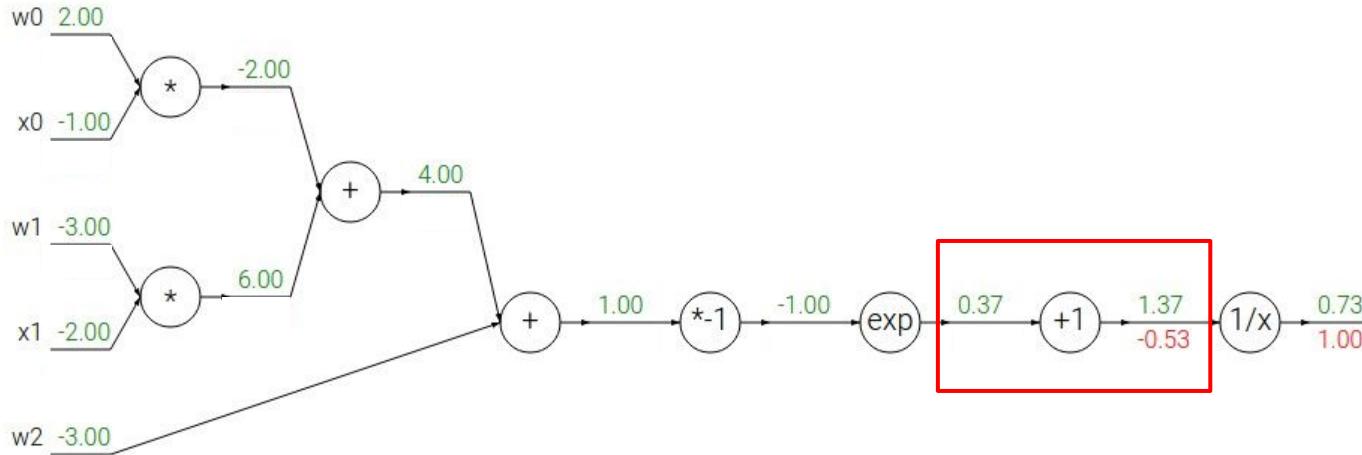
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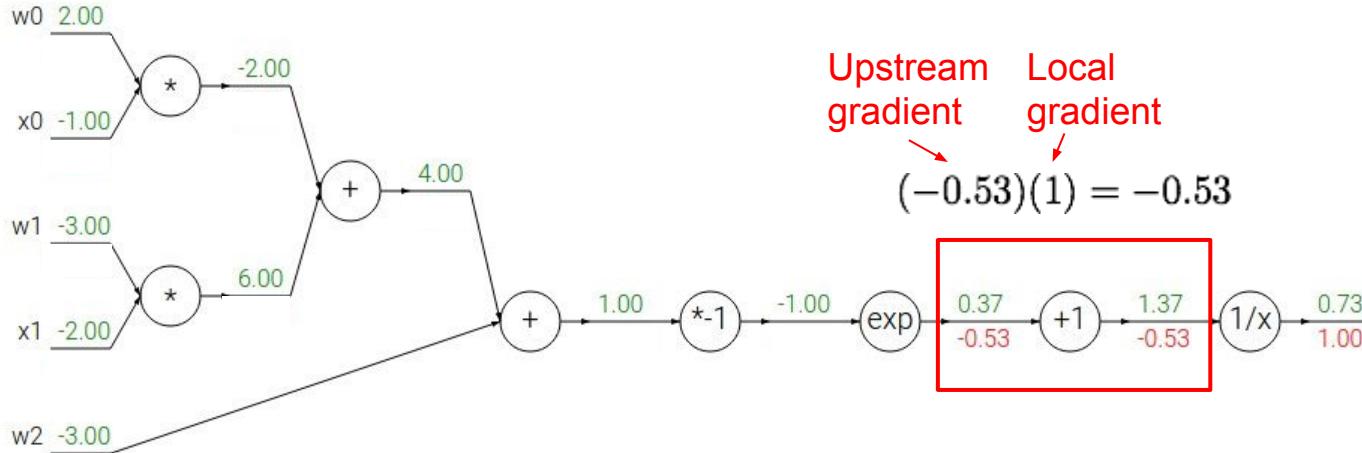
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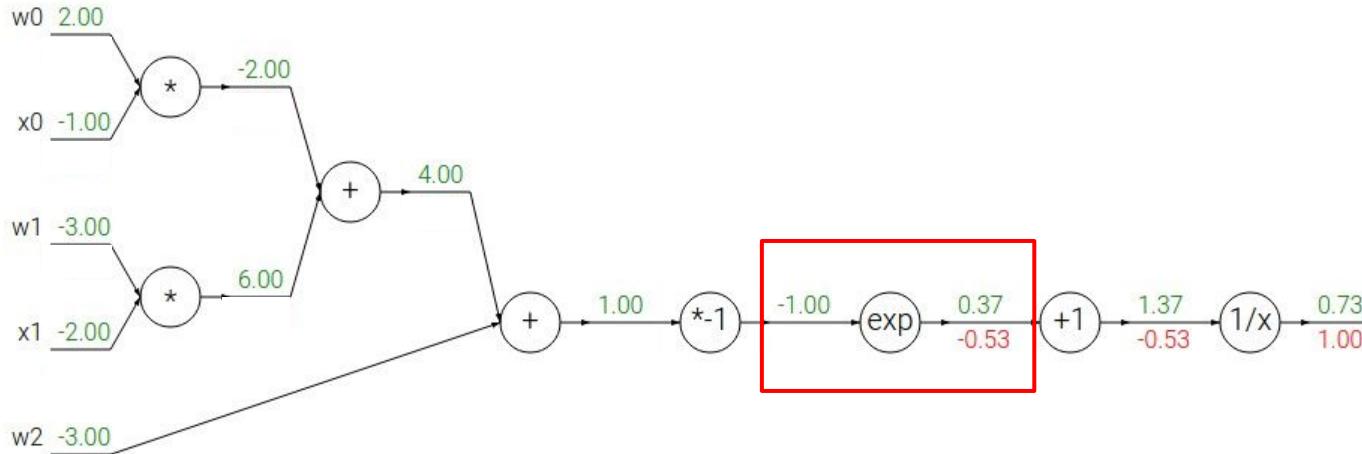
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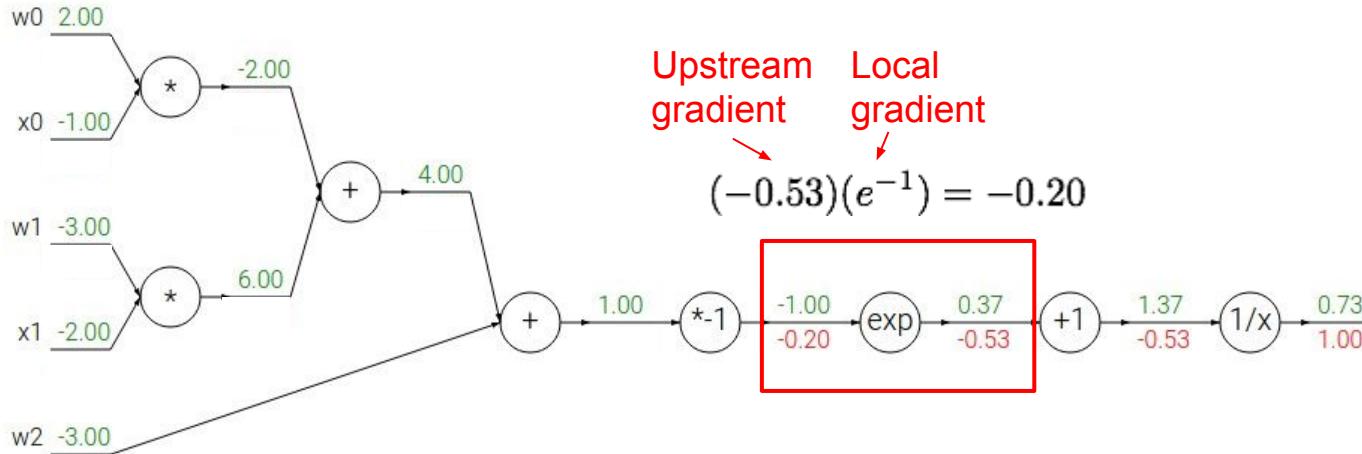
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\rightarrow

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

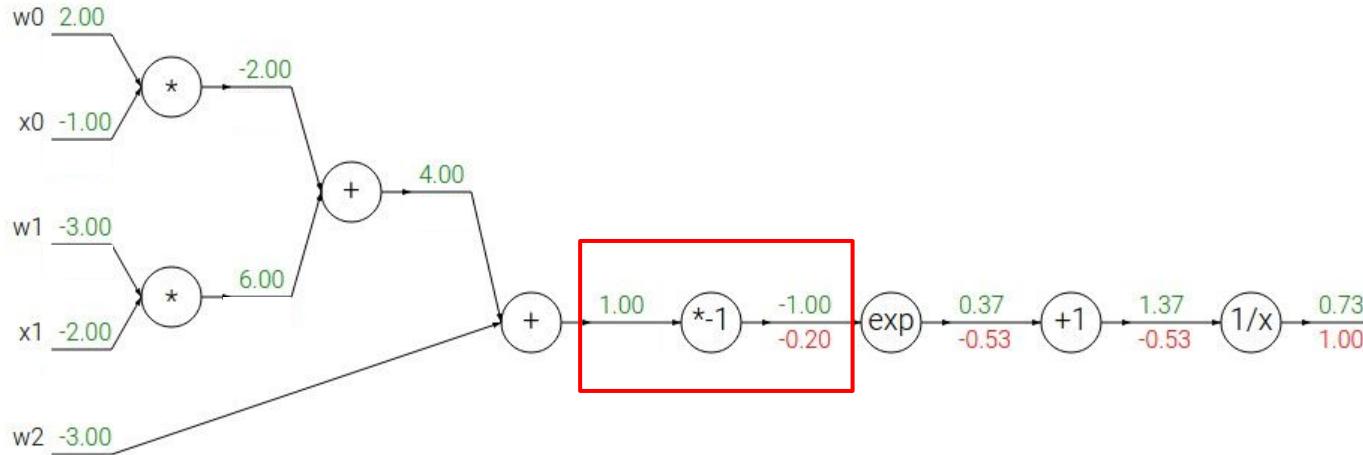
$$f_c(x) = c + x$$

\rightarrow

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

Another example:

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



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

\rightarrow

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

$$f_a(x) = ax$$

\rightarrow

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

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

\rightarrow

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

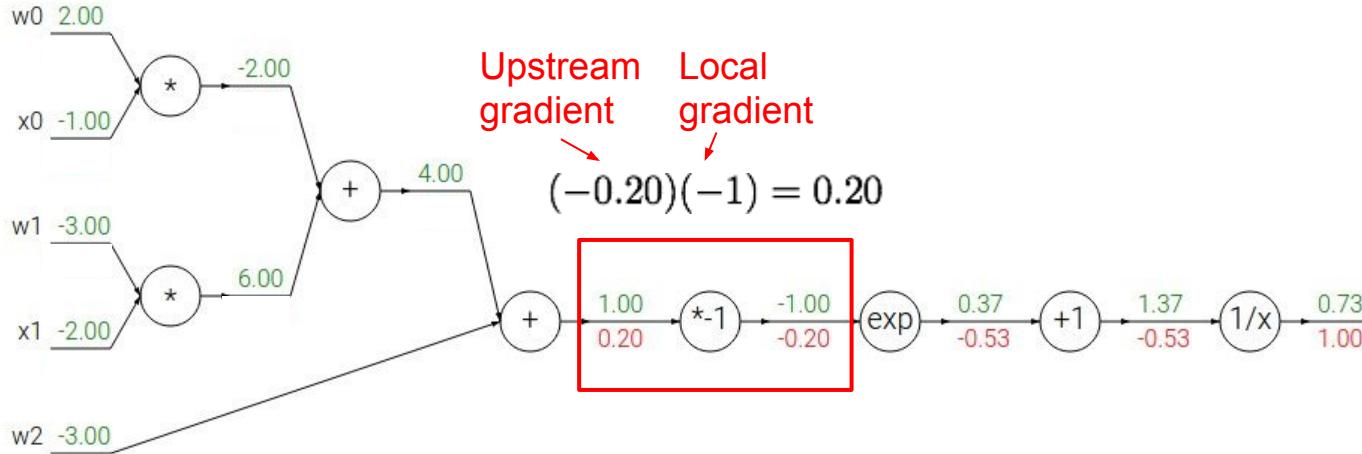
$$f_c(x) = c + x$$

\rightarrow

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

Another example:

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



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

\rightarrow

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

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\rightarrow

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

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

\rightarrow

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

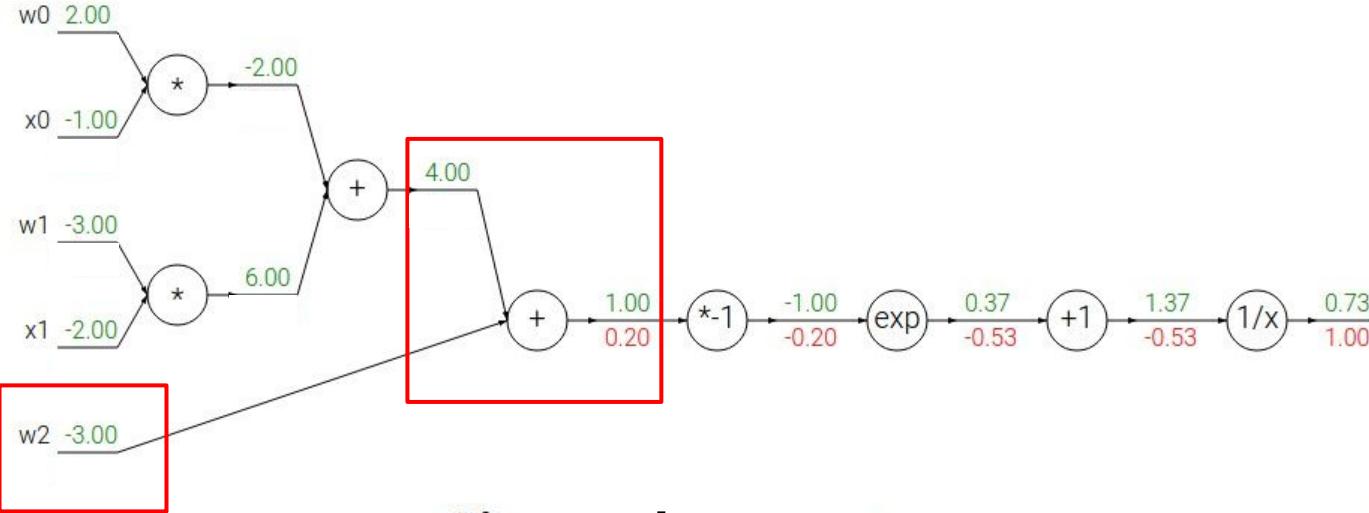
$$f_c(x) = c + x$$

\rightarrow

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

Another example:

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



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

→

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→

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

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

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

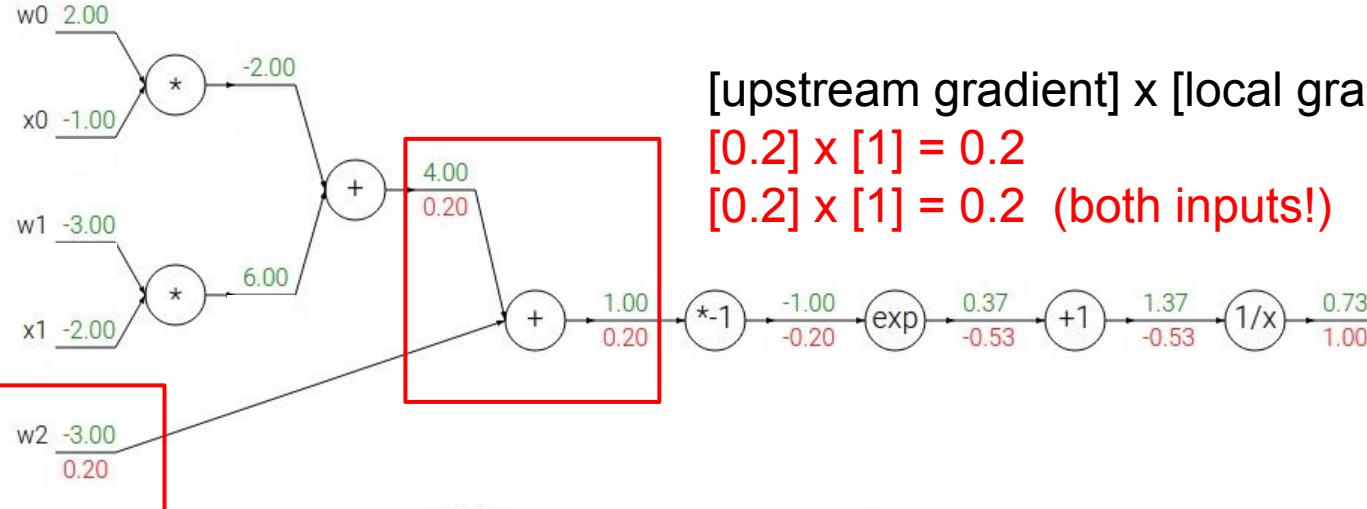
→

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

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

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

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

\rightarrow

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

$$f_a(x) = ax$$

\rightarrow

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

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

\rightarrow

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

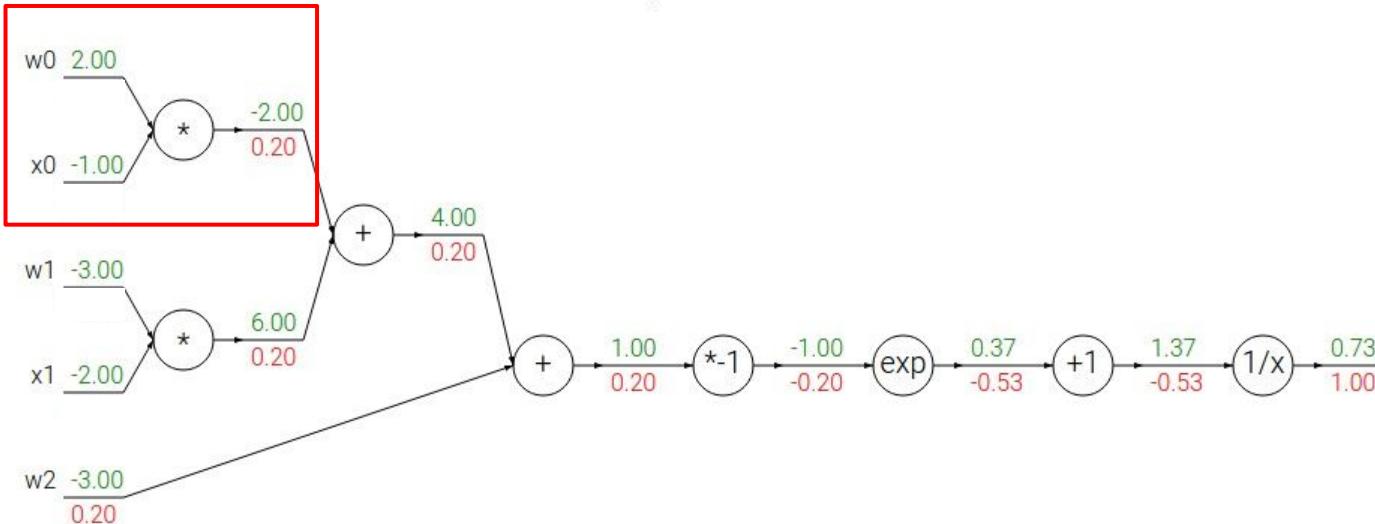
$$f_c(x) = c + x$$

\rightarrow

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

Another example:

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



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

→

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

$$f_a(x) = ax$$

→

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

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

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

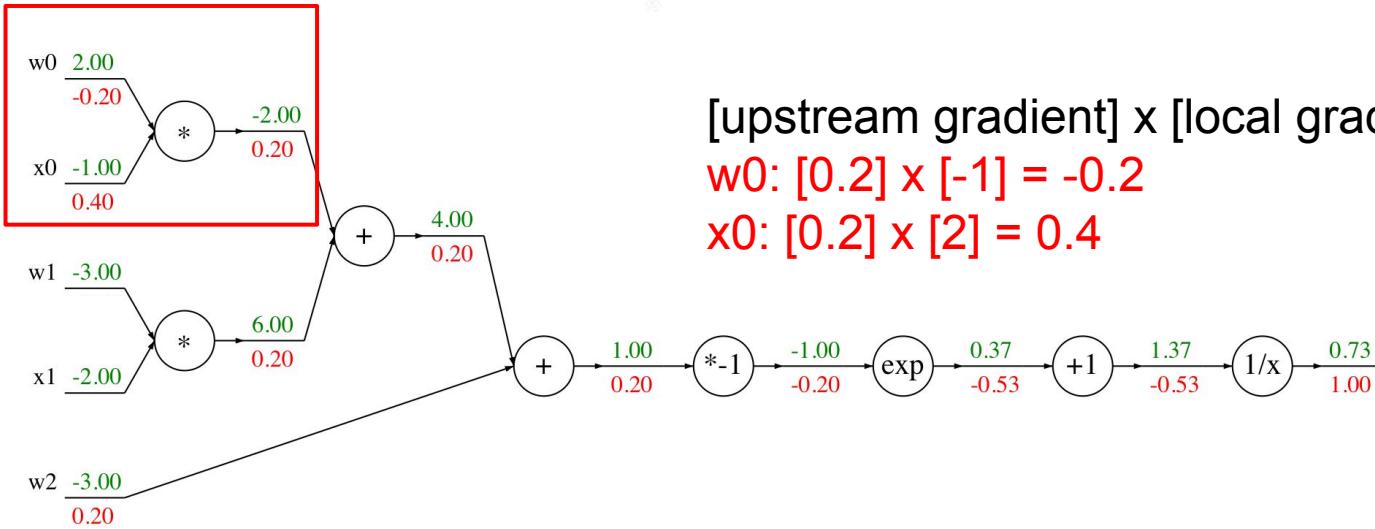
→

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

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

Another example:

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



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

→

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

$$f_a(x) = ax$$

→

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

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

→

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

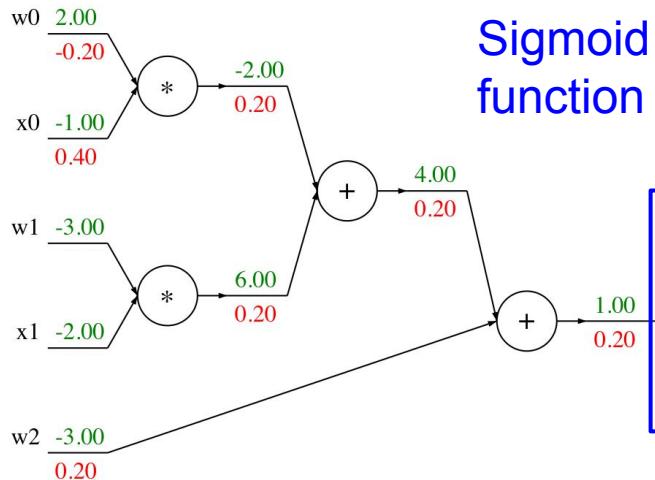
$$f_c(x) = c + x$$

→

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

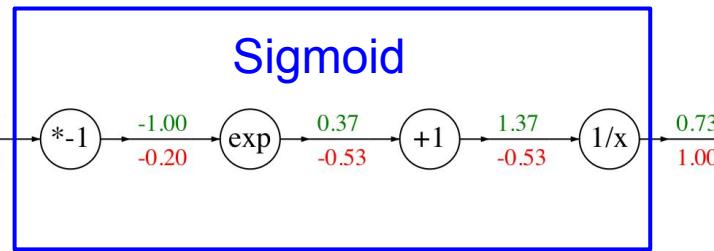
Another example:

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



Sigmoid
function

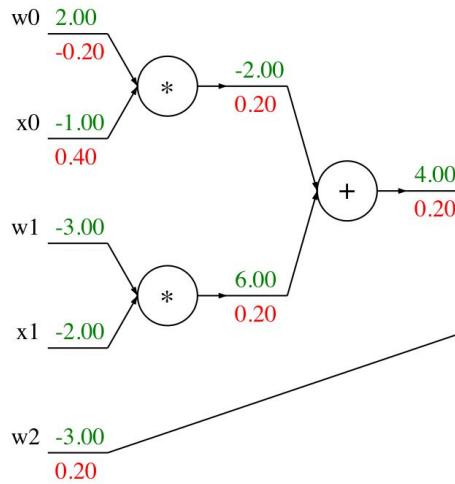
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



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

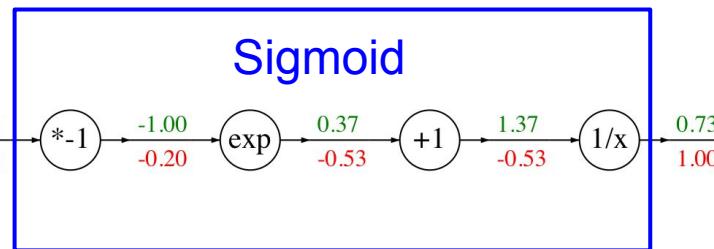
Another example:

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



Sigmoid
function

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



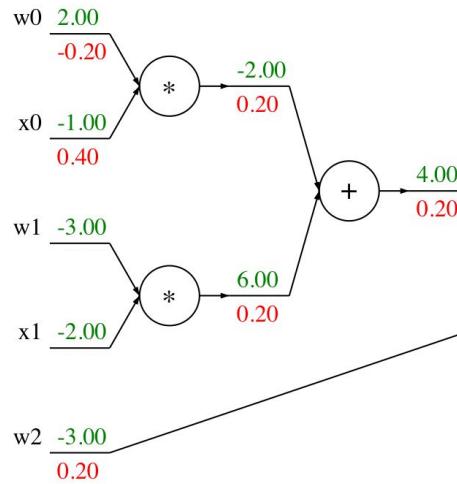
Sigmoid local
gradient:

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

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

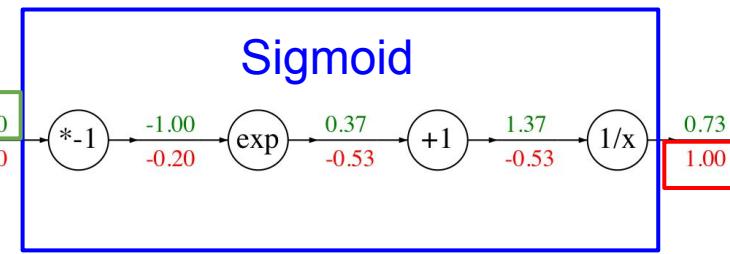
Another example:

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



Sigmoid
function

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



[upstream gradient] \times [local gradient]
 $[1.00] \times [(1 - 1/(1+e^1)) (1/(1+e^1))] = 0.2$

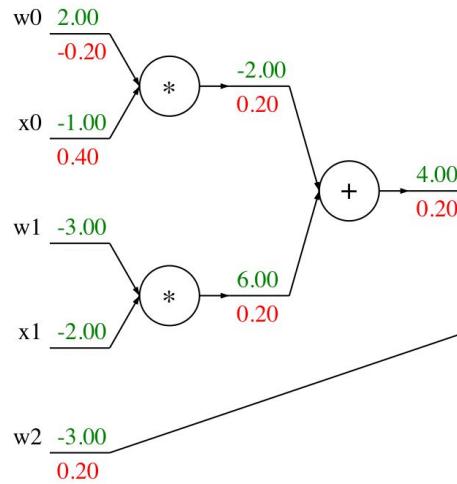
Sigmoid local
gradient:

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

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

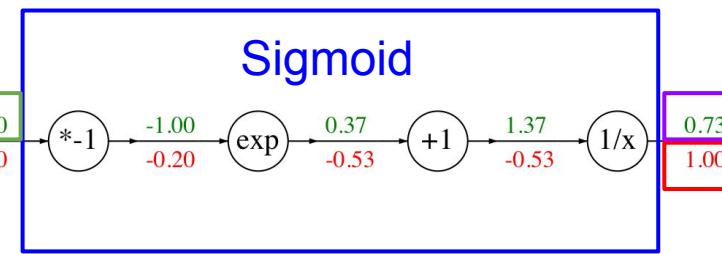
Another example:

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



Sigmoid
function

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



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

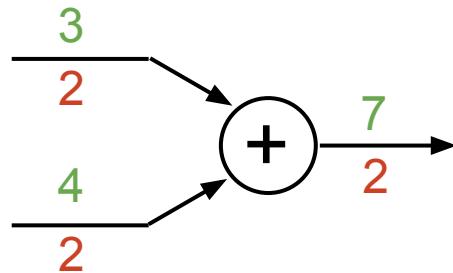
Sigmoid local
gradient:

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

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

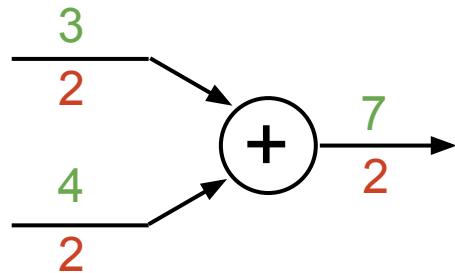
Patterns in gradient flow

add gate: gradient distributor

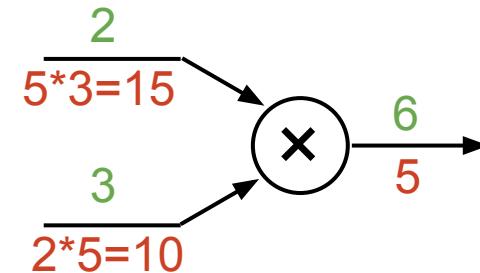


Patterns in gradient flow

add gate: gradient distributor

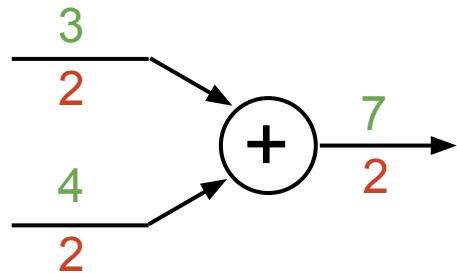


mul gate: “swap multiplier”

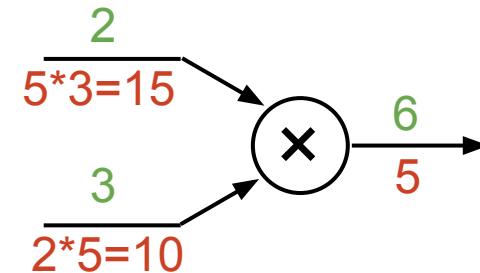


Patterns in gradient flow

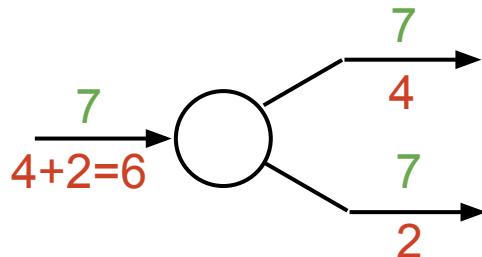
add gate: gradient distributor



mul gate: “swap multiplier”

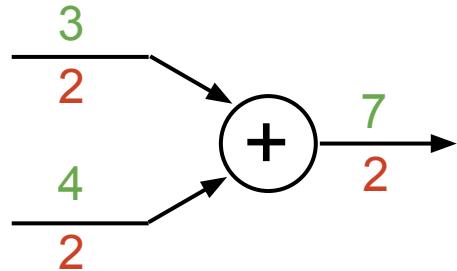


copy gate: gradient adder

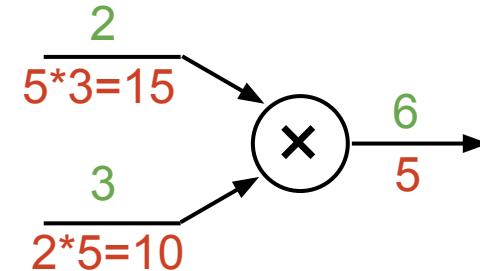


Patterns in gradient flow

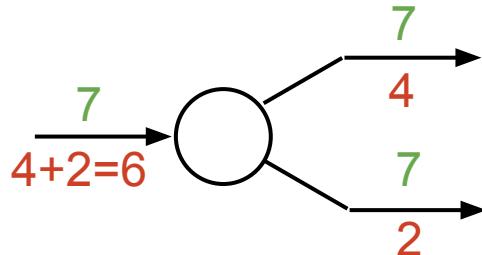
add gate: gradient distributor



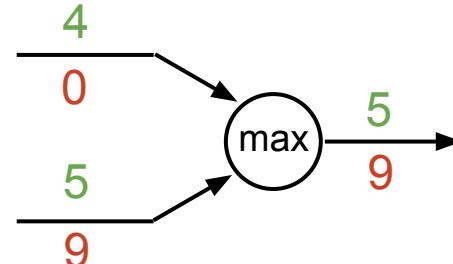
mul gate: “swap multiplier”



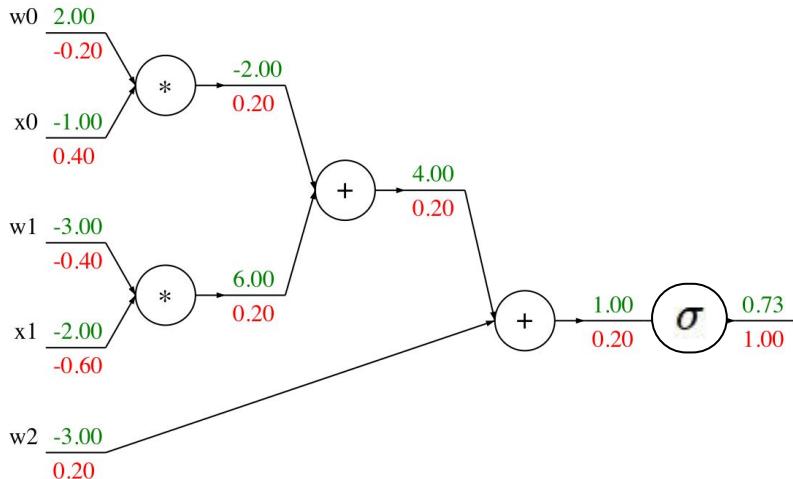
copy gate: gradient adder



max gate: gradient router



Backprop Implementation: “Flat” code



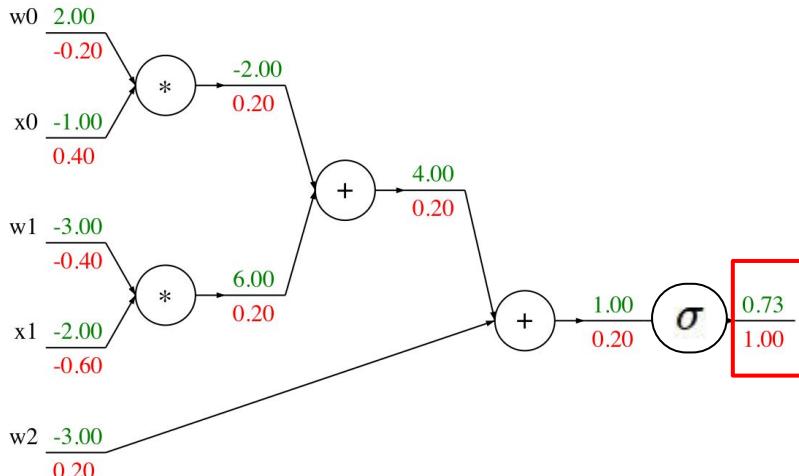
Forward pass:
Compute output

```
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

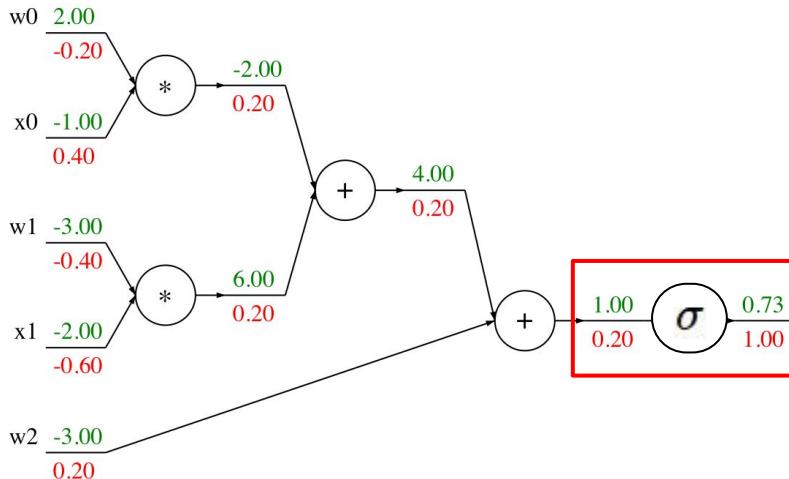
```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

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



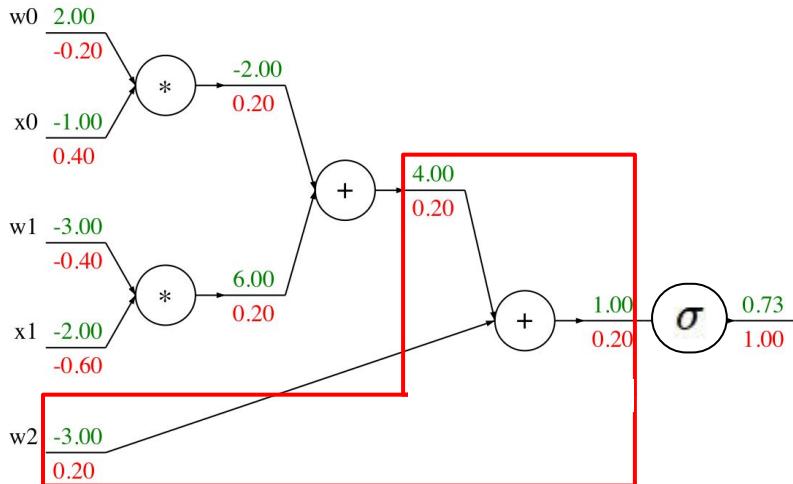
Forward pass:
Compute output

Sigmoid

```
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
```

Backprop Implementation: “Flat” code



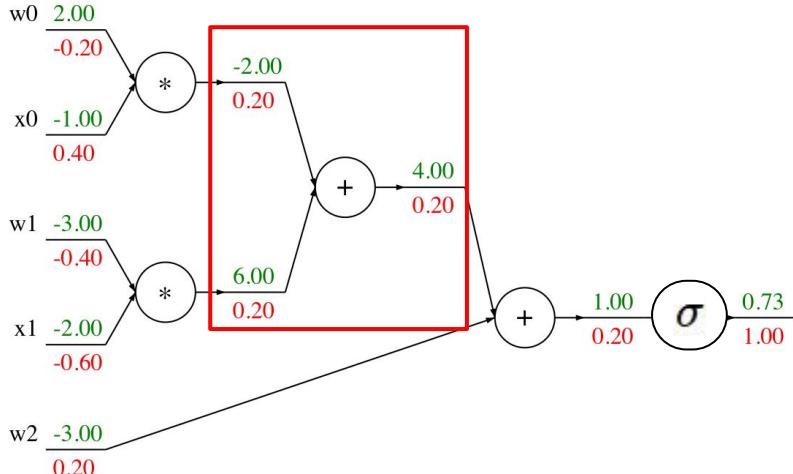
Forward pass:
Compute output

```
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



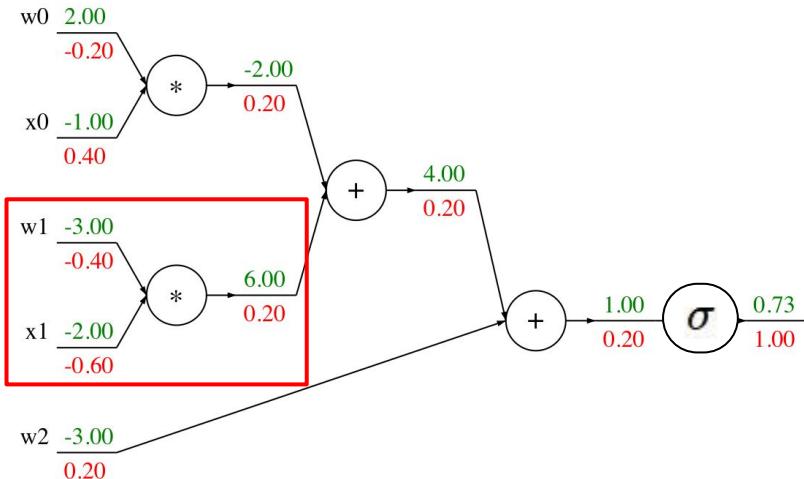
Forward pass:
Compute output

Add gate

```
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
```

Backprop Implementation: “Flat” code



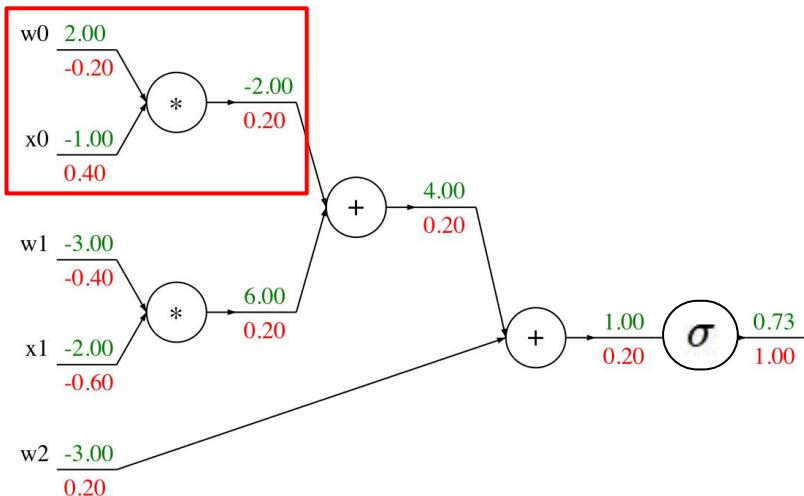
Forward pass:
Compute output

```
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
```

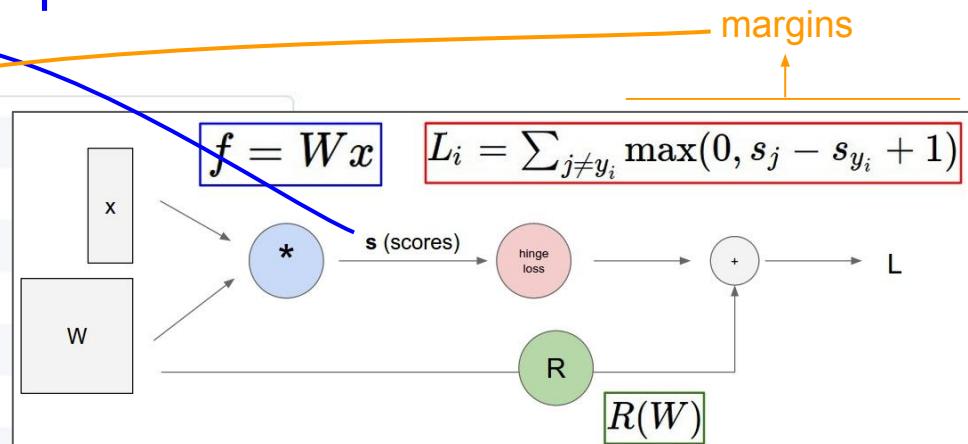
Multiply gate

“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 6 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 = #...
```



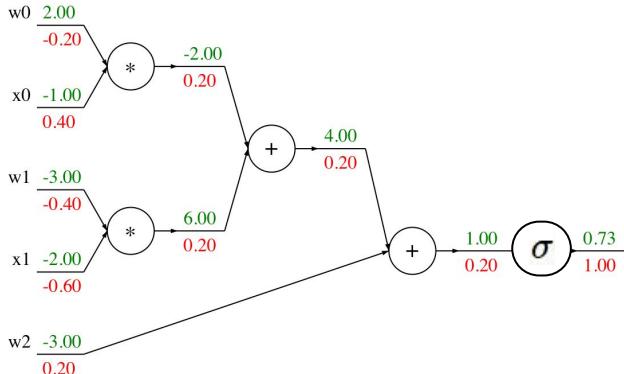
“Flat” Backprop: Do this for assignment 1!

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

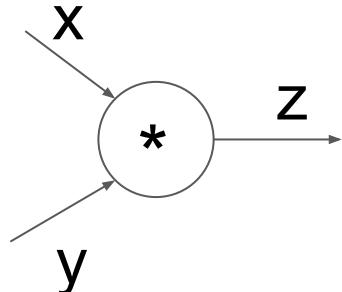
Graph (or Net) object (*rough pseudo code*)



```
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		
Code	Issues 2,286	Pull requests 561
Tree: 517c7c9861 → pytorch / aten / src / THNN / generic /	Create new file	Upload files
ezyang and facebook-github-bot Canonicalize all includes in PyTorch. (#14849)	Latest commit 517c7c9 on Dec 8, 2018	
..		
AbsCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
BCECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ClassNLLCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Col2im.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ELU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
FeatureLPPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
GatedLinearUnit.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
HardTanh.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Im2Col.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
IndexLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LeakyReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LogSigmoid.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MSECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MultiLabelMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MultiMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
RReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Sigmoid.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SmoothL1Criterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SoftMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SoftPlus.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SoftShrink.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SparseLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialAdaptiveAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialAdaptiveMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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
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VolumetricReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricUpSamplingNearest.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

```
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 }
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
```

Forward

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

[Source](#)

PyTorch sigmoid layer

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23         *gradInput_data = *gradOutput_data * (1. - z) * z;
24     );
25 }
26
27 #endif
```

Forward

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

```
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...](#)

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

[Source](#)

PyTorch sigmoid layer

```
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 }
26
27 #endif
```

Forward

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

```
static void sigmoid_kernel(TensorIterator& iter) {
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            [=](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

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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

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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

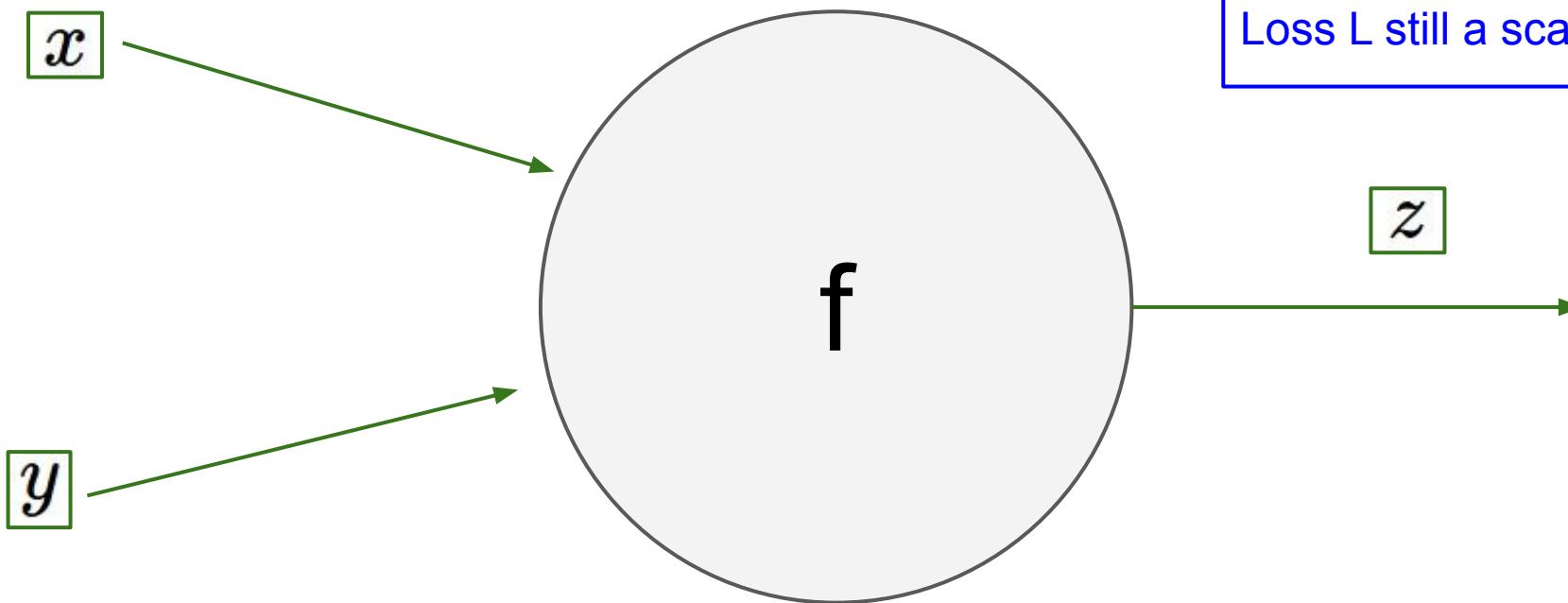
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

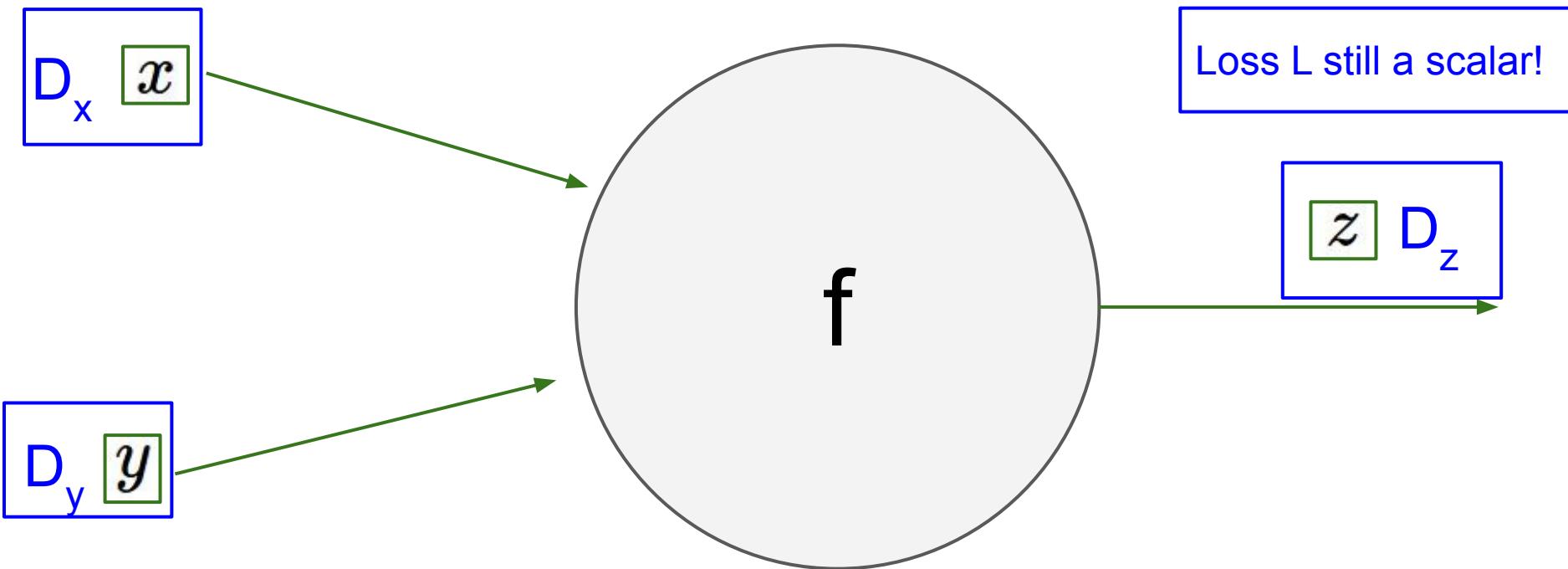
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x} \right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

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

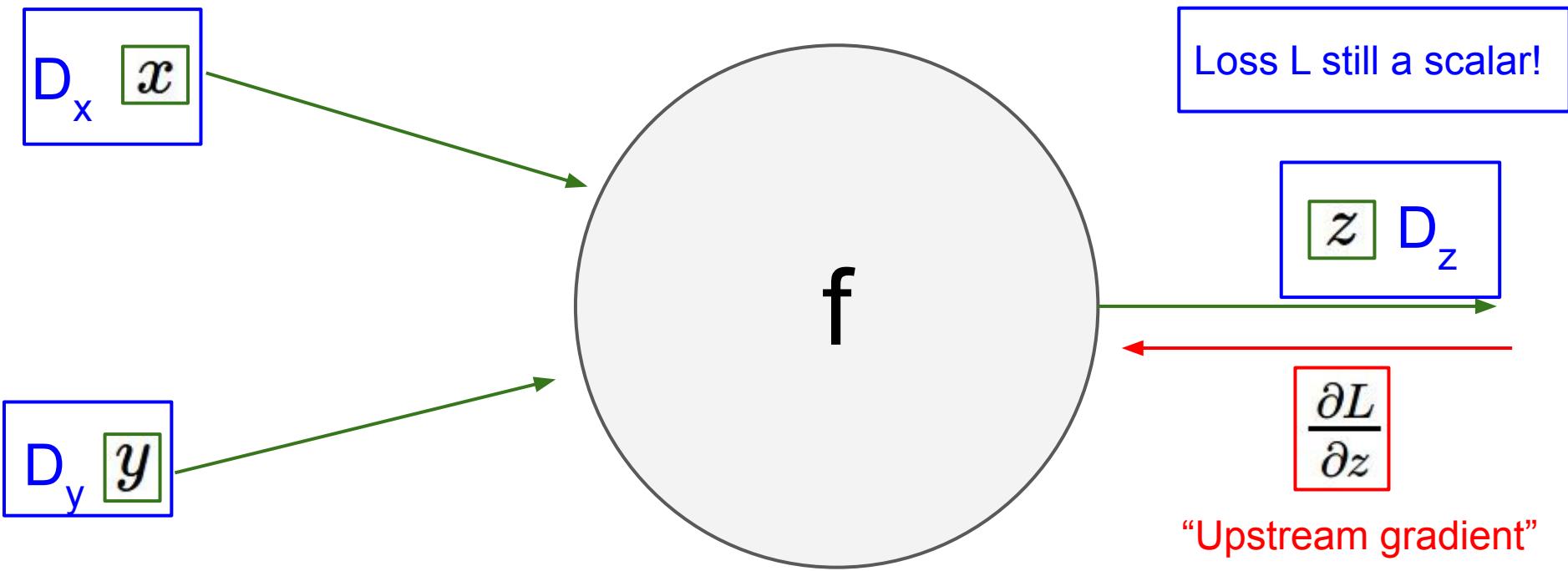
Backprop with Vectors



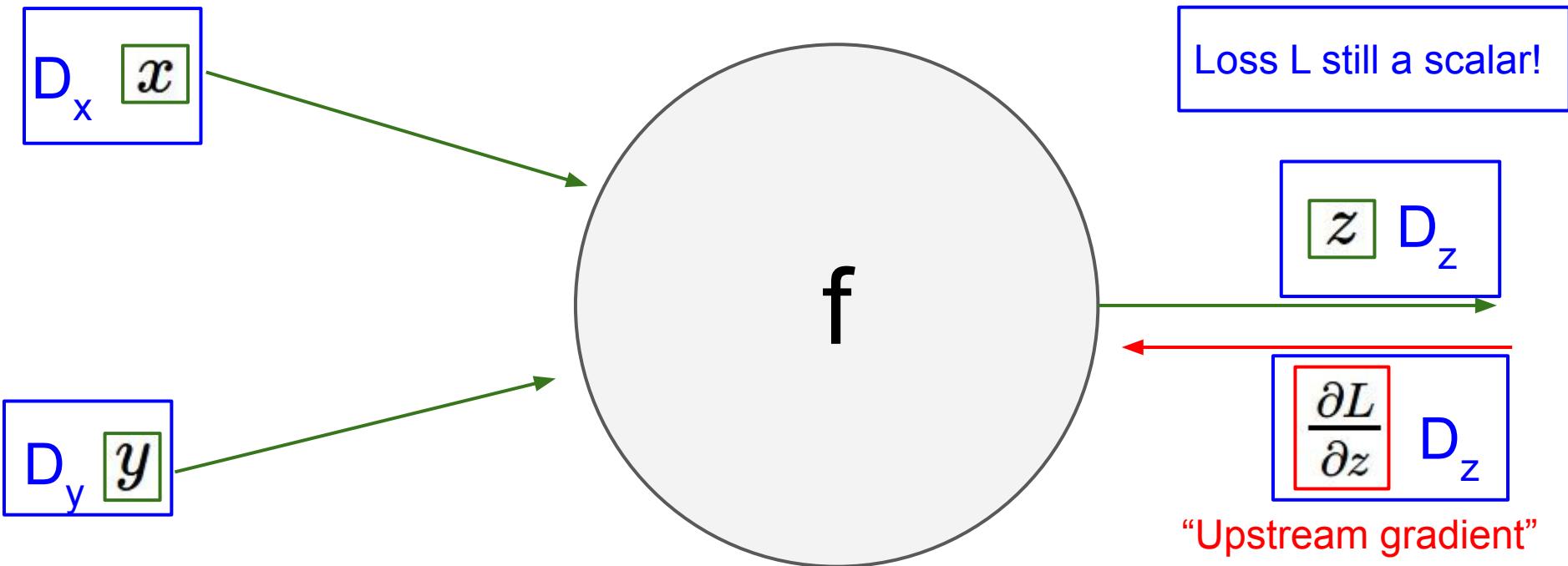
Backprop with Vectors



Backprop with Vectors



Backprop with Vectors



Loss L still a scalar!

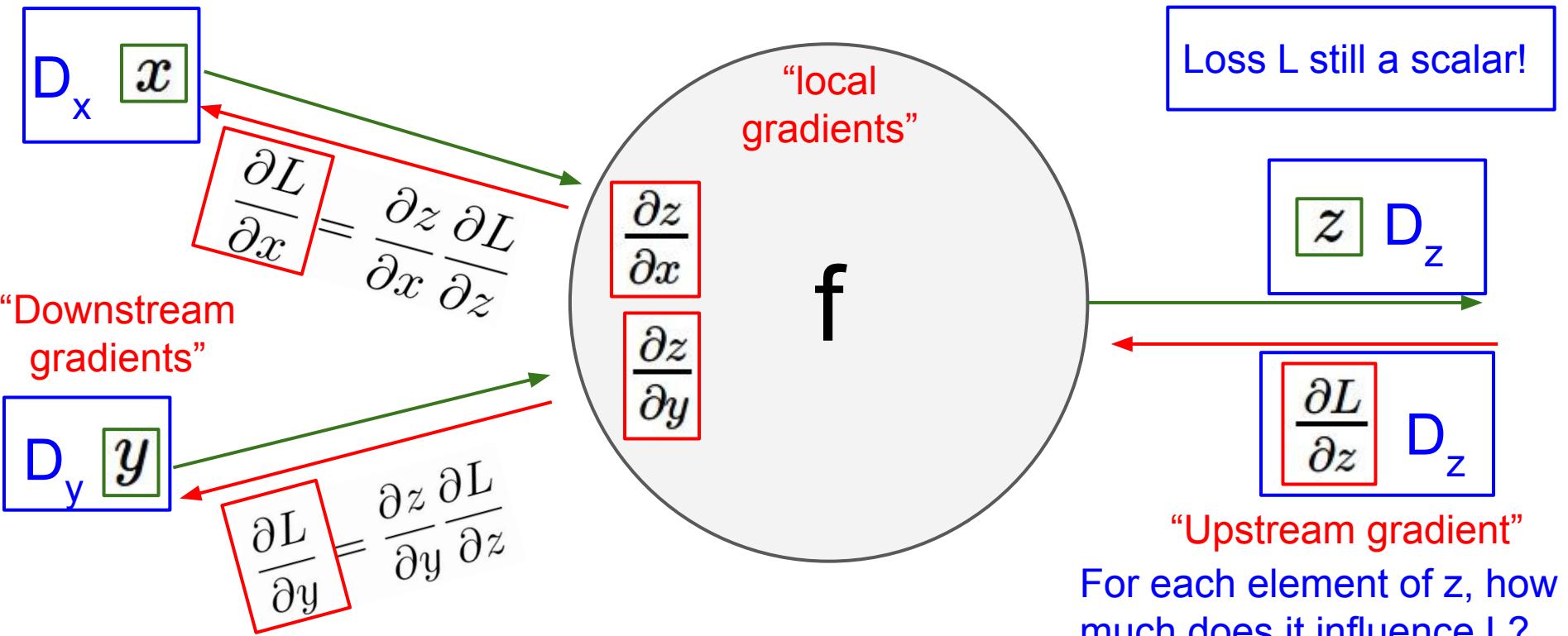
$$z \quad D_z$$

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

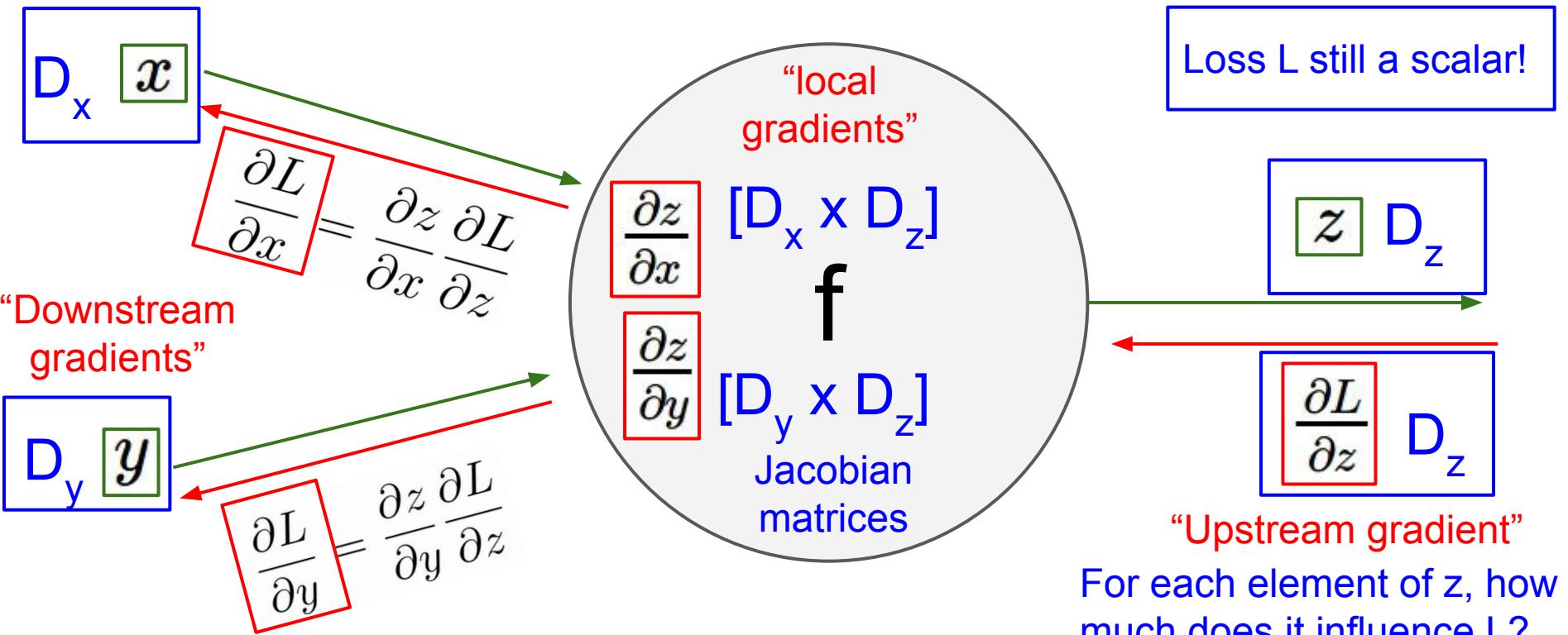
"Upstream gradient"

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

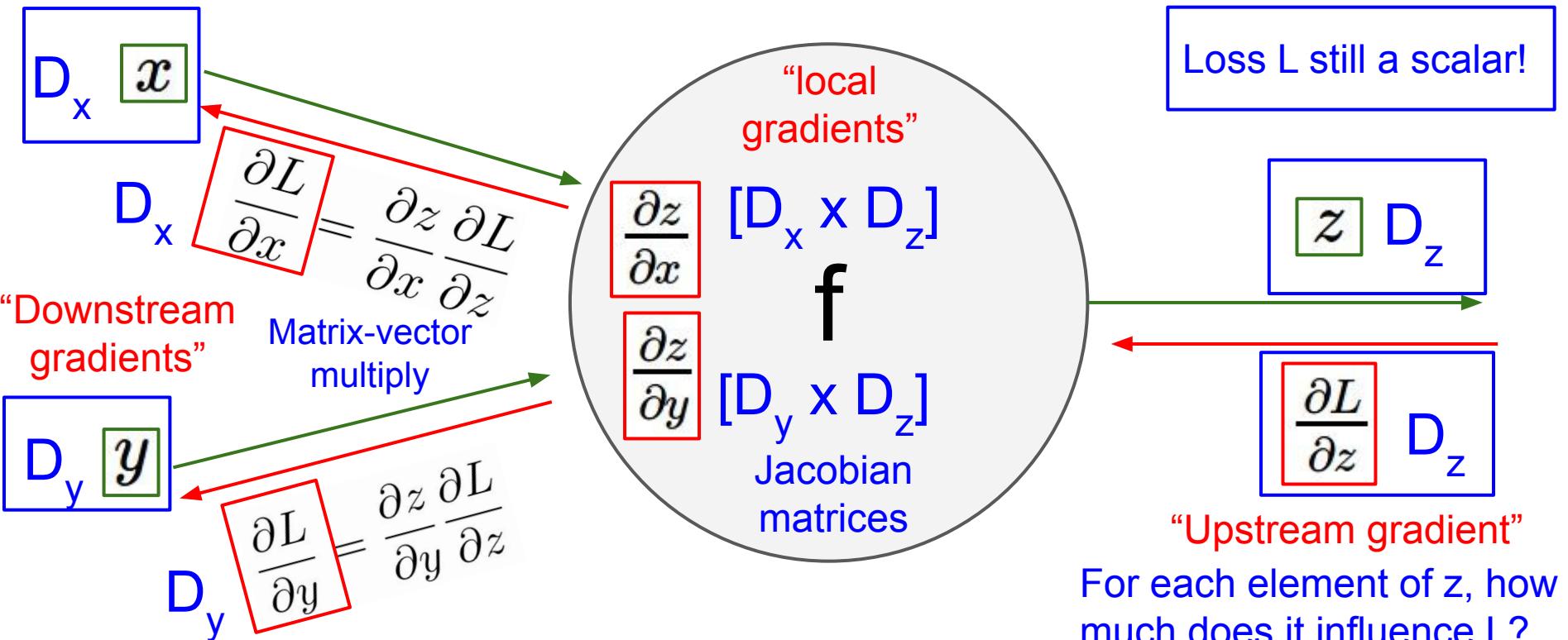
Backprop with Vectors



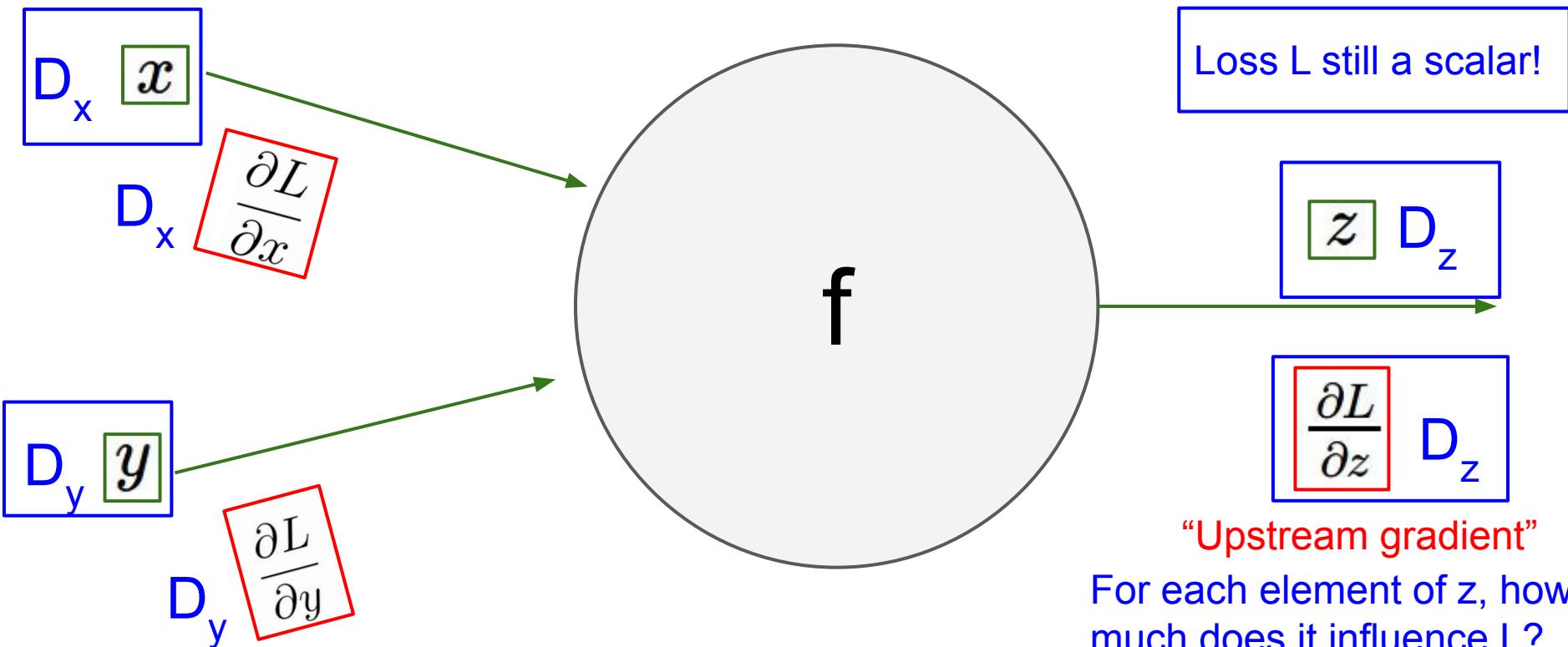
Backprop with Vectors



Backprop with Vectors



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



Backprop with Vectors

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\hspace{1cm}} \begin{array}{c} \text{f}(x) = \max(0, x) \\ (\text{elementwise}) \end{array}$$

4D output z :

$$\begin{array}{l} \xrightarrow{\hspace{1cm}} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix} \\ \xrightarrow{\hspace{1cm}} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 3 \end{bmatrix} \\ \xrightarrow{\hspace{1cm}} \begin{bmatrix} 3 \\ 0 \\ 0 \\ 1 \end{bmatrix} \\ \xrightarrow{\hspace{1cm}} \begin{bmatrix} 0 \\ 3 \\ 1 \\ 0 \end{bmatrix} \end{array}$$

Backprop with Vectors

4D input x :

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$$\begin{array}{l} \xrightarrow{\quad} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix} \end{array}$$

4D dL/dz :

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

Upstream
gradient

Backprop with Vectors

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\quad} \begin{array}{c} f(x) = \max(0, x) \\ (\text{elementwise}) \end{array}$$

4D output z :

$$\begin{array}{c} \xrightarrow{\quad} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix} \\ \xrightarrow{\quad} \\ \xrightarrow{\quad} \\ \xrightarrow{\quad} \end{array}$$

Jacobian $\frac{dz}{dx}$

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

4D $\frac{dL}{dz}$:

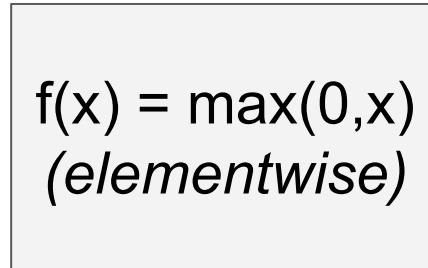
$$\begin{array}{c} \leftarrow \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array}$$

Upstream
gradient

Backprop with Vectors

4D input x :

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



4D output z :

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

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

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

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

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

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

4D dL/dz :

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

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

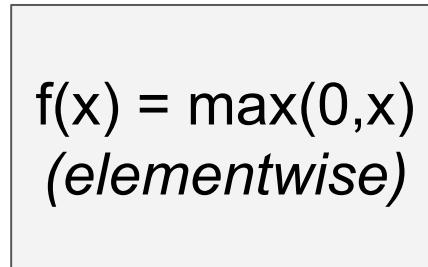
$$\leftarrow \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow$$

Upstream
gradient

Backprop with Vectors

4D input x :

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4D output z :

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

4D dL/dx :

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

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

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

4D dL/dz :

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

Upstream
gradient

Backprop with Vectors

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\quad} \begin{array}{c} f(x) = \max(0, x) \\ (\text{elementwise}) \end{array}$$

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

4D output z :

$$\begin{array}{c} \xrightarrow{\quad} [1] \\ \xrightarrow{\quad} [0] \\ \xrightarrow{\quad} [3] \\ \xrightarrow{\quad} [0] \end{array}$$

4D dL/dx :

$$\begin{array}{l} [4] \\ [0] \\ [5] \\ [0] \end{array} \xleftarrow{\quad} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

4D dL/dz :

$$\begin{array}{l} [4] \\ [-1] \\ [5] \\ [9] \end{array} \xleftarrow{\quad}$$

Upstream
gradient

Backprop with Vectors

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\quad} \begin{array}{c} f(x) = \max(0, x) \\ (\text{elementwise}) \end{array}$$

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4D output z :

$$\begin{array}{l} \xrightarrow{\quad} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix} \end{array}$$

4D dL/dx :

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

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

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

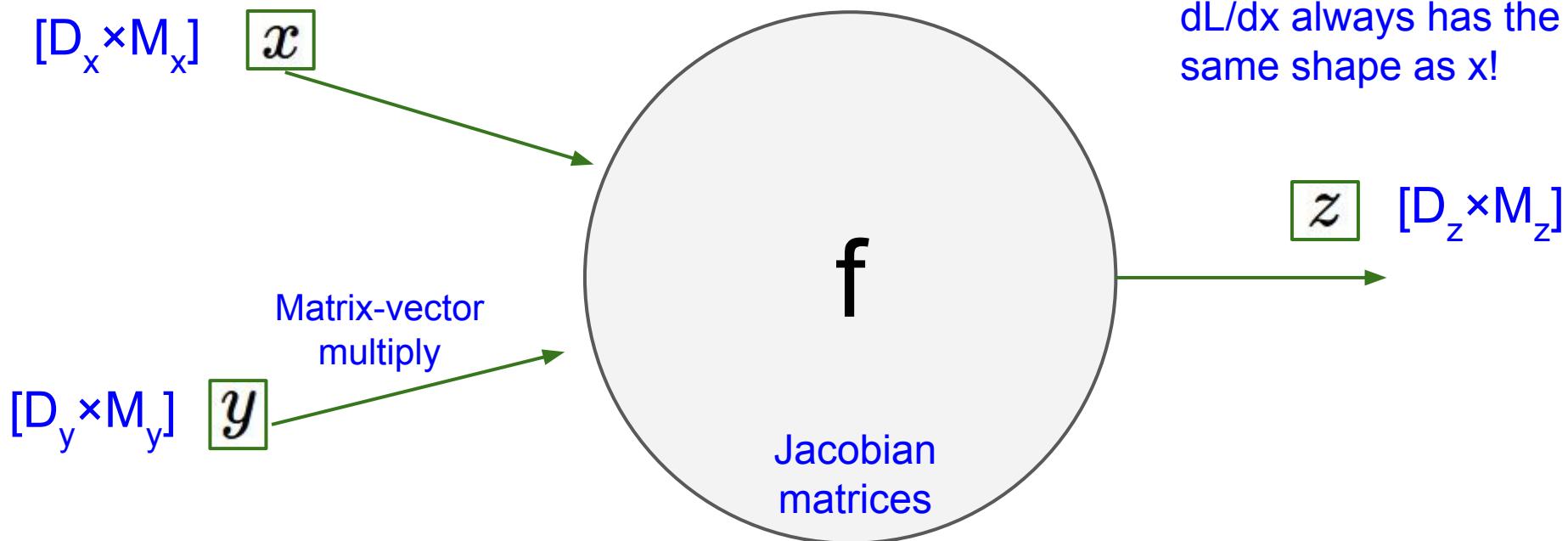
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$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow$$

Upstream
gradient

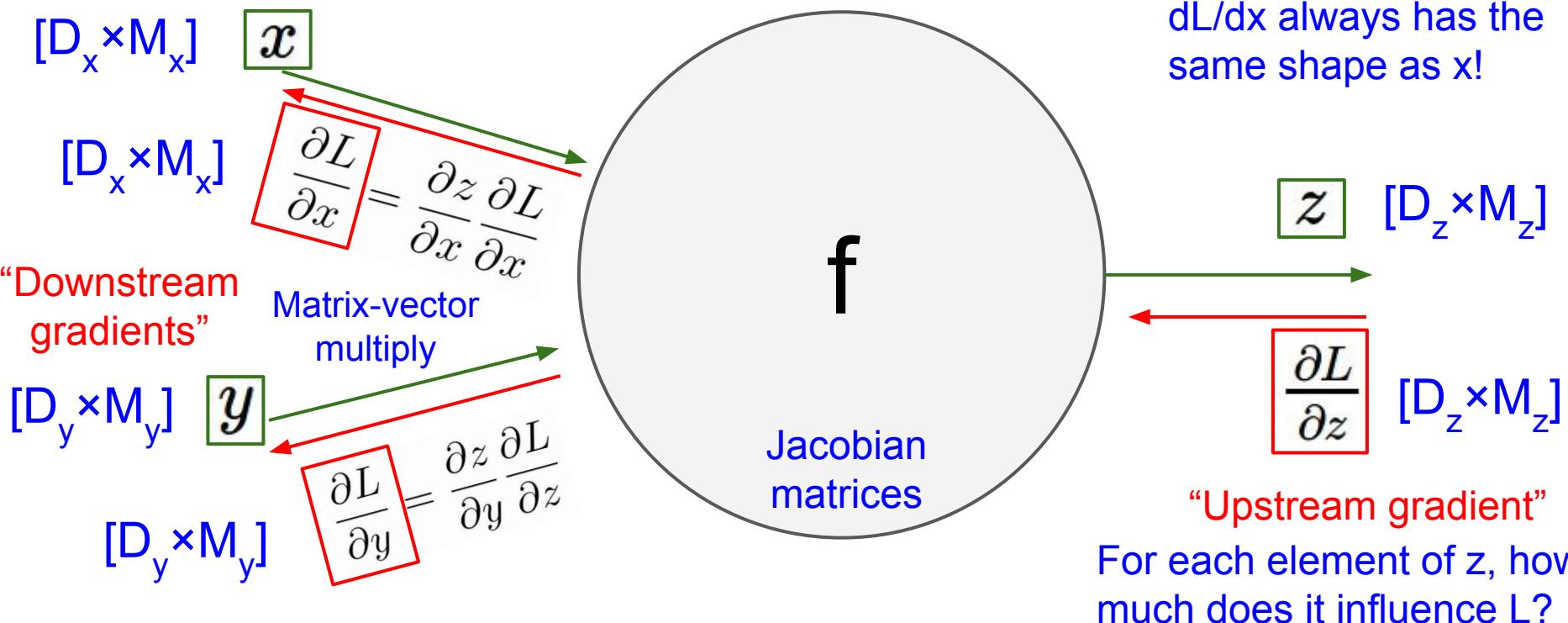
Backprop with Matrices (or Tensors)

Loss L still a scalar!



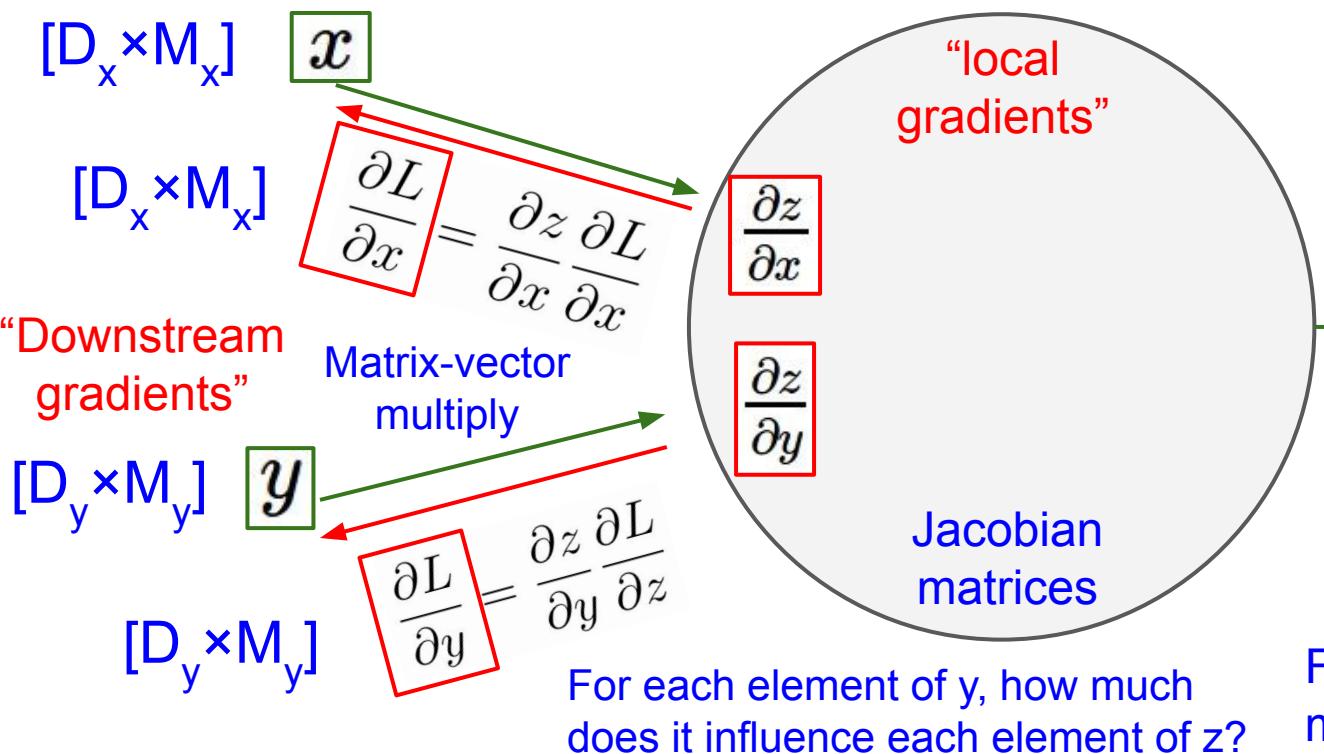
Backprop with Matrices (or Tensors)

Loss L still a scalar!

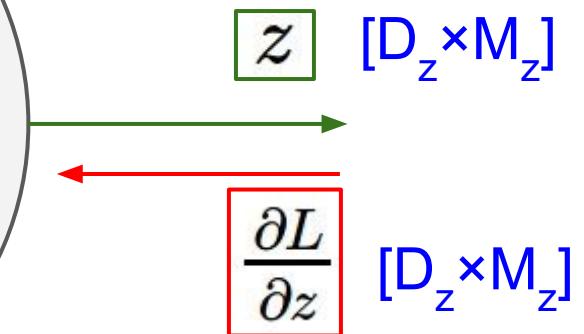


Backprop with Matrices (or Tensors)

Loss L still a scalar!

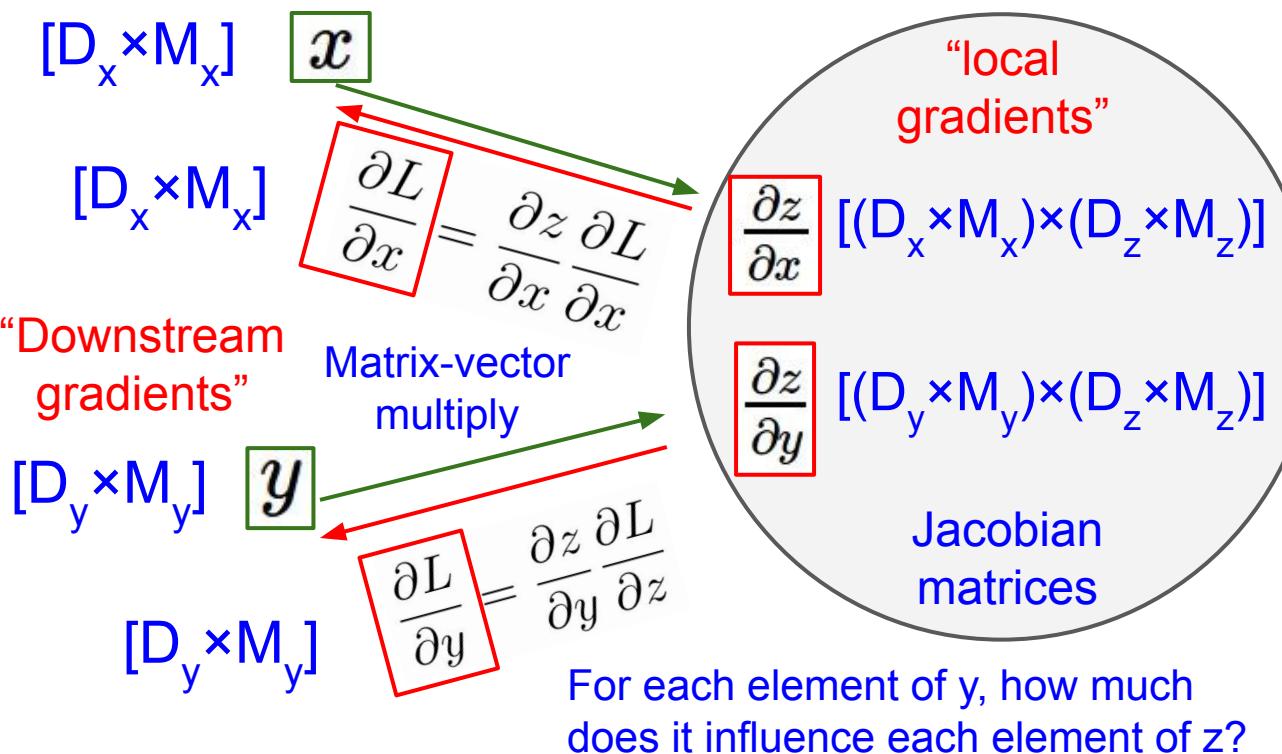


dL/dx always has the same shape as x!



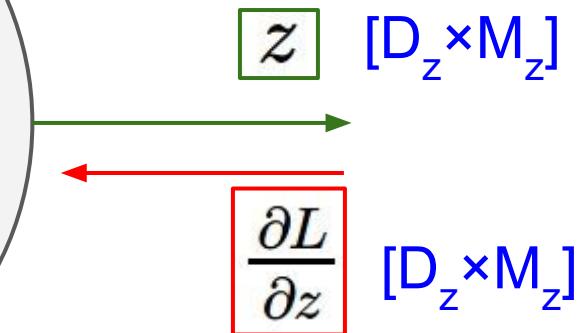
“Upstream gradient”
For each element of z, how much does it influence L?

Backprop with Matrices (or Tensors)



Loss L still a scalar!

dL/dx always has the same shape as x !



“Upstream gradient”

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

Backprop with Matrices

x: [N×D]

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

w: [D×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×M]

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

dL/dy: [N×M]

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

Also see derivation in the course notes:

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

Backprop with Matrices

$x: [N \times D]$

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

$w: [D \times M]$

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

Matrix Multiply

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

Jacobians:

$$\begin{aligned} dy/dx &: [(N \times D) \times (N \times M)] \\ dy/dw &: [(D \times M) \times (N \times M)] \end{aligned}$$

$y: [N \times M]$

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

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

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

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]

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

w: [D×M]

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

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

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

y: [N×M]

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

dL/dy: [N×M]

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Backprop with Matrices

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$y: [N \times M]$

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

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

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

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

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

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

Backprop with Matrices

$x: [N \times D]$

[2 **1** -3]

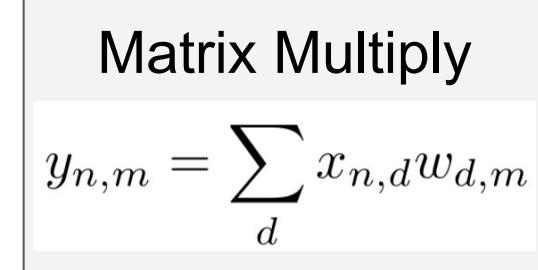
[-3 4 2]

$w: [D \times M]$

[3 2 1 -1]

[2 1 3 2]

[3 2 1 -2]



$y: [N \times M]$

13	9	-2	-6
5	2	17	1

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

2	3	-3	9
-8	1	4	6

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

$x: [N \times D]$

[2 **1** -3]

[-3 4 2]

$w: [D \times M]$

[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 $y_{n,:}$.

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

$y: [N \times M]$

[13 9 **-2** -6]

[5 2 17 1]

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

[2 3 -3 9]

[-8 1 4 6]

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

Backprop with Matrices

x: [N×D]

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

w: [D×M]

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

[N×D] [N×M] [M×D]

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

Matrix Multiply

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

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: $w_{d,m}$

y: [N×M]

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

dL/dy: [N×M]

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

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

Backprop with Matrices

$x: [N \times D]$

[2 **1** -3]

[-3 4 2]

$w: [D \times M]$

[3 2 1 -1]

[2 1 **3** 2]

[3 2 1 -2]

Matrix Multiply

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

$y: [N \times M]$

[13 9 **-2** -6]

[5 2 17 1]

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

[2 3 -3 9]

[-8 1 4 6]

By similar logic:

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

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

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

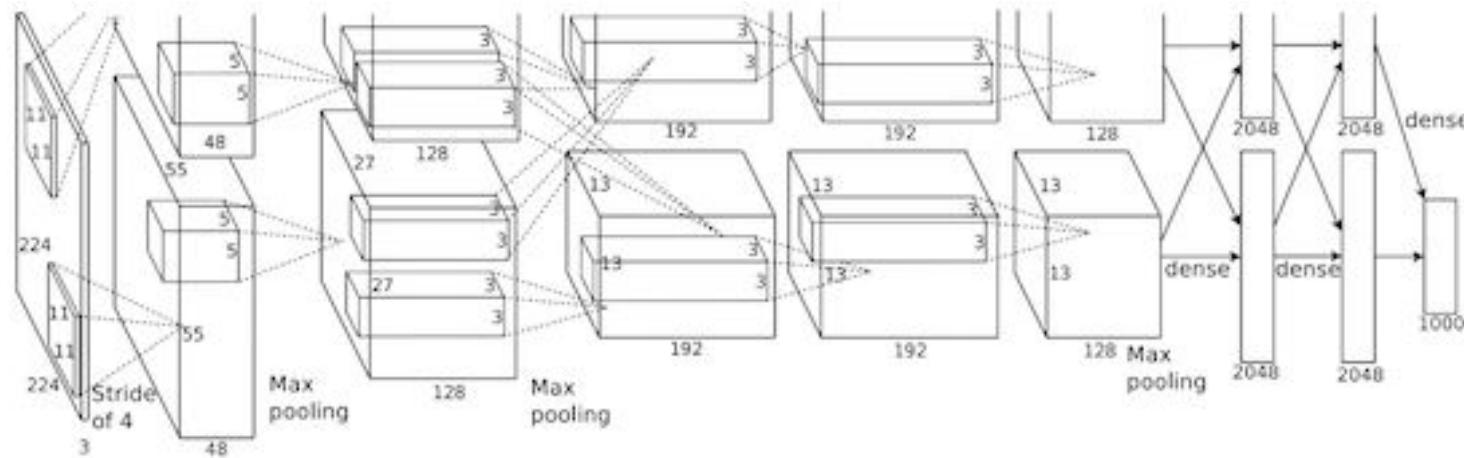
$$\frac{\partial L}{\partial w} = x^T \left(\frac{\partial L}{\partial y} \right)$$

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!

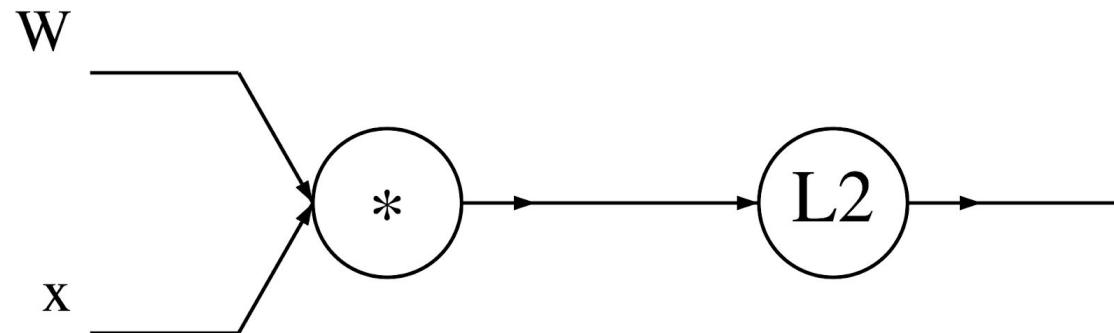


A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$

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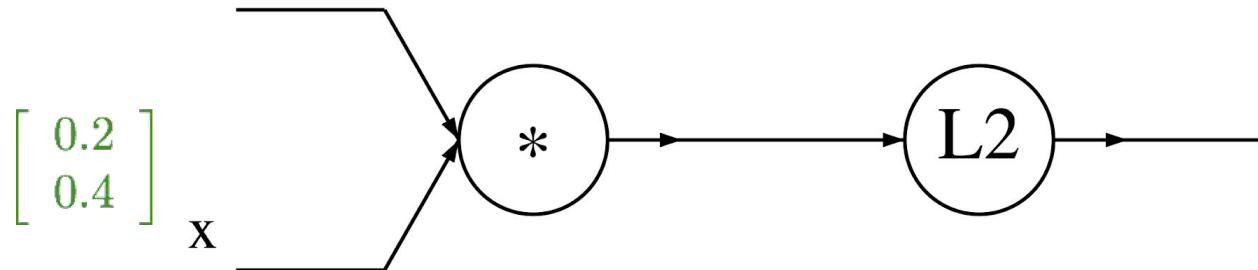
\downarrow \downarrow
 $\in \mathbb{R}^n$ $\in \mathbb{R}^{n \times n}$

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

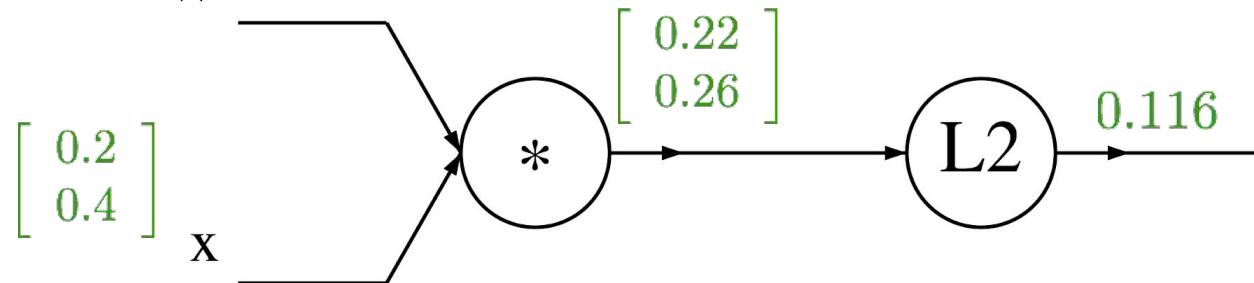


$$q = W \cdot x = \begin{pmatrix} W_{1,1}x_1 + \cdots + W_{1,n}x_n \\ \vdots \\ W_{n,1}x_1 + \cdots + W_{n,n}x_n \end{pmatrix}$$

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

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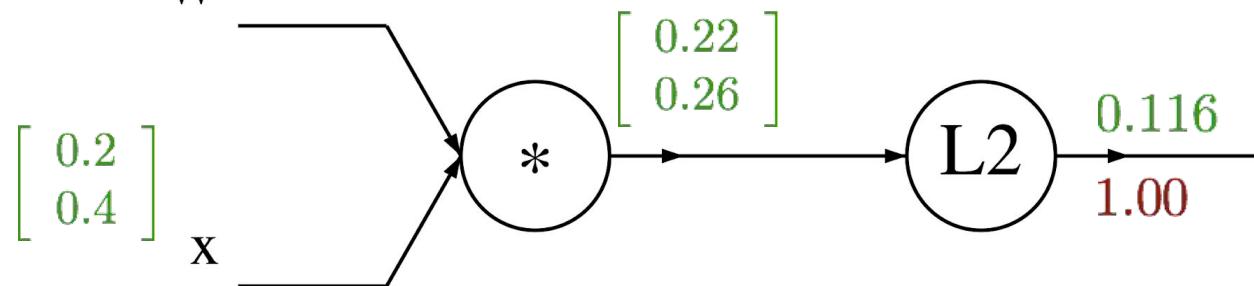


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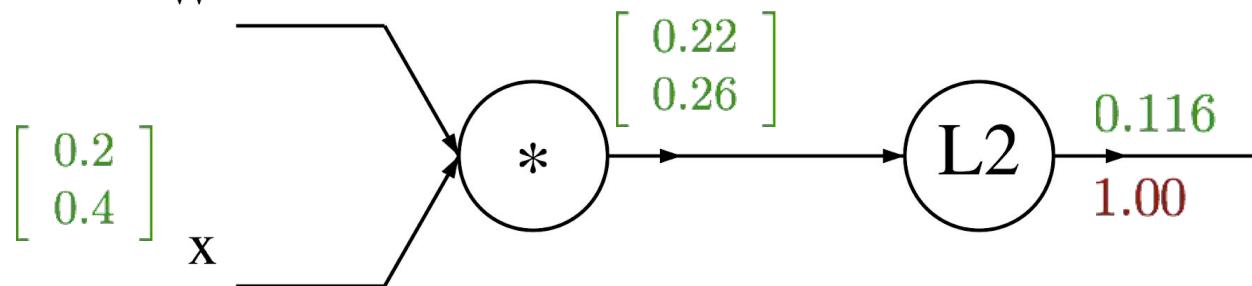


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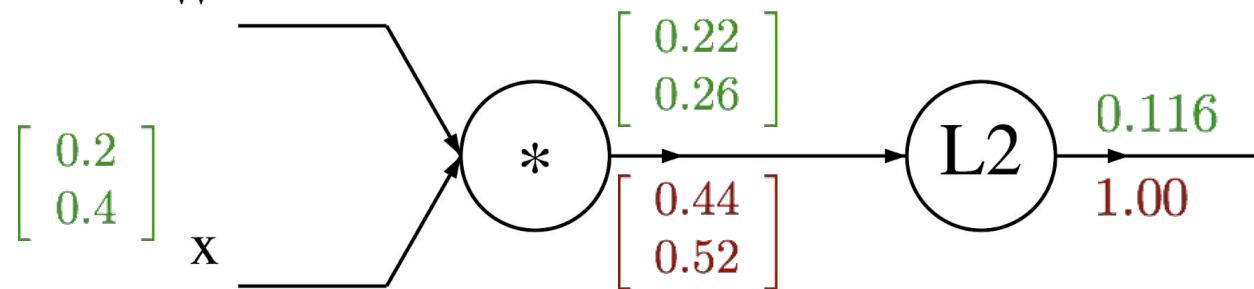
$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

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

$$\nabla_q f = 2q$$

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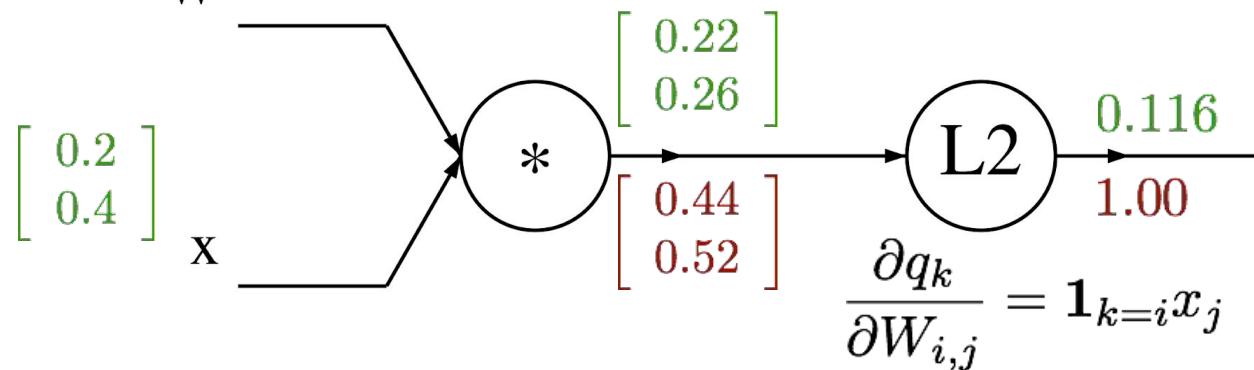
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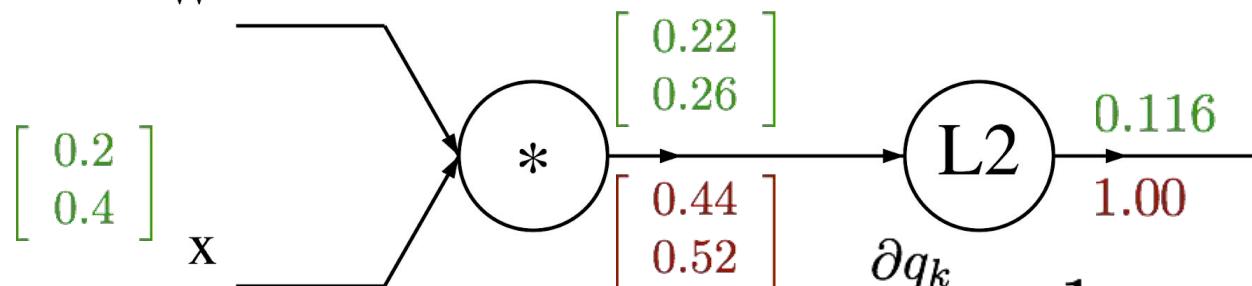
$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

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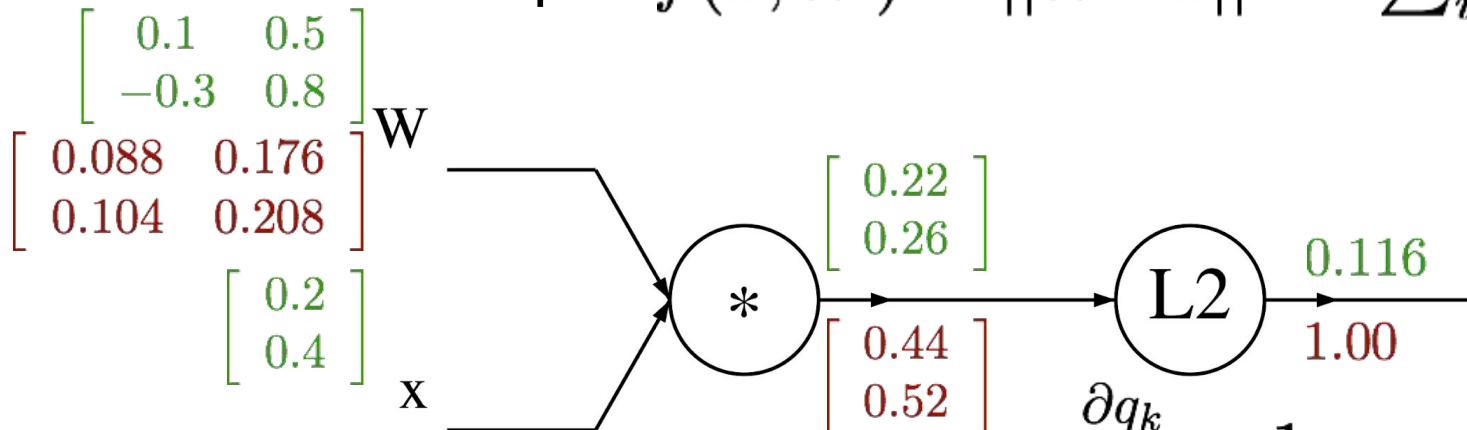
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$$= \sum_k (2q_k)(\mathbf{1}_{k=i} x_j)$$

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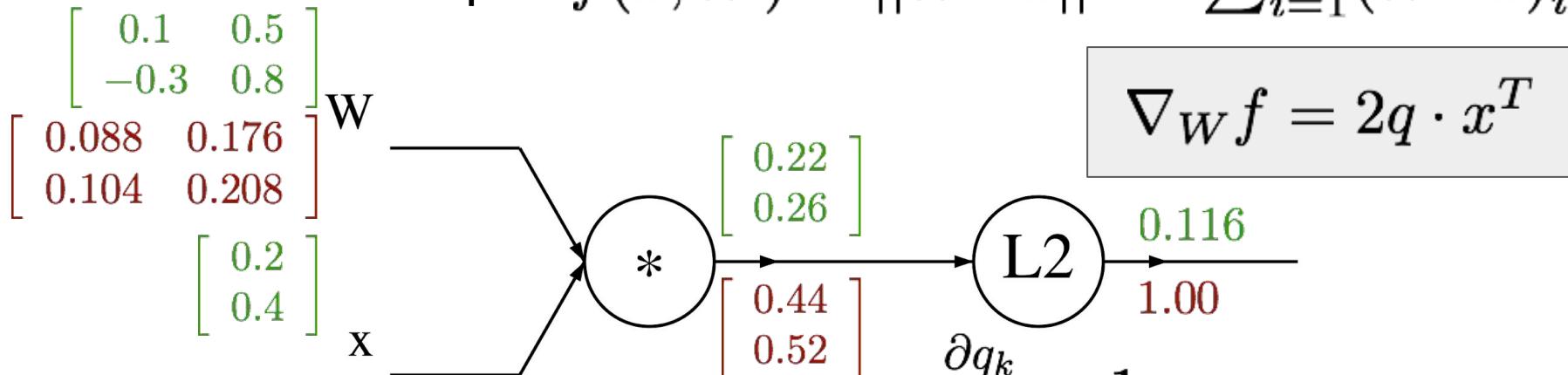
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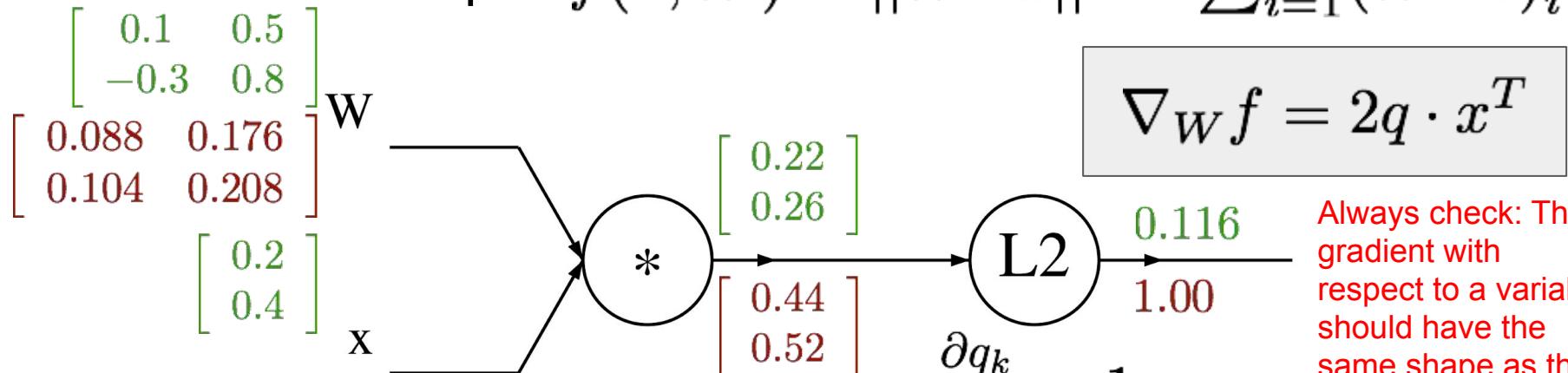
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Always check: The gradient with respect to a variable should have the same shape as the variable

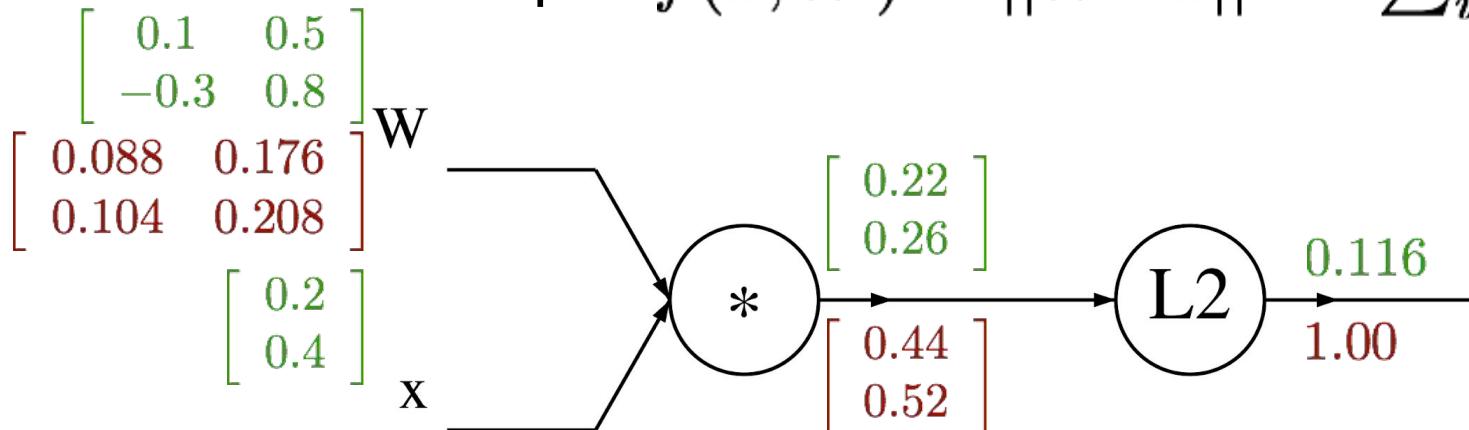
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$$f(q) = \|q\|^2 = q_1^2 + \cdots + q_n^2$$

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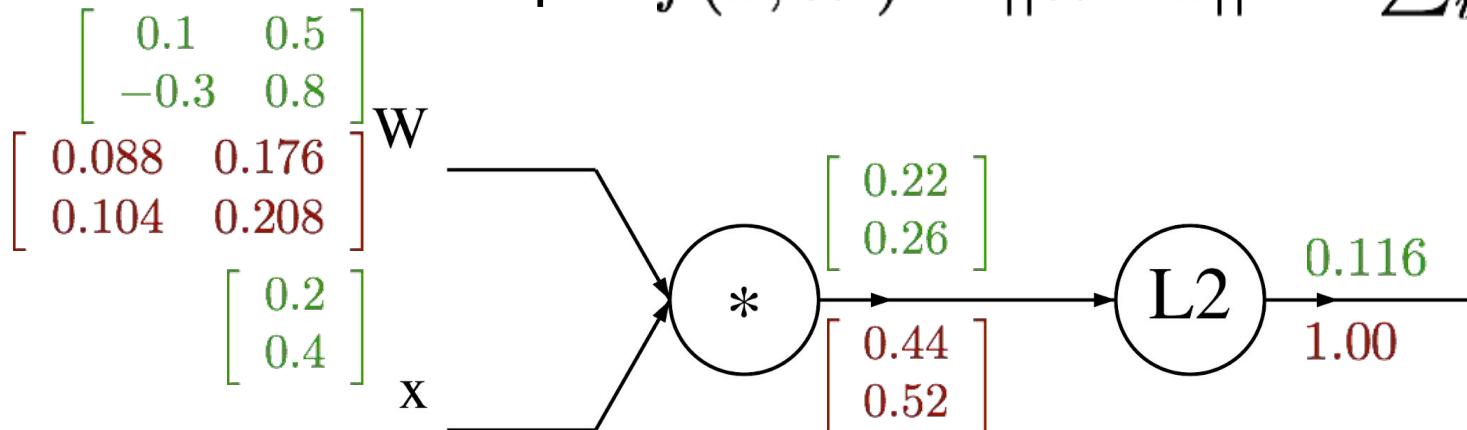


$$\frac{\partial q_k}{\partial x_i} = W_{k,i}$$

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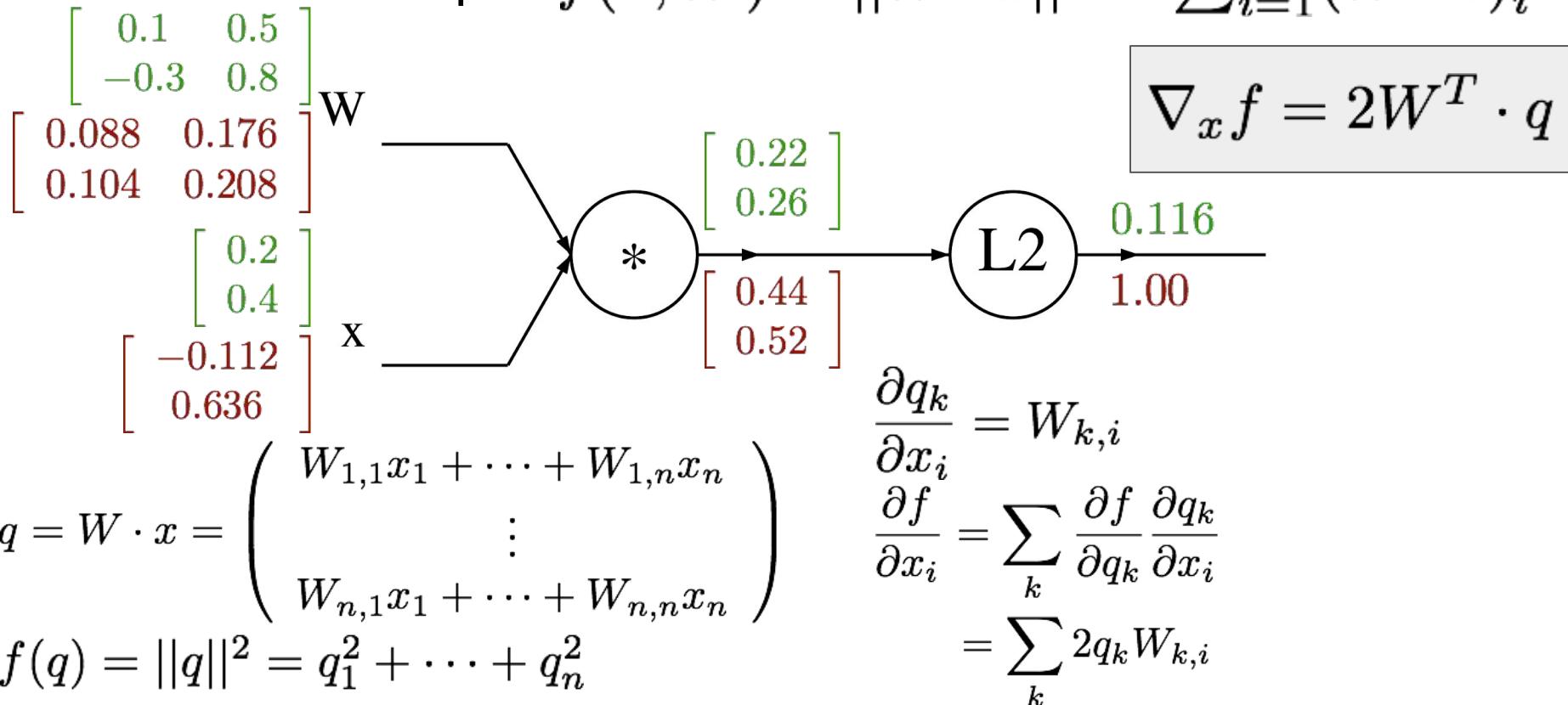


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A vectorized example: $f(x, W) = ||W \cdot x||^2 = \sum_{i=1}^n (W \cdot x)_i^2$



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

In discussion section: A matrix example...

$$z_1 = XW_1$$

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

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

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

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

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

