Lecture 4:
Neural Networks and Backpropagation

Administrative: Assignment 1

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

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

We will distribute Google Cloud coupons by this weekend

Administrative: Alternate Midterm Time

If you need to request an alternate midterm time:

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

Administrative: Project Proposal

Project proposal due 4/24

Administrative: Discussion Section

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

How to pick a project / How to read a paper

Where we are...

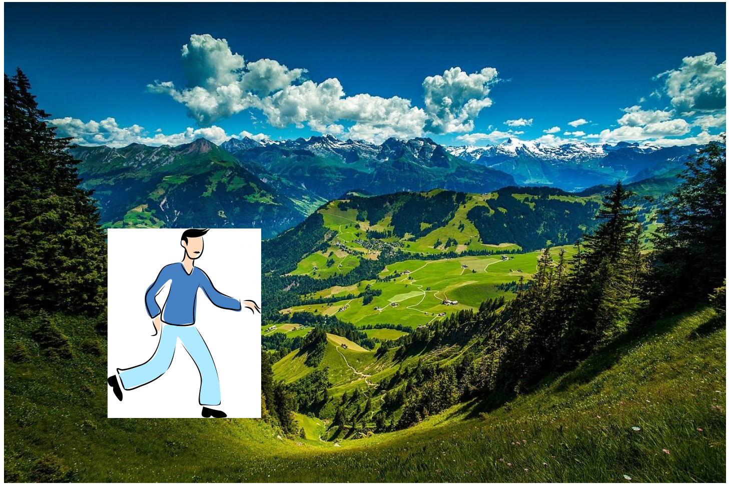
$$s = f(x; W) = Wx$$ Linear score function

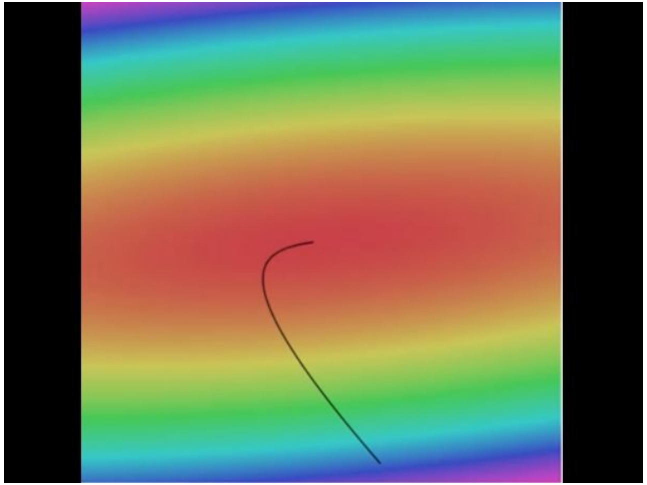
$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$ SVM loss (or softmax)

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

How to find the best W?

Finding the best W: Optimize with Gradient Descent





```
# Vanilla Gradient Descent

while True:
  weights_grad = evaluate_gradient(loss_fun, data, weights)
  weights += - step_size * weights_grad # perform parameter update
```

Gradient descent

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

Numerical gradient: slow :(, approximate :(, easy to write :)
Analytic gradient: fast :), exact :), error-prone :(

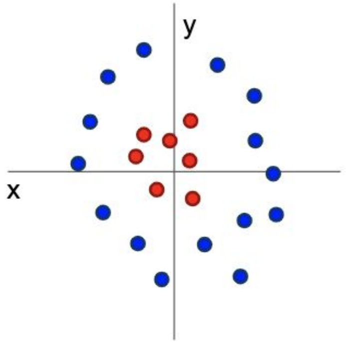
In practice: Derive analytic gradient, check your implementation with numerical gradient

Problem: Linear Classifiers are not very powerful

Visual Viewpoint

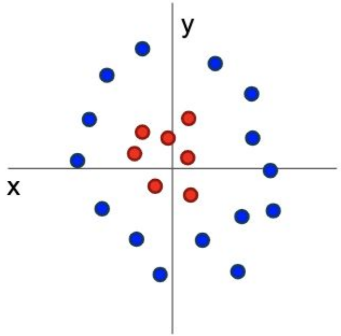
Linear classifiers learn one template per class

Geometric Viewpoint



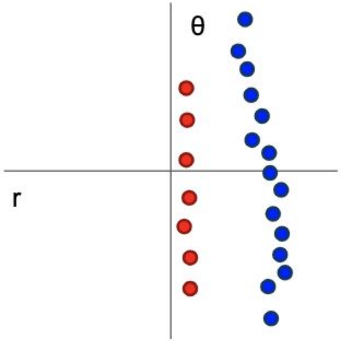
Linear classifiers can only draw linear decision boundaries

One Solution: Feature Transformation

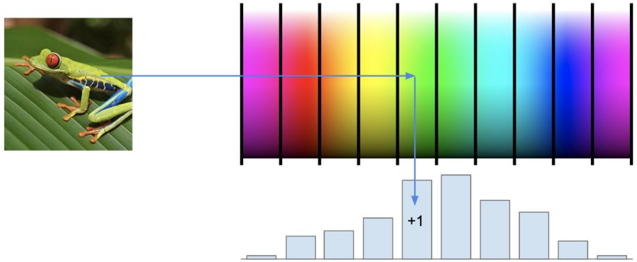


$f(x, y) = (r(x, y), \theta(x, y))$

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



Color Histogram



Histogram of Oriented Gradients (HoG)

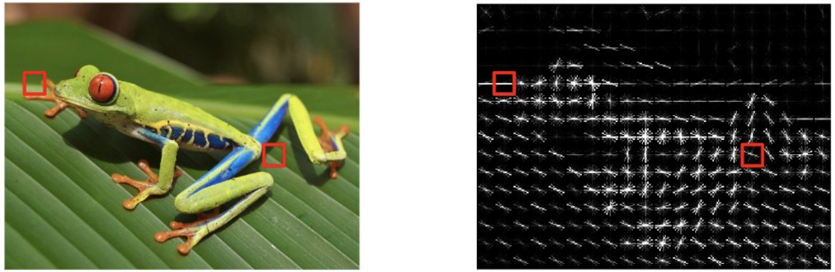
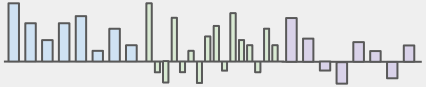


Image features vs ConvNets

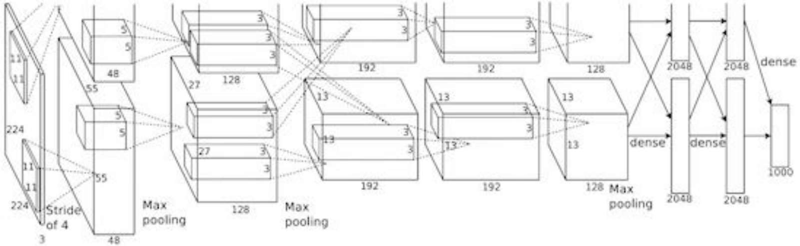
Feature Extraction



f

10 numbers giving scores for classes

training



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

10 numbers giving scores for classes

training

Today: Neural Networks

Neural networks: without the brain stuff

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

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

Neural networks: without the brain stuff

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

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

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

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

Neural networks: without the brain stuff

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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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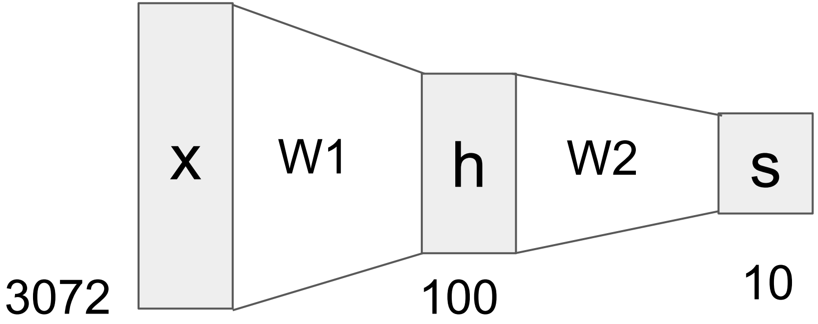

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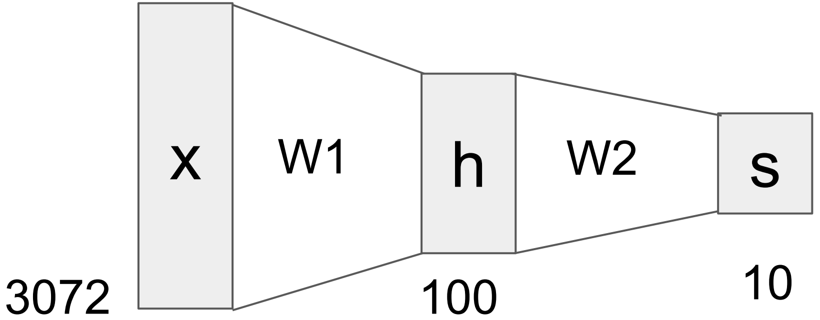
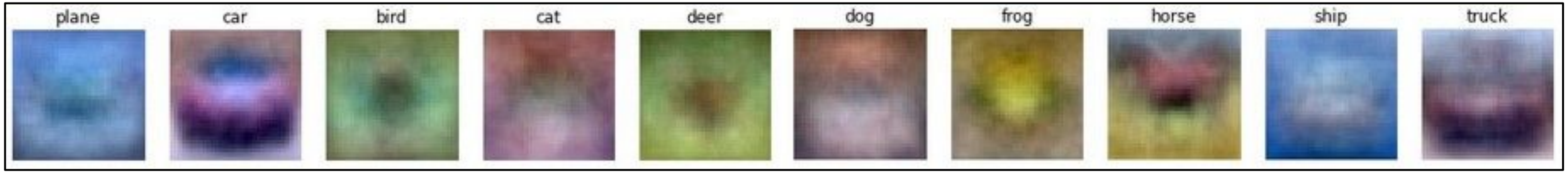




Neural networks: without the brain stuff

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

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

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: $f = Wx$

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

The function $\max(0, z)$ is called the **activation function.**
Q: What if we try to build a neural network without one?

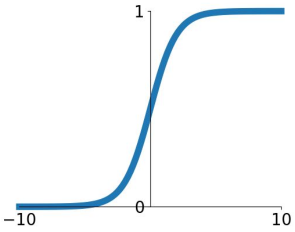
$$f = W_2 W_1 x \qquad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

A: We end up with a linear classifier again!

Activation functions

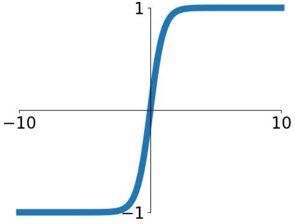
Sigmoid

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



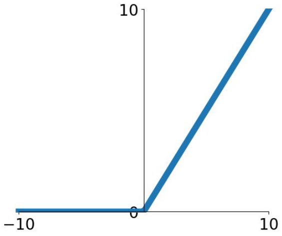
tanh

$\tanh(x)$



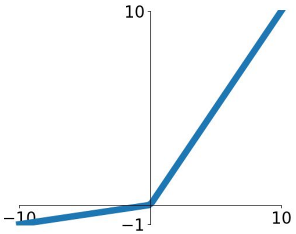
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

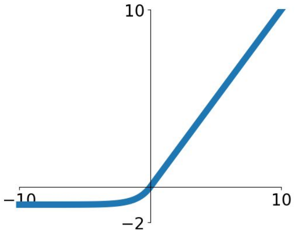


Maxout

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

ELU

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

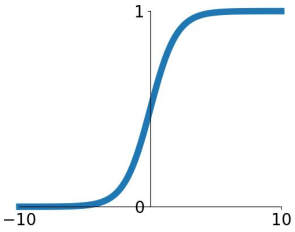


Activation functions

ReLU is a good default choice for most problems

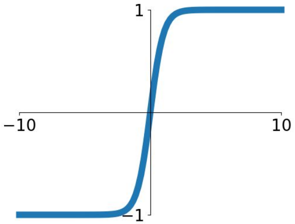
Sigmoid

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



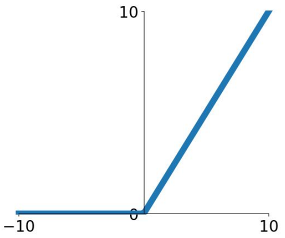
tanh

$\tanh(x)$



ReLU

$\max(0, x)$



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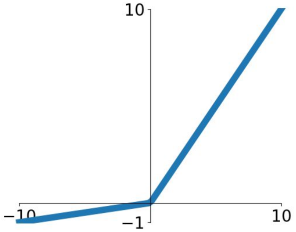

Maxout

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

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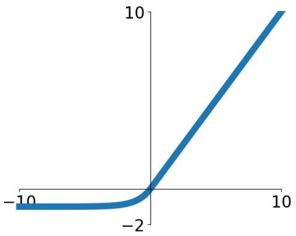
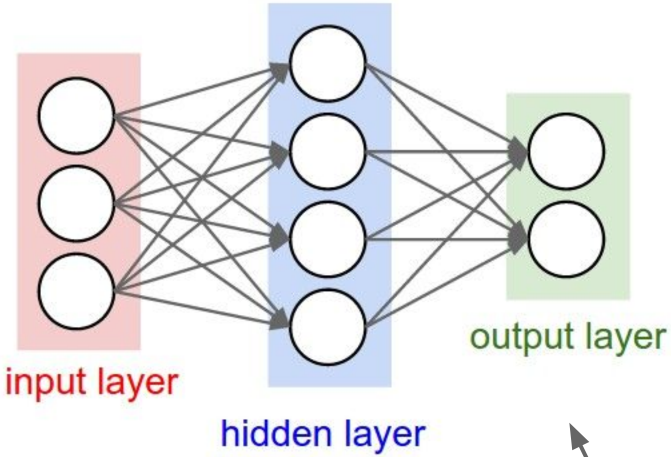
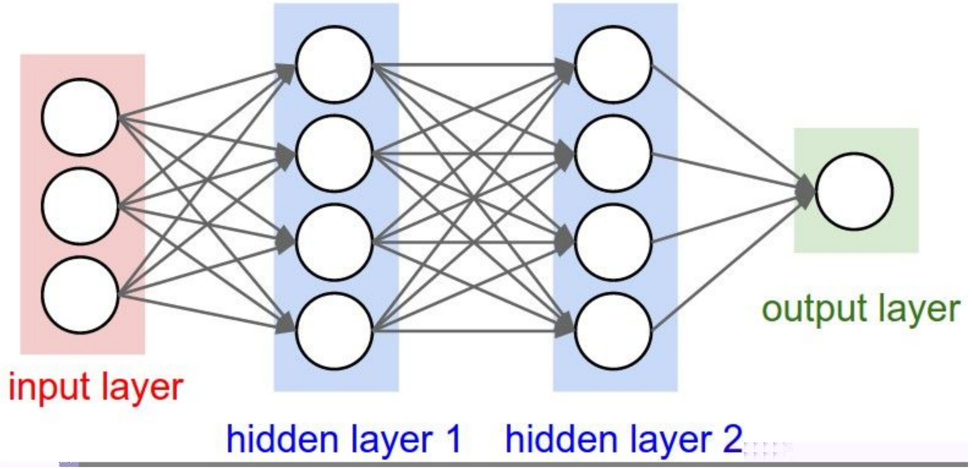


Neural networks: Architectures



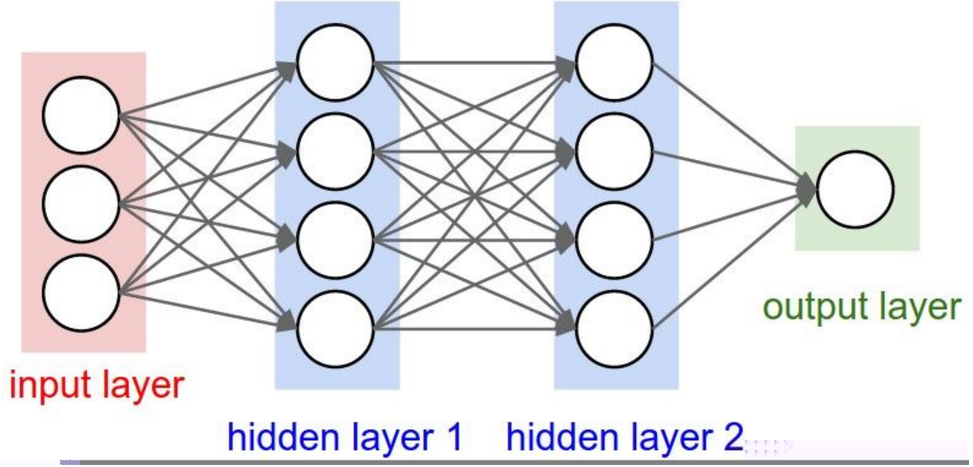


“2-layer Neural Net”, or
“1-hidden-layer Neural Net”

“Fully-connected” layers

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

Example feed-forward computation of a neural network




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

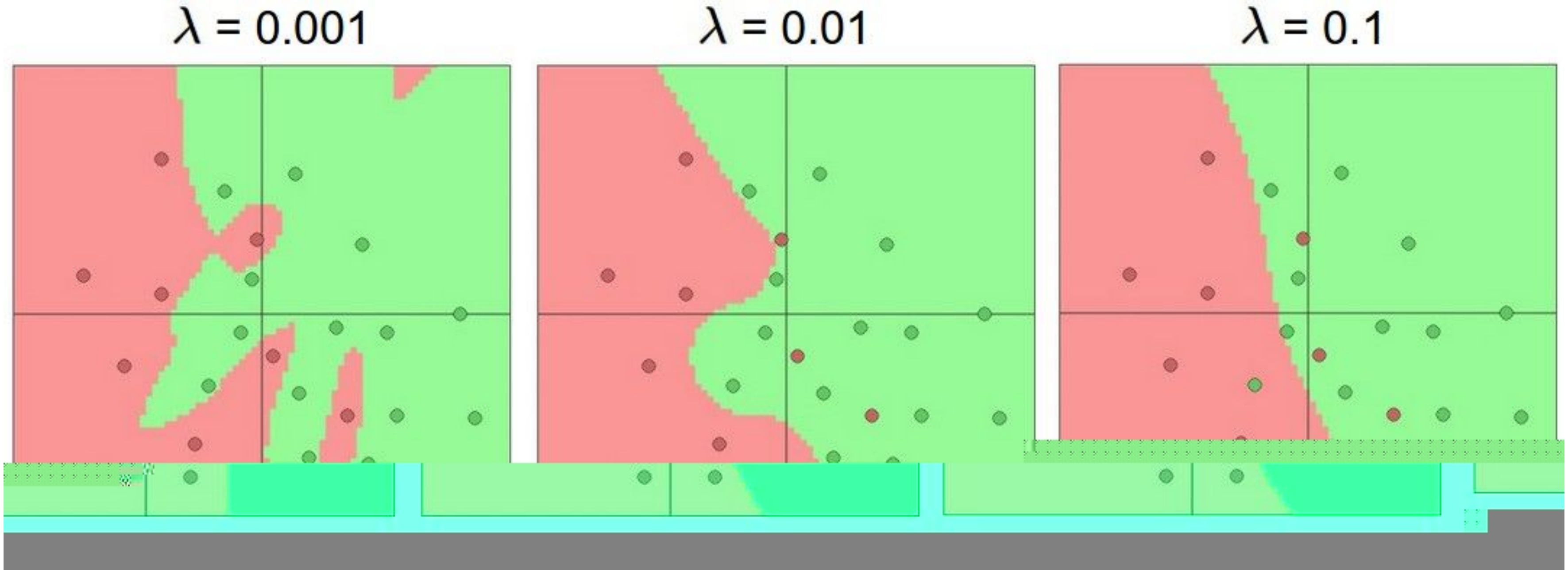
Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
import numpy as np
from numpy
```

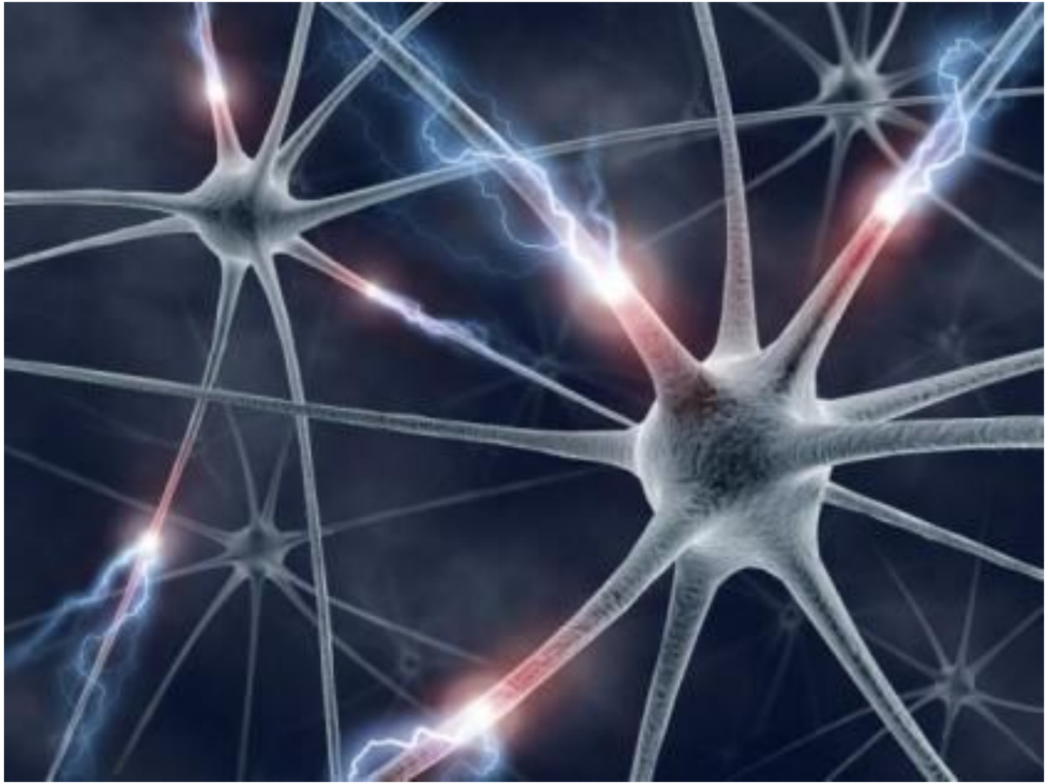
Setting the number of layers and their sizes

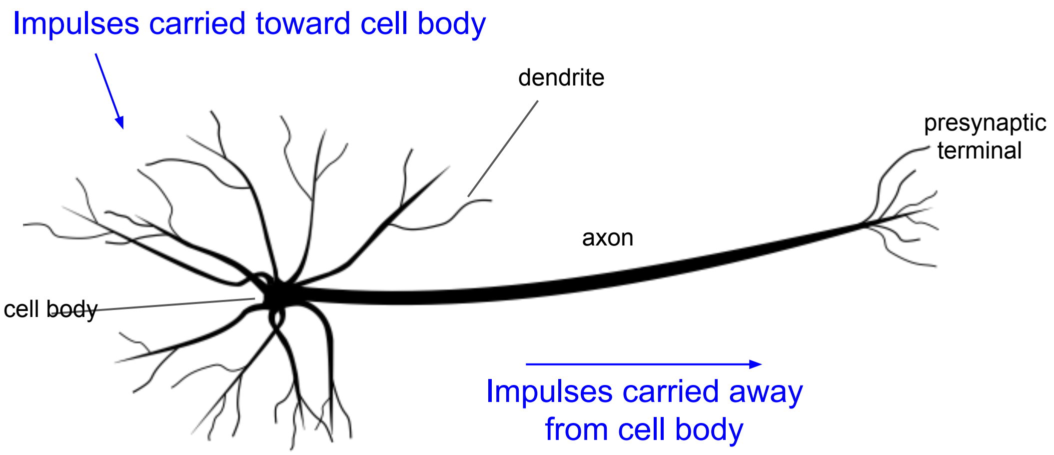
more neurons = more capacity

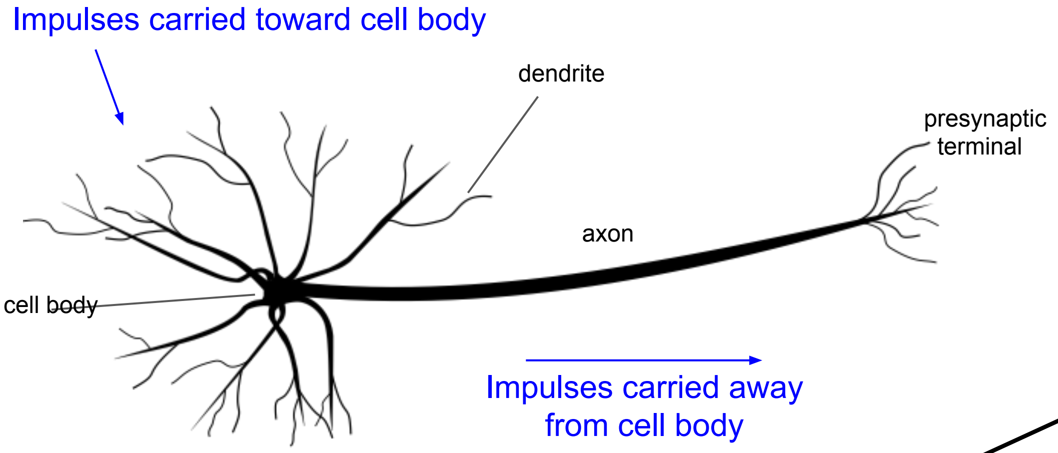
Do not use size of neural network as a regularizer. Use stronger regularization instead:



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




Impulses carried toward cell body
dendrite
presynaptic
terminal
axon
cell body
Impulses carried away
from cell body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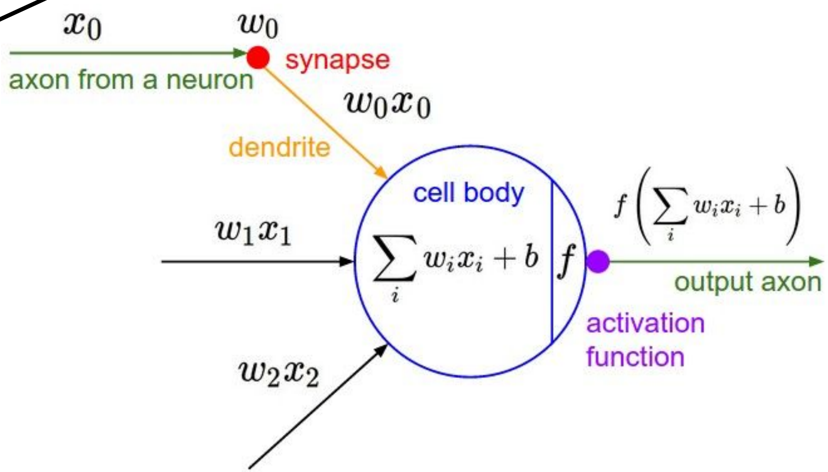
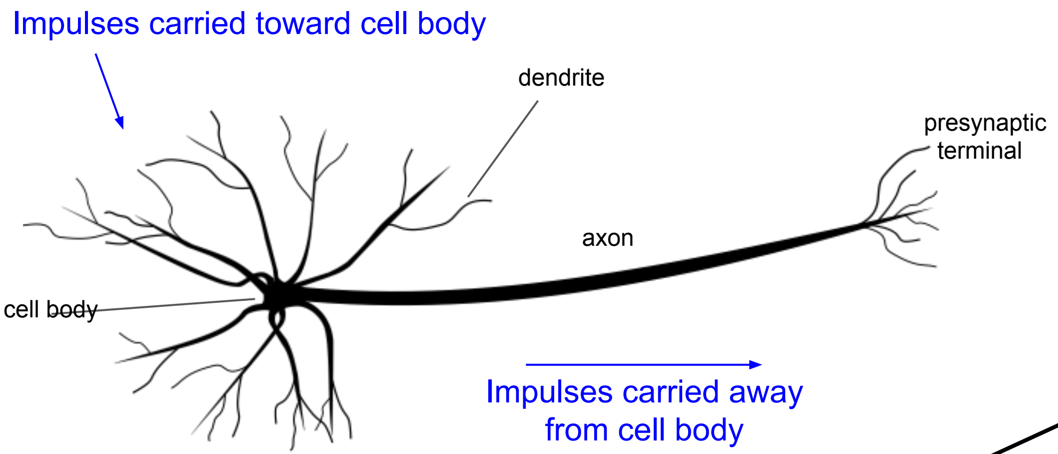
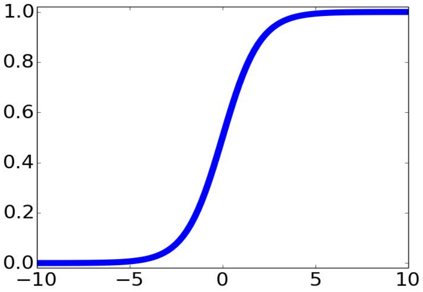
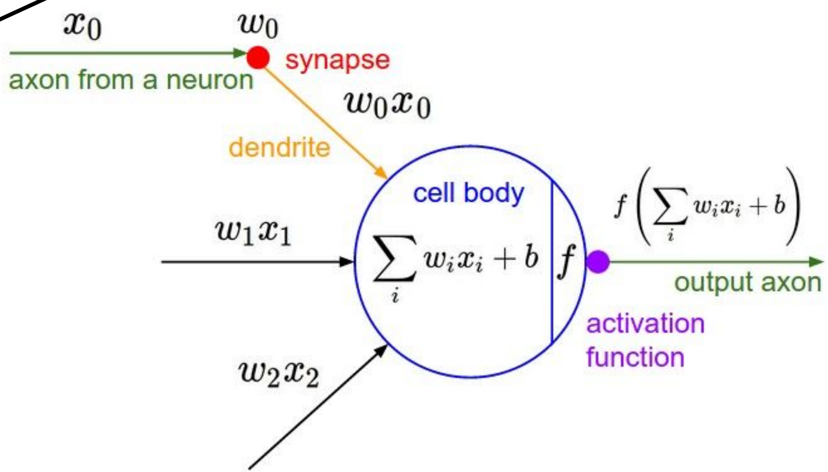

x_0
w_0
synapse
axon from a neuron
$w_0 x_0$
dendrite
cell body
$\sum_i w_i x_i + b$
f
$f\left(\sum_i w_i x_i + b\right)$
$w_1 x_1$
output axon
activation
function
$w_2 x_2$

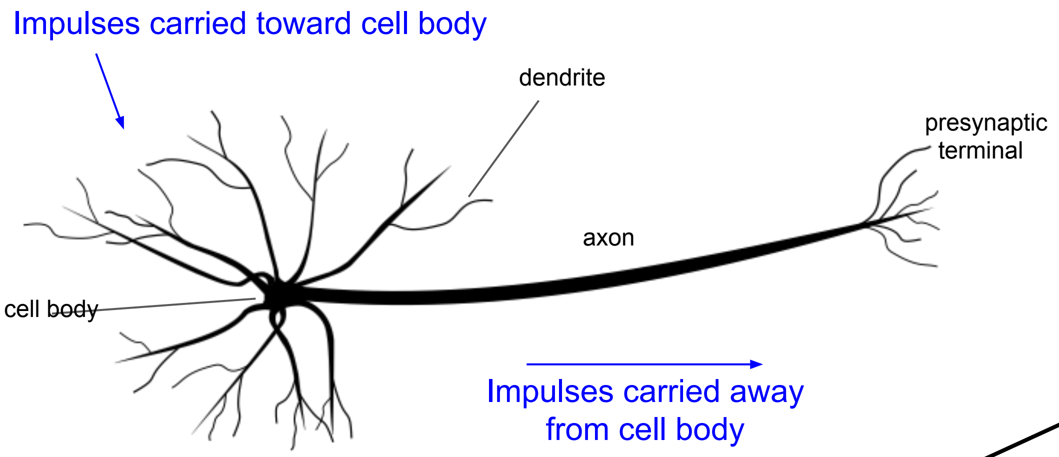


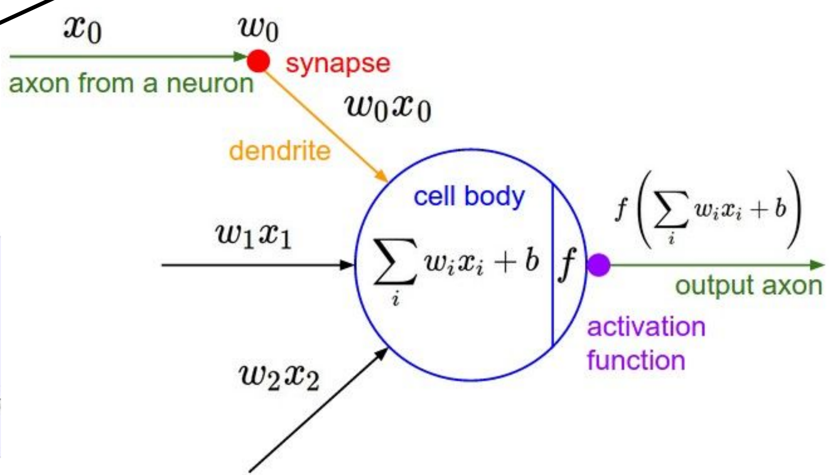


sigmoid activation function

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

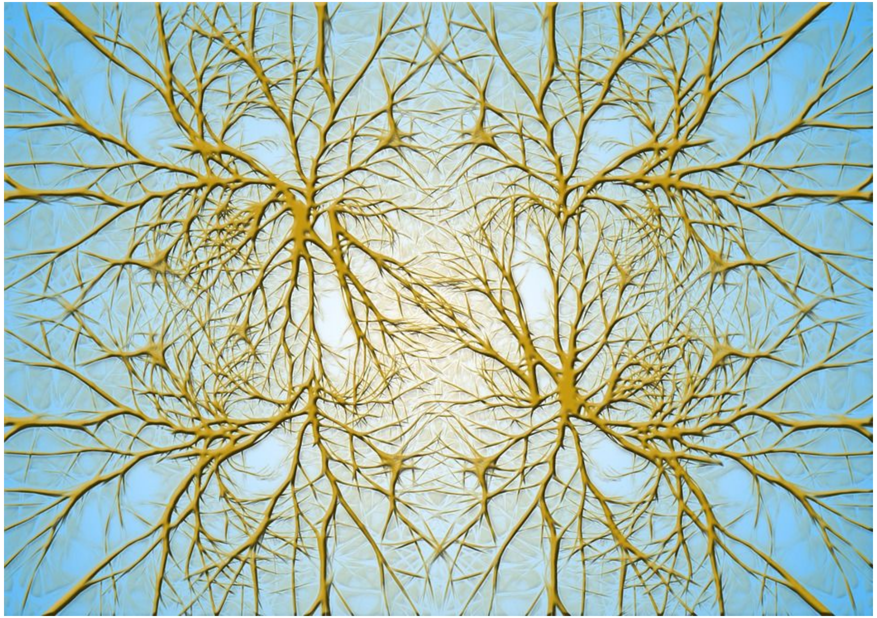







```python
class Neuron:
  # ...
  def neuron_tick(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation func
    return firing_rate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

Biological Neurons:
Complex connectivity patterns



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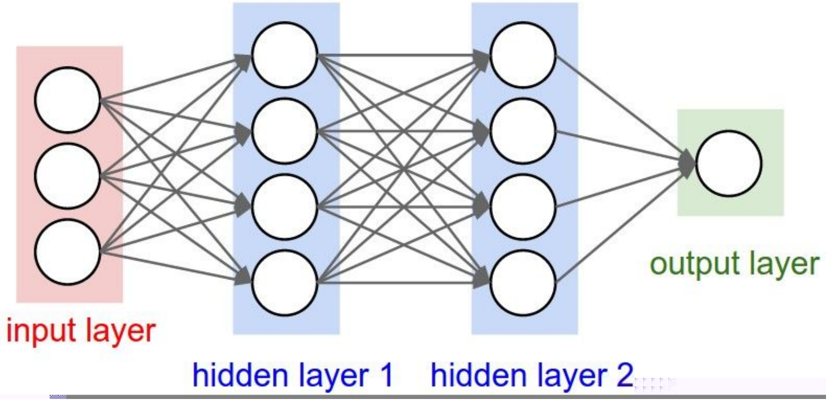
Neurons in a neural network:
Organized into regular layers for computational efficiency



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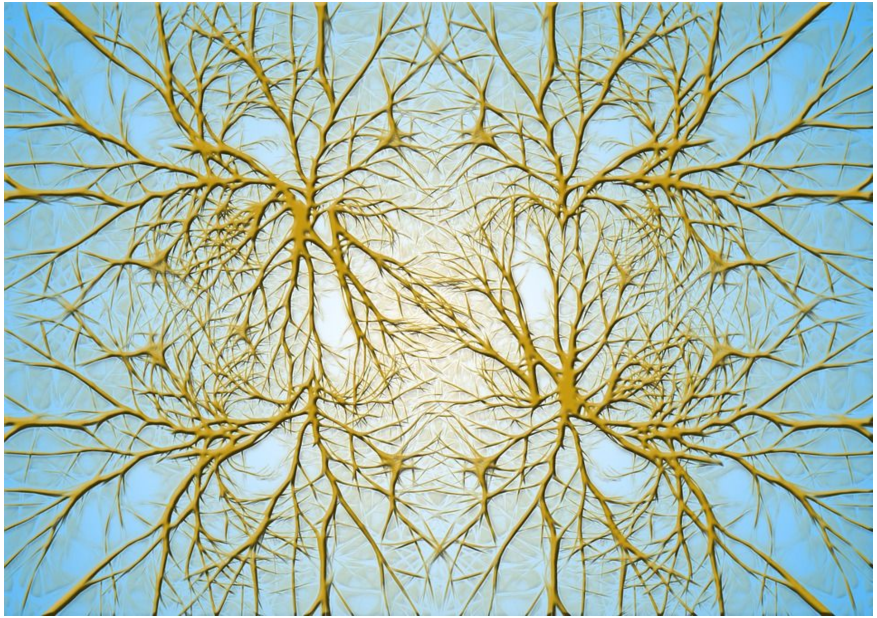

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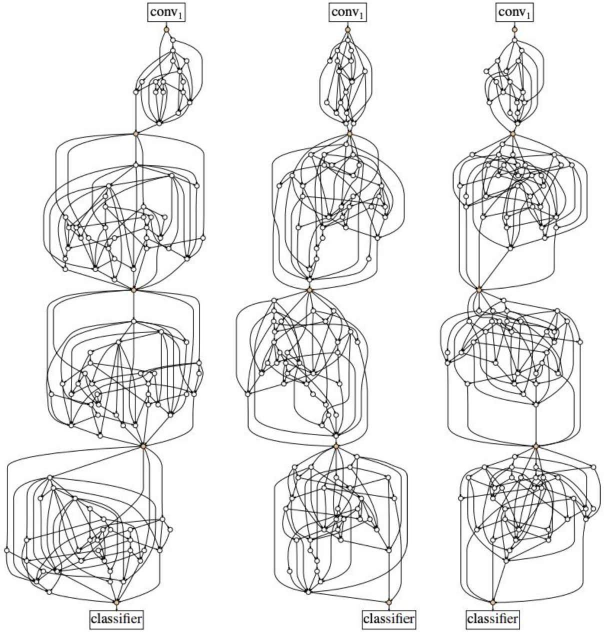
But neural networks with random connections can work too!



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

Be very careful with your brain analogies!

Biological Neurons:

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

[Dendritic Computation. London and Hausser]

Problem: How to compute gradients?

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

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

$$R(W) = \sum_k W_k^2$$ Regularization

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

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

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

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

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

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

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

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

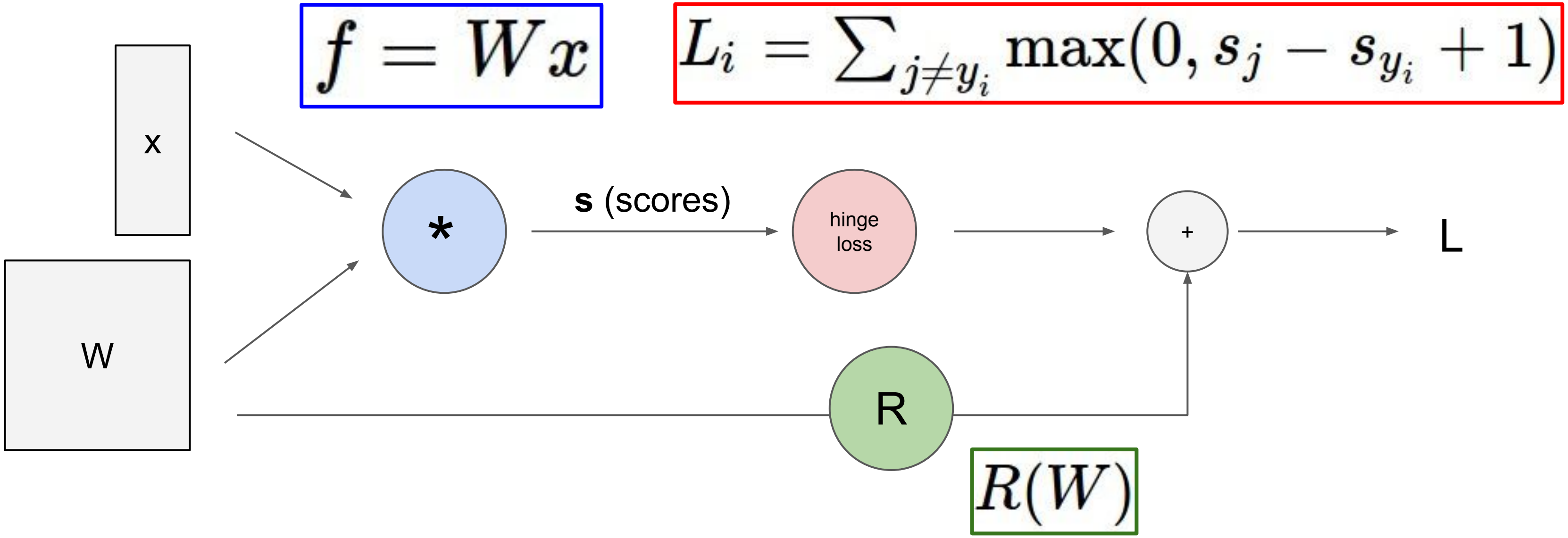
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

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

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

Problem: Not feasible for very complex models!

Better Idea: Computational graphs + Backpropagation



Convolutional network (AlexNet)

input image

weights

loss

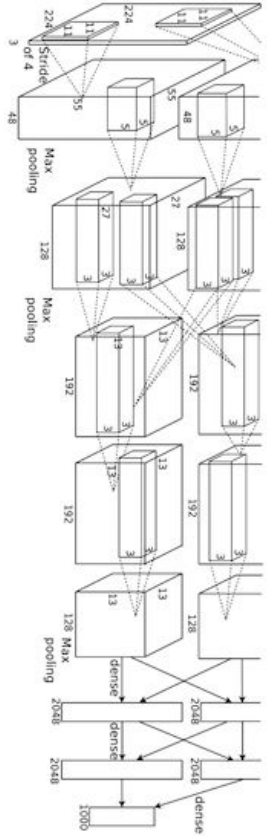
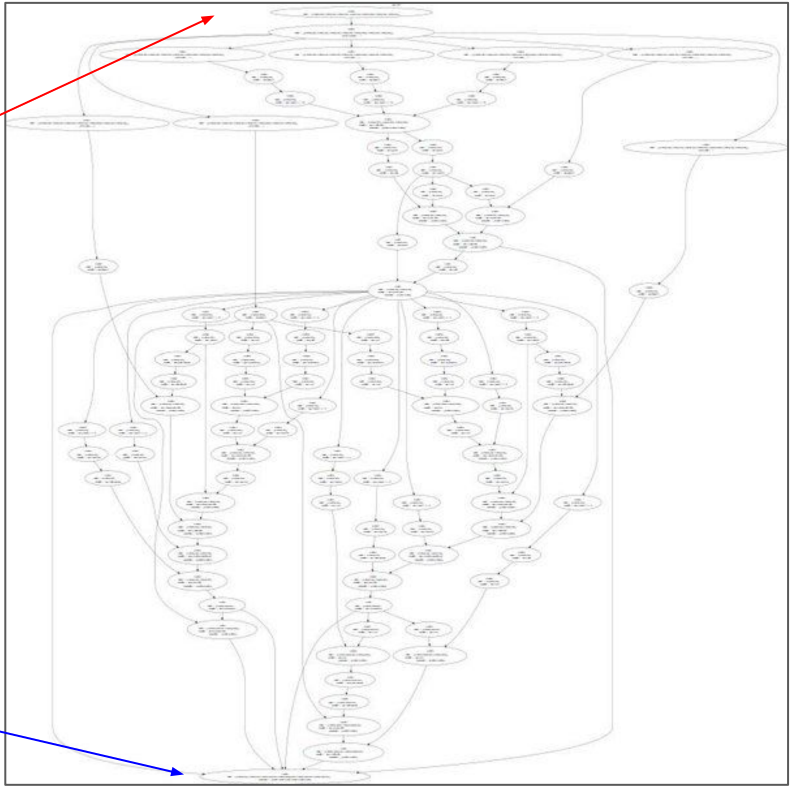


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

Neural Turing Machine

input image

loss



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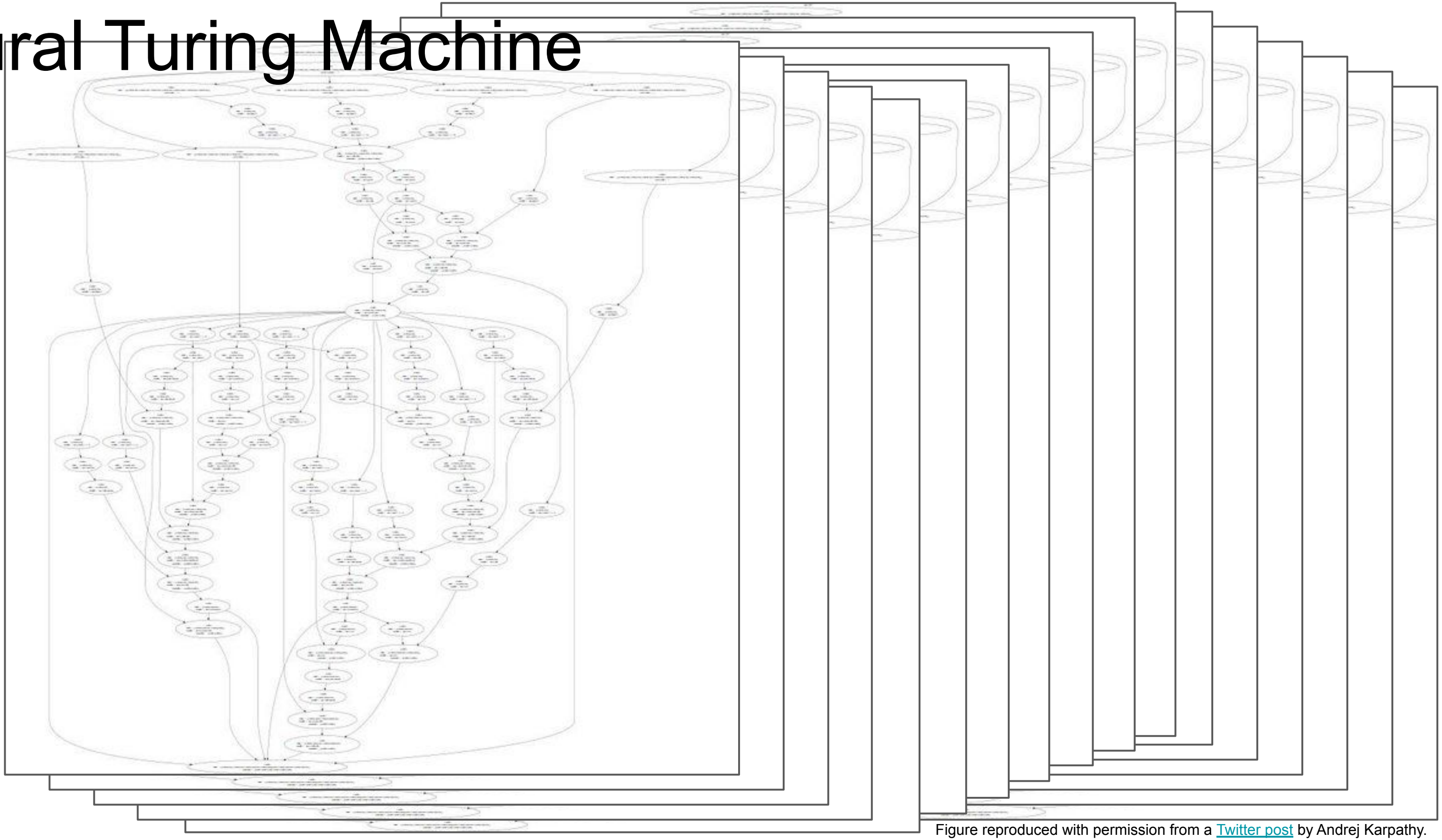
Neural Turing Machine



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Backpropagation: a simple example

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

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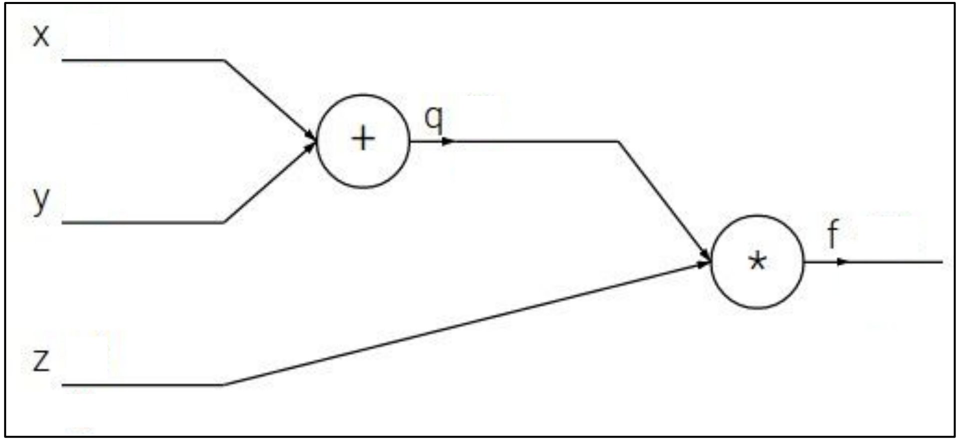
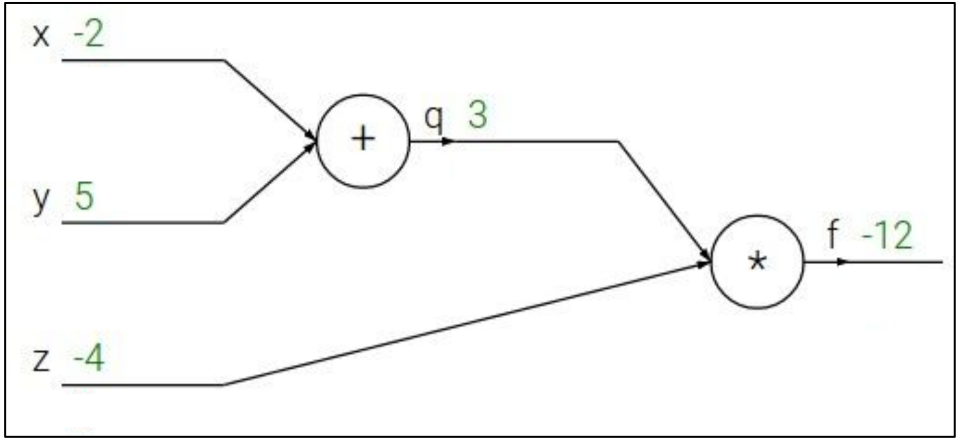


Backpropagation: a simple example

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

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



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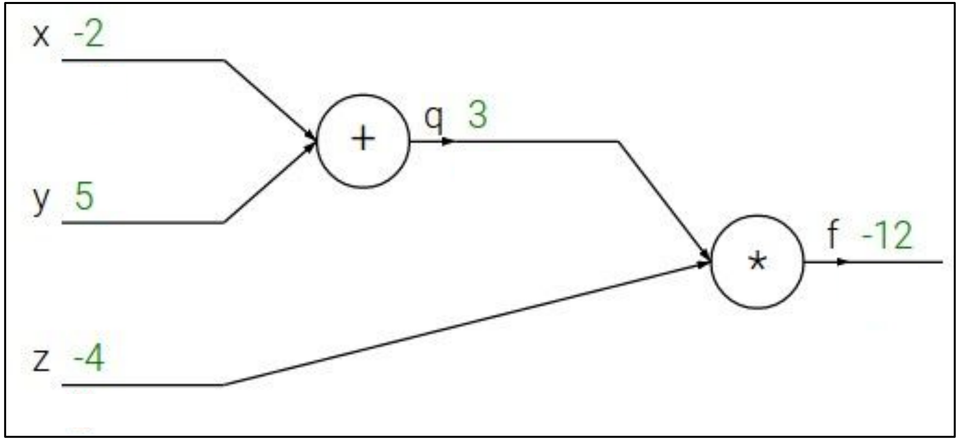
$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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

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



Backpropagation: a simple example

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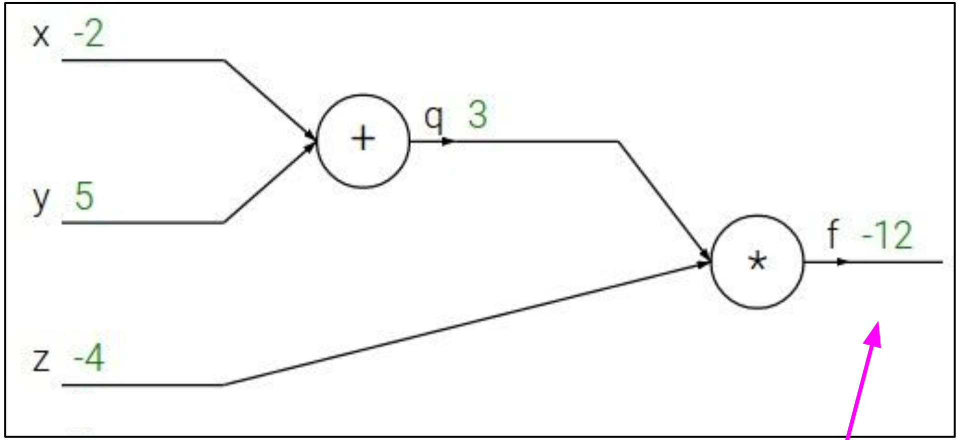
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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

Backpropagation: a simple example

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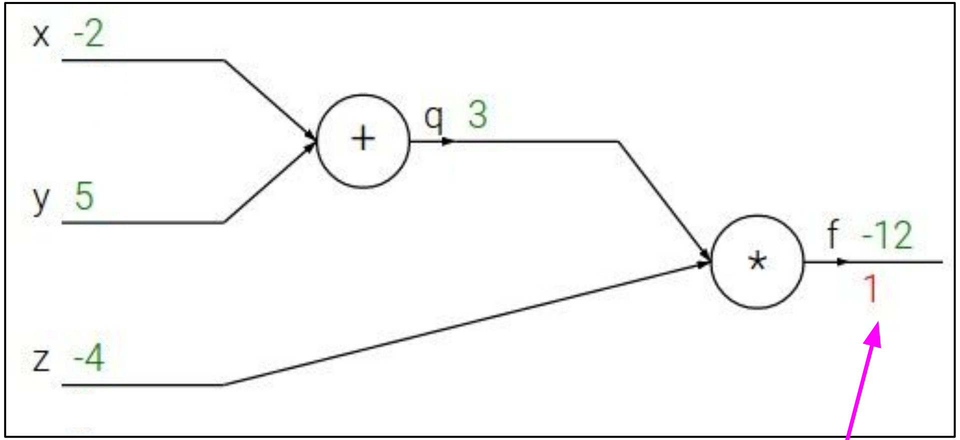

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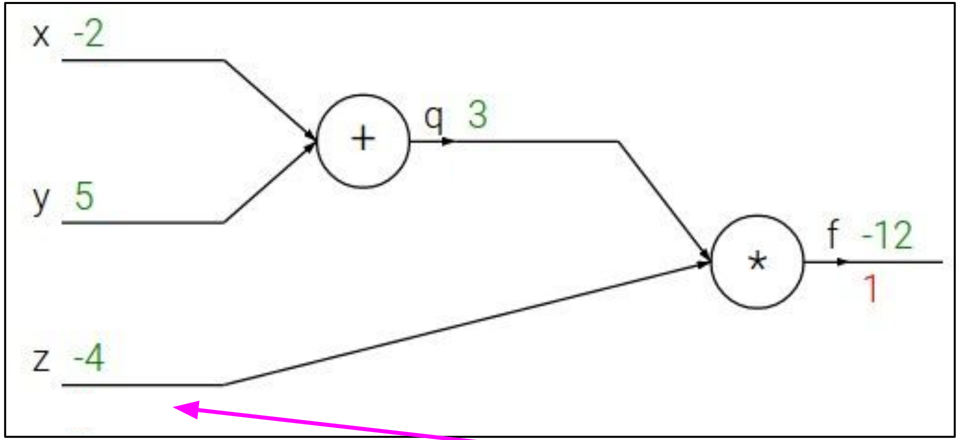
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Backpropagation: a simple example

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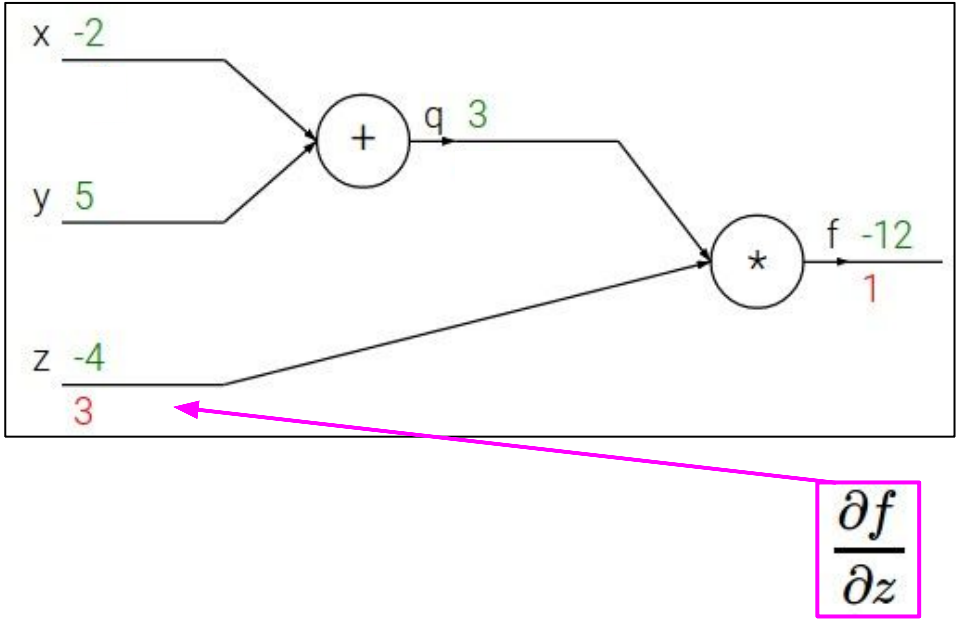

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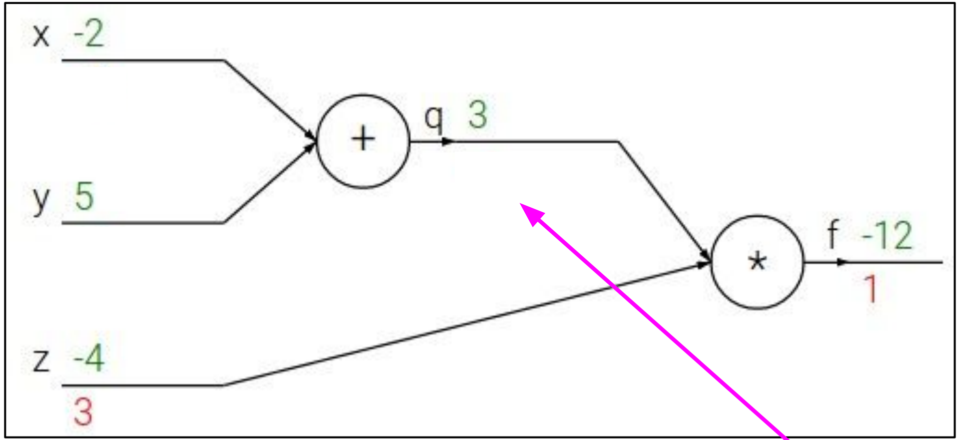
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Backpropagation: a simple example

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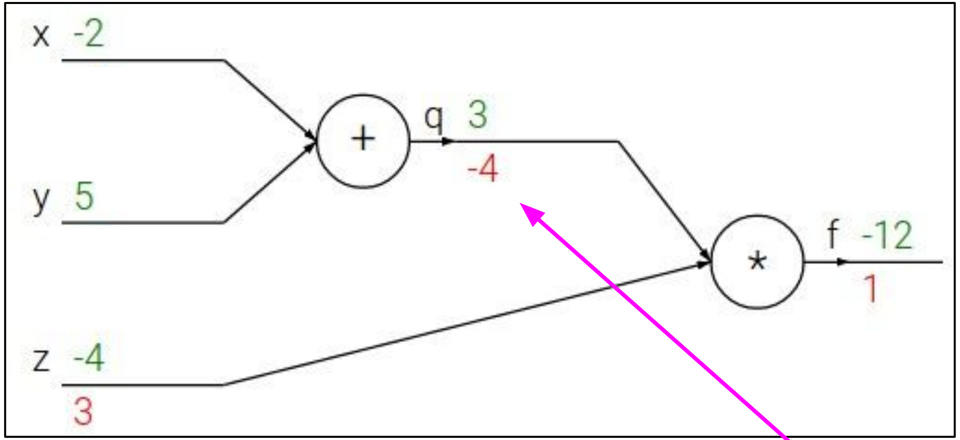
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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



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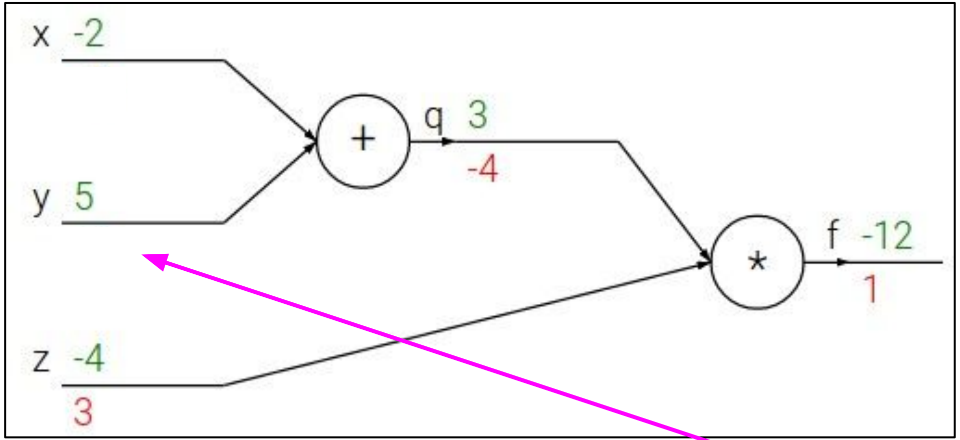

$$\frac{\partial f}{\partial y}$$

Chain rule:

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

Upstream gradient

Local gradient

Backpropagation: a simple example

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

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

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

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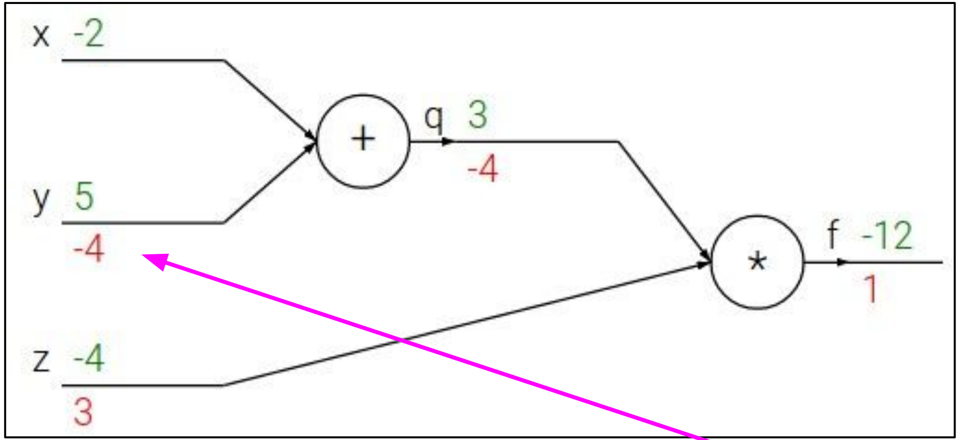
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Chain rule:

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

Upstream gradient

Local gradient

Backpropagation: a simple example

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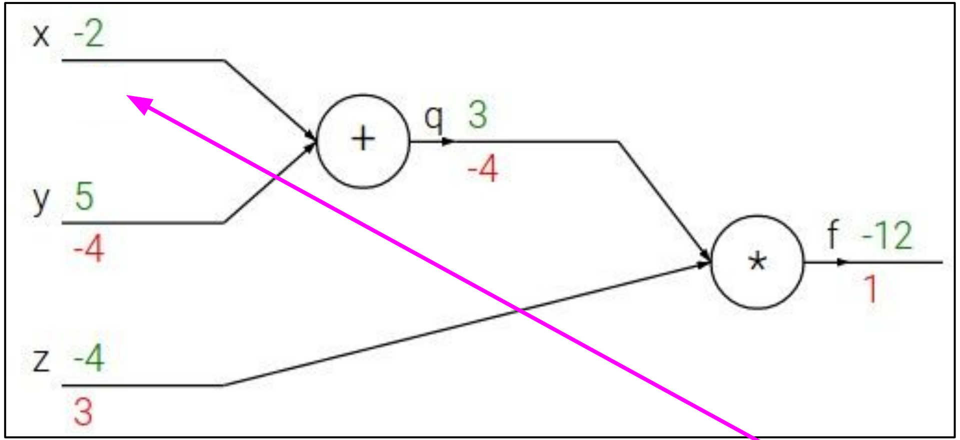
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

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

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

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

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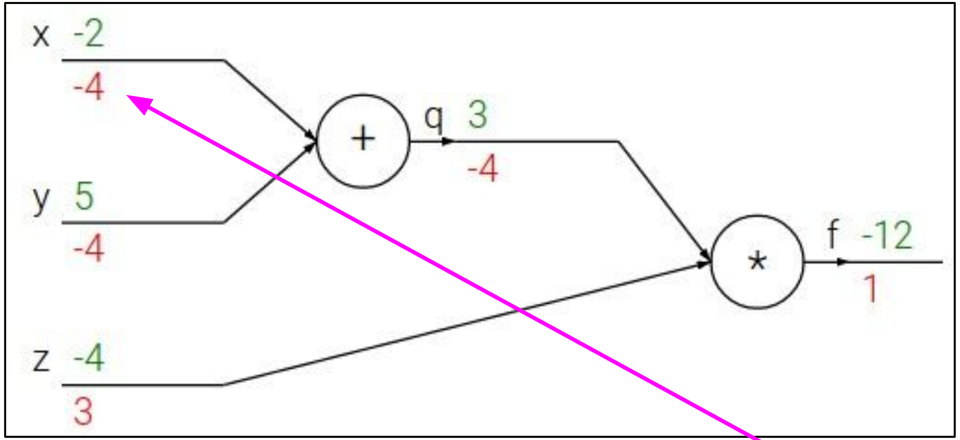


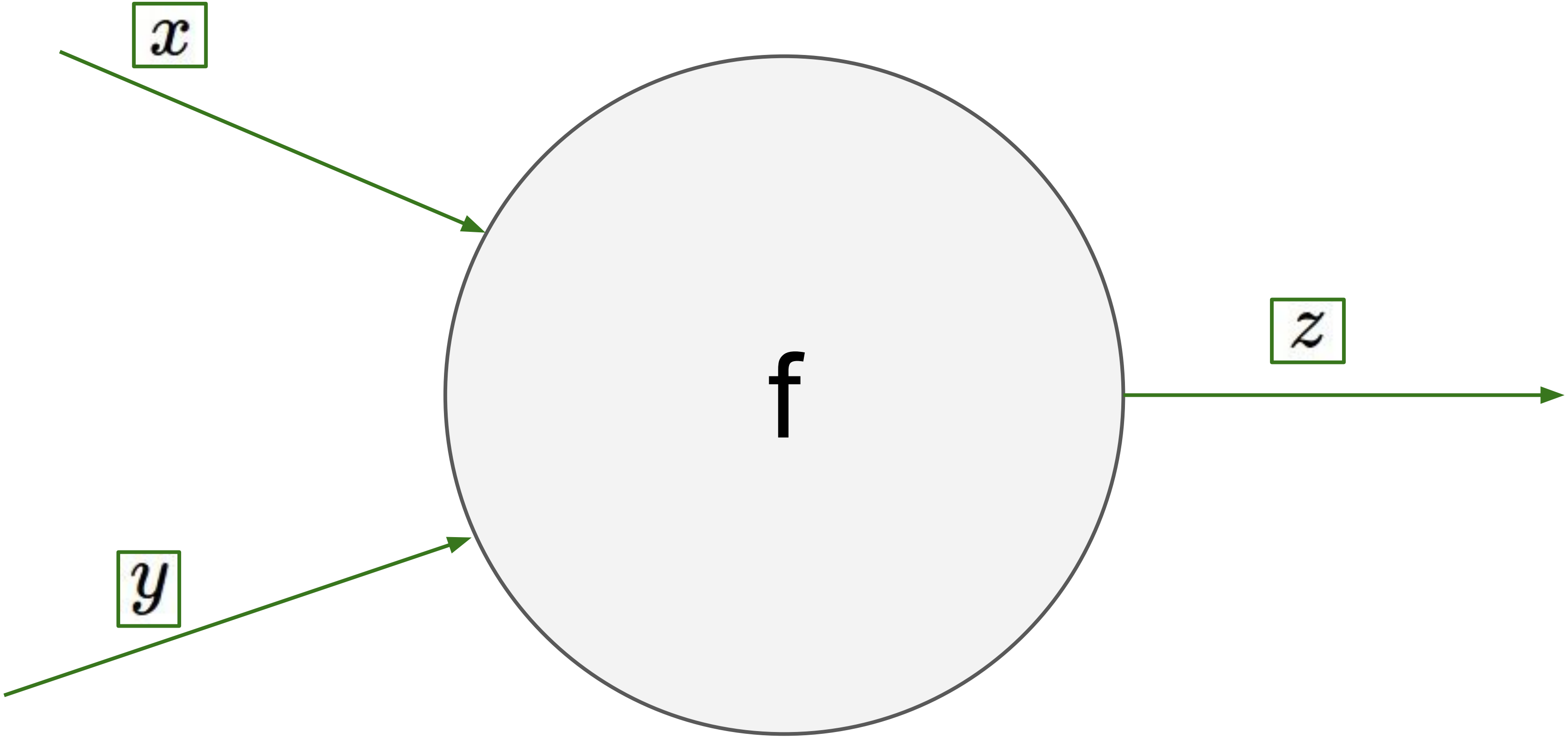
$$\boxed{\frac{\partial f}{\partial x}}$$

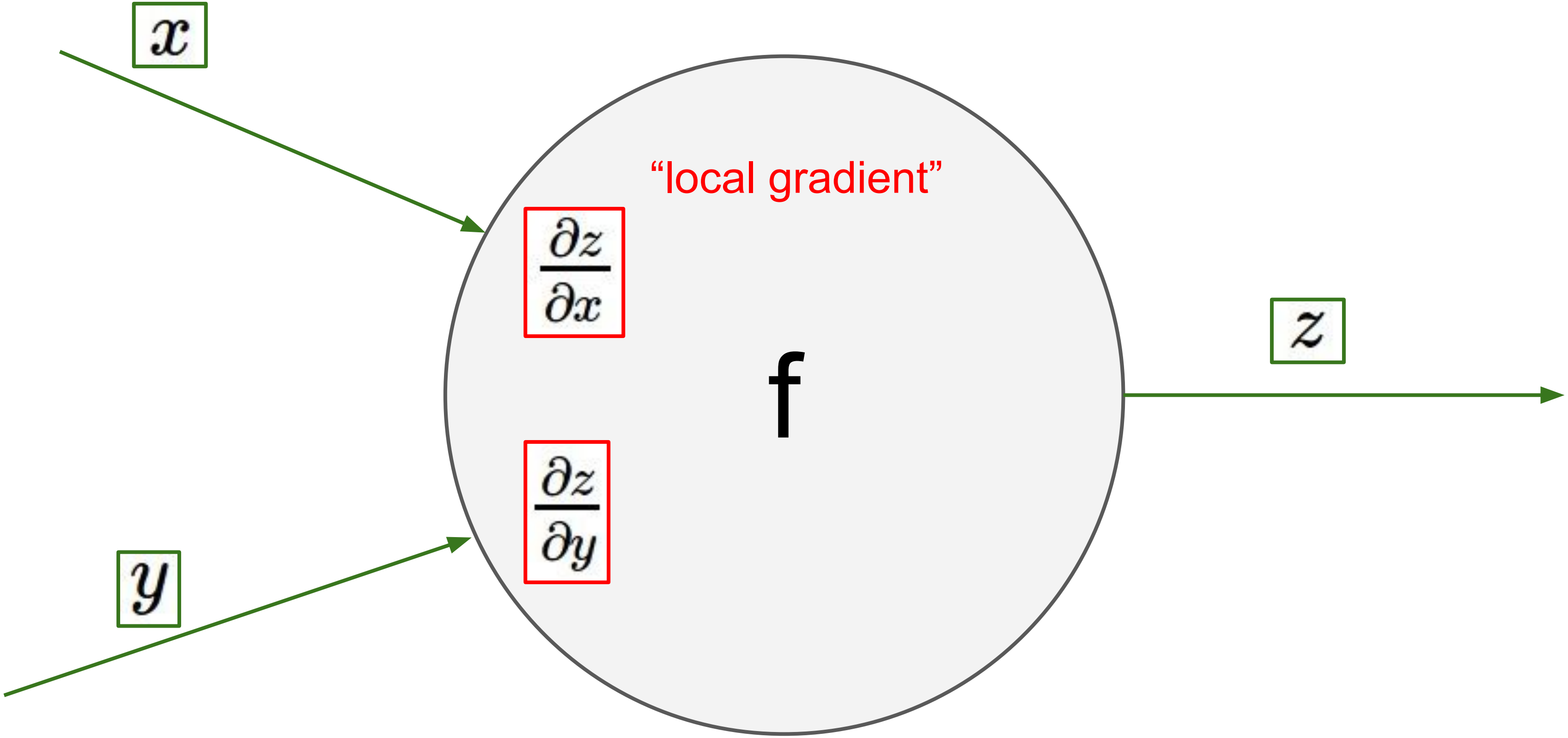
Chain rule:

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

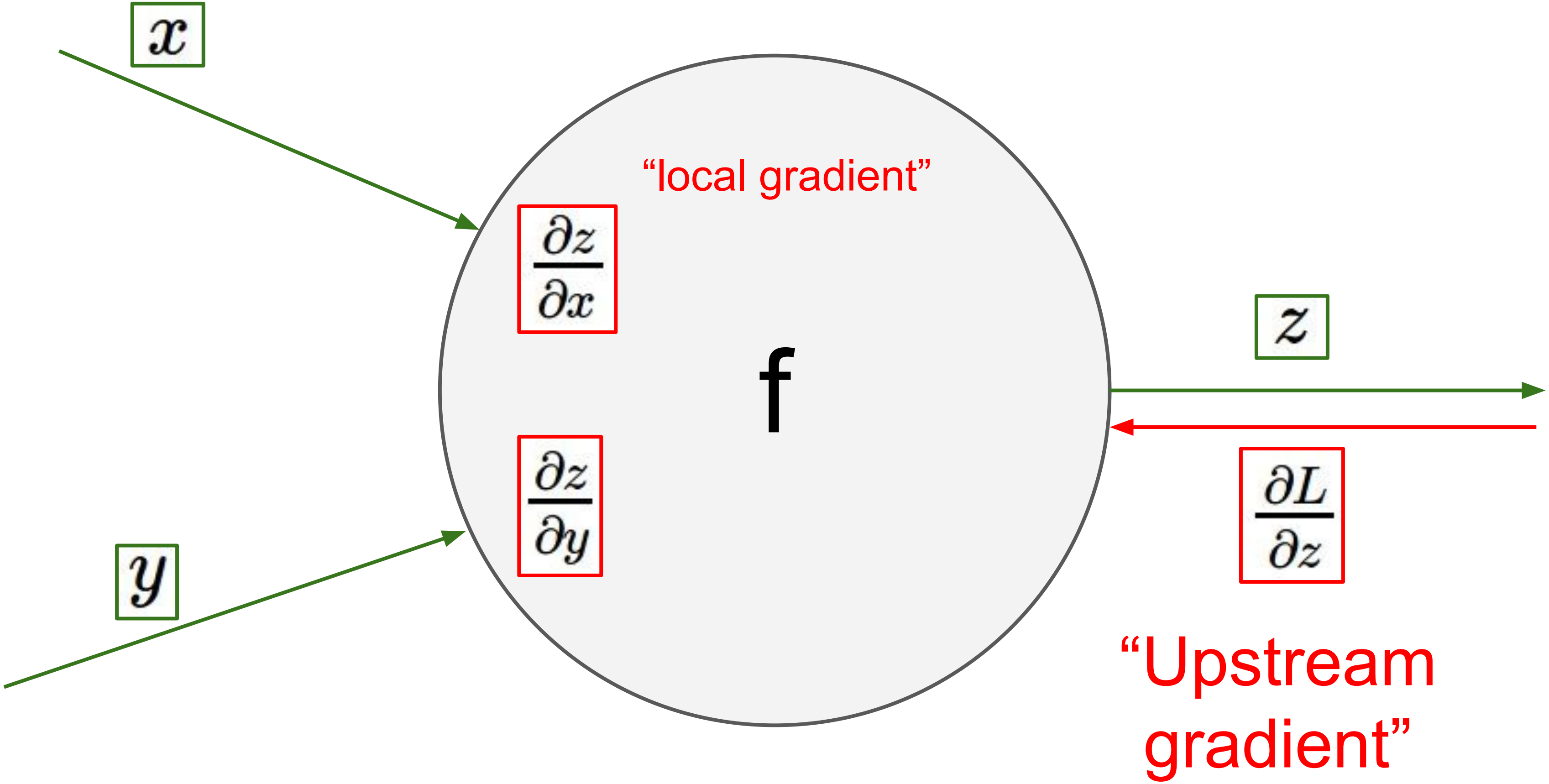
Upstream gradient

Local gradient

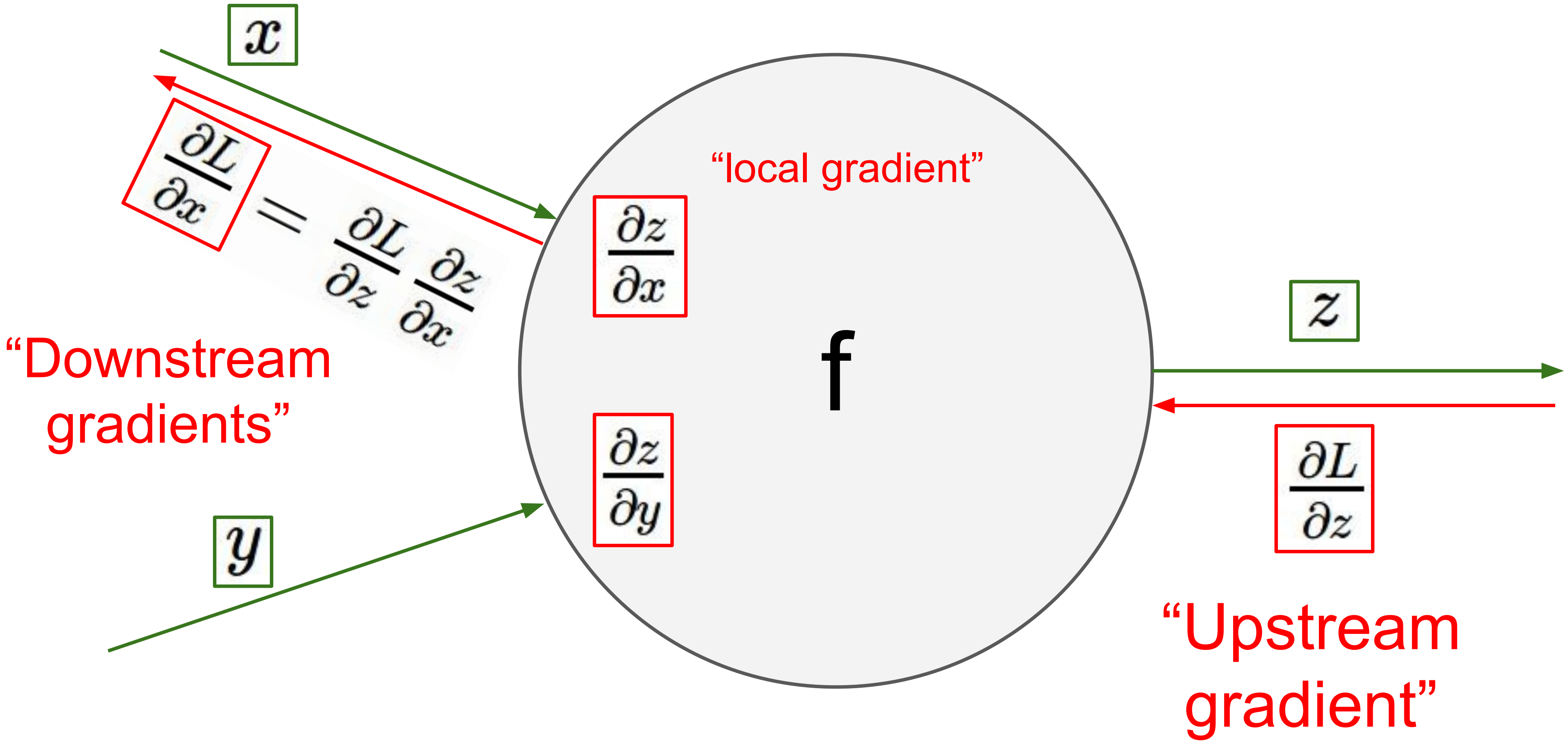

x
y
f
z



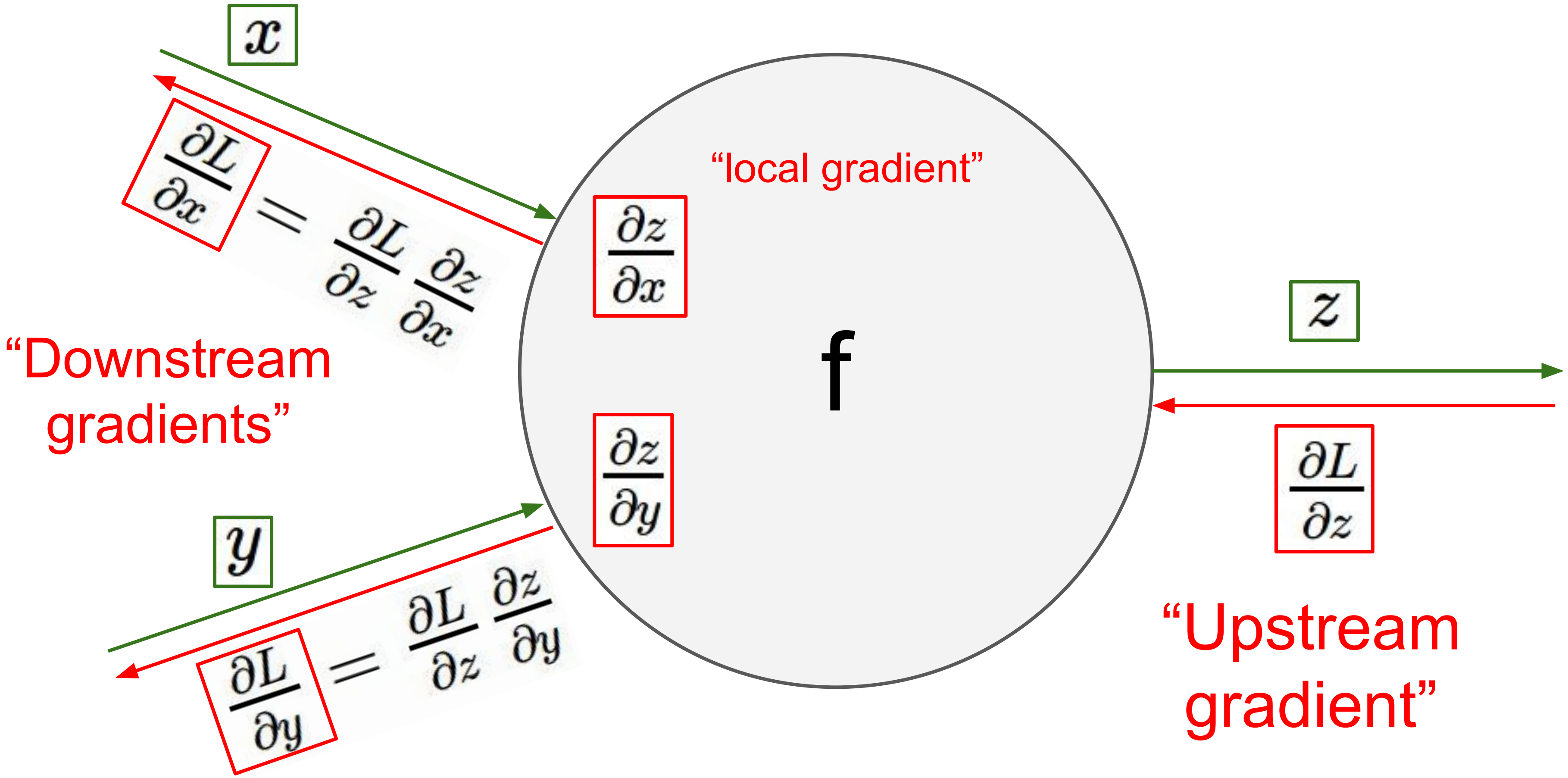
x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
y



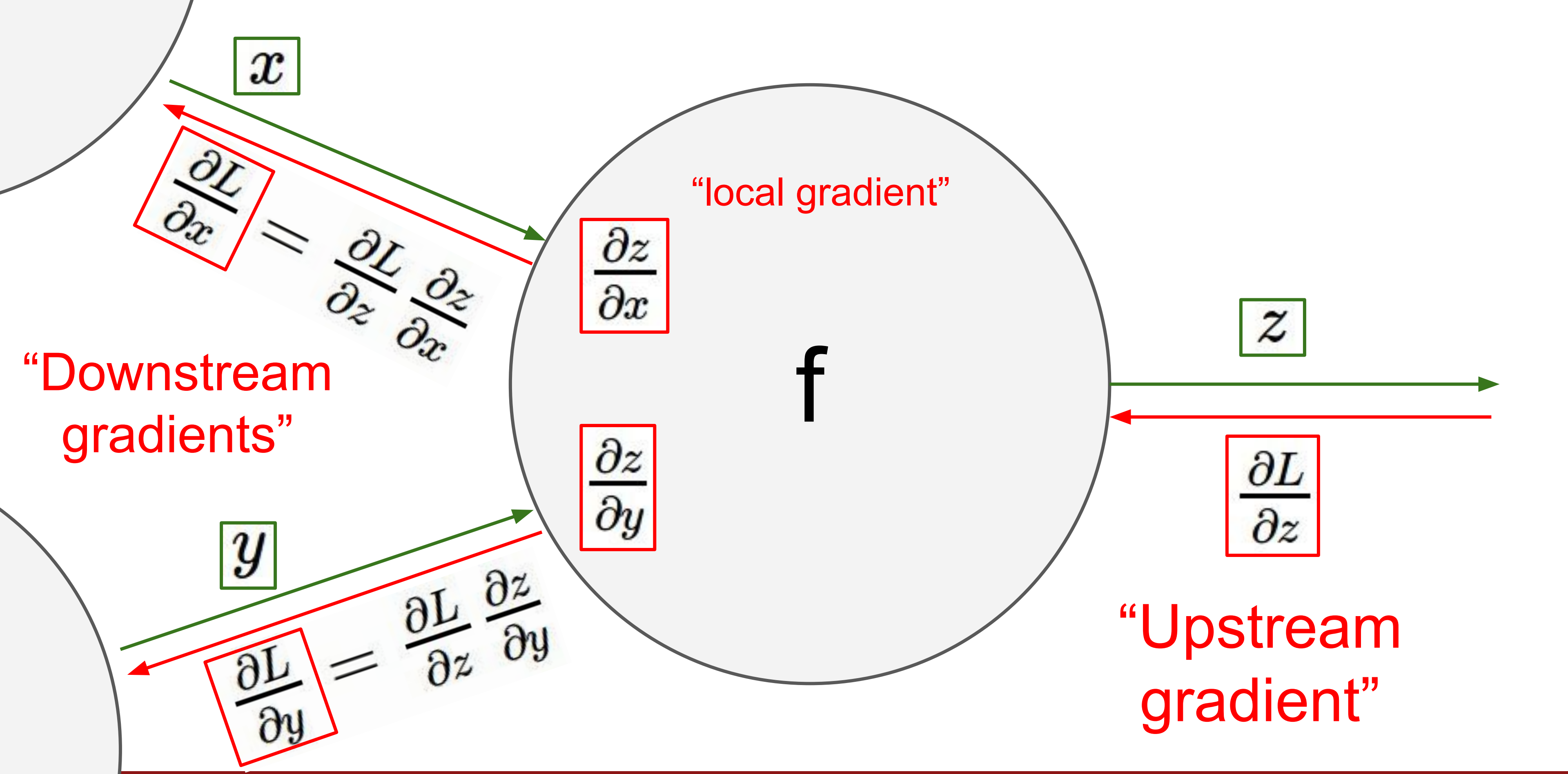
x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
y
$\frac{\partial L}{\partial z}$
"Upstream gradient"



x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"Downstream gradients"
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z
$\frac{\partial L}{\partial z}$
"Upstream gradient"
y

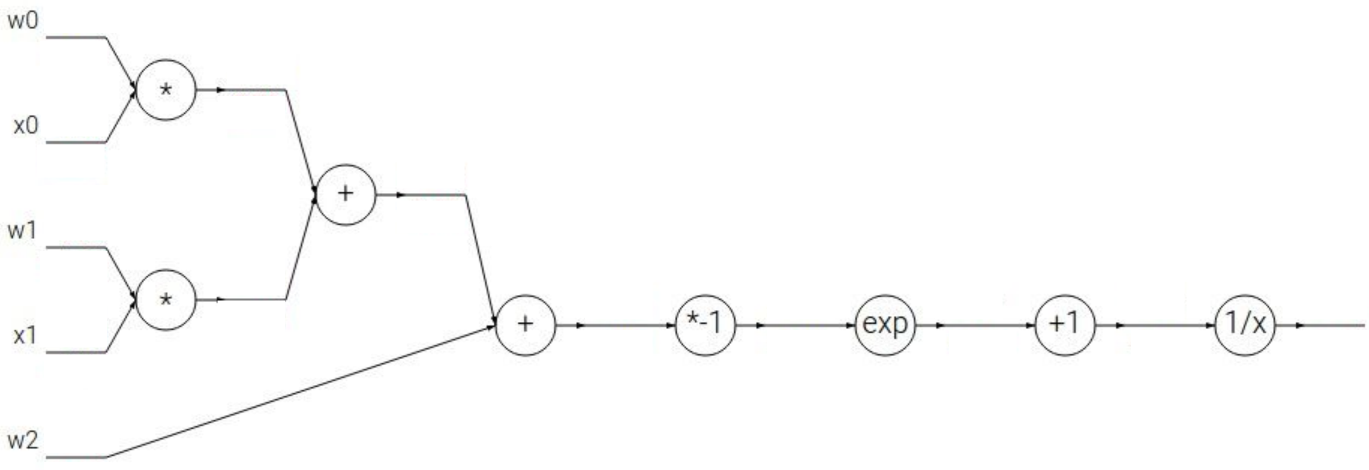


x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"Downstream gradients"
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z
$\frac{\partial L}{\partial z}$
"Upstream gradient"

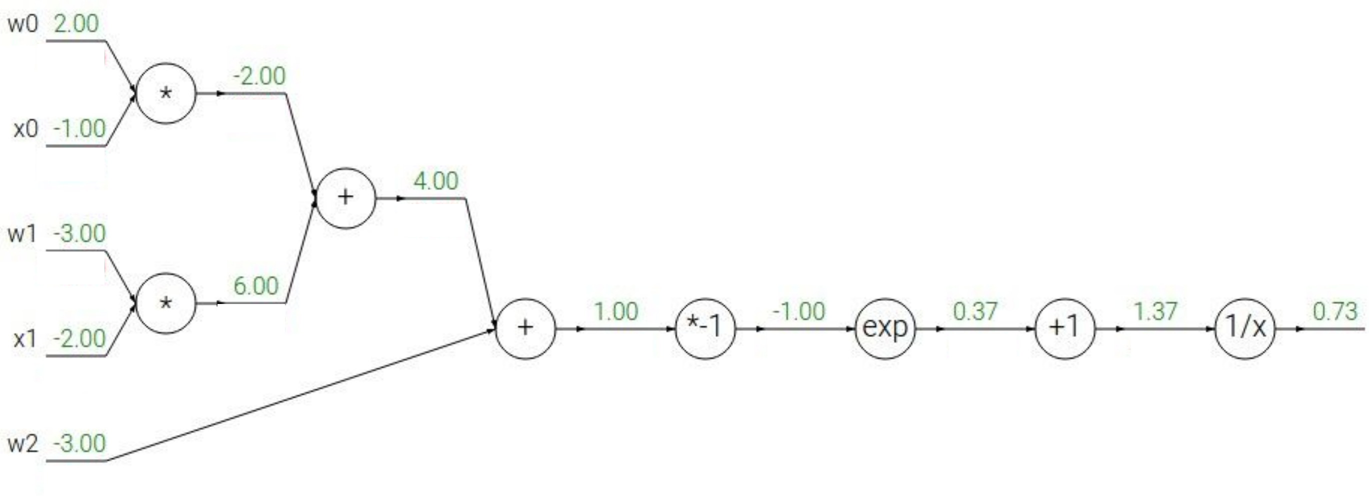


x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"Downstream gradients"
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
"local gradient"
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
z
$\frac{\partial L}{\partial z}$
"Upstream 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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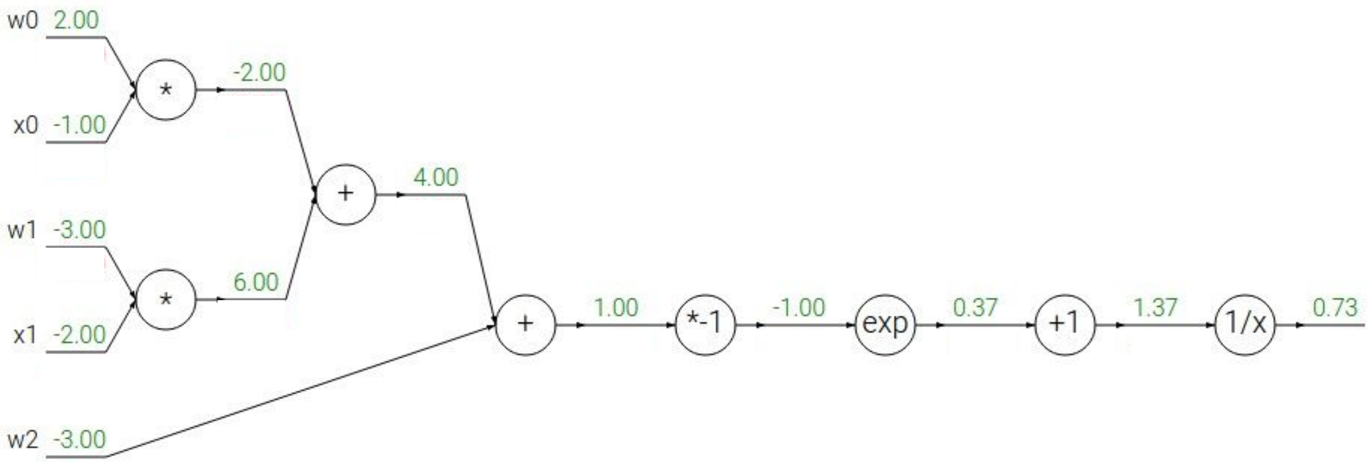

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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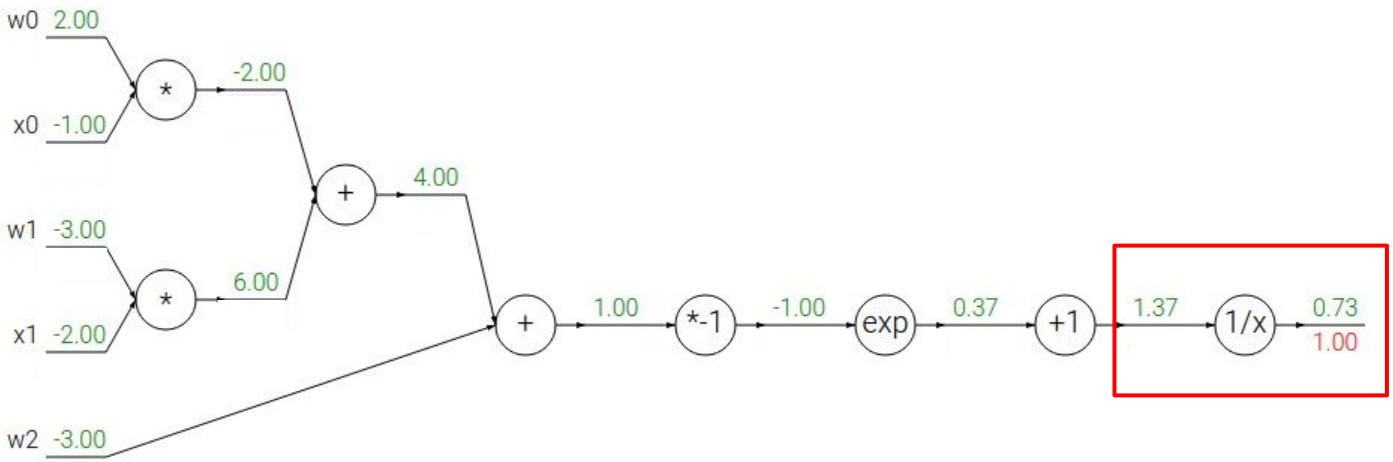

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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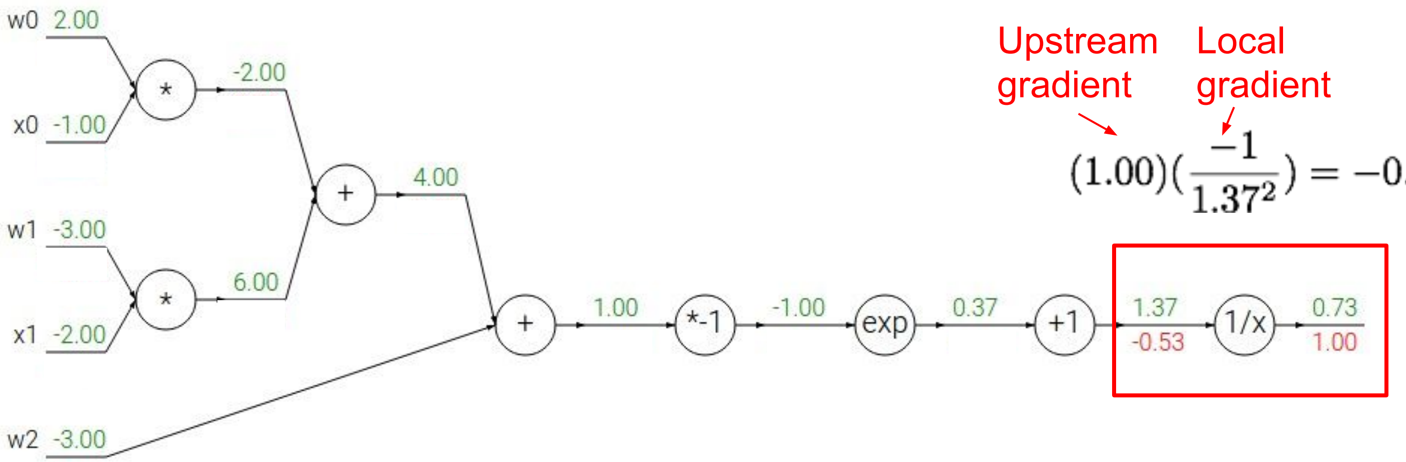

Upstream gradient

Local gradient

$$(1.00)\left(\frac{-1}{1.37^2}\right) = -0.53$$

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

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

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

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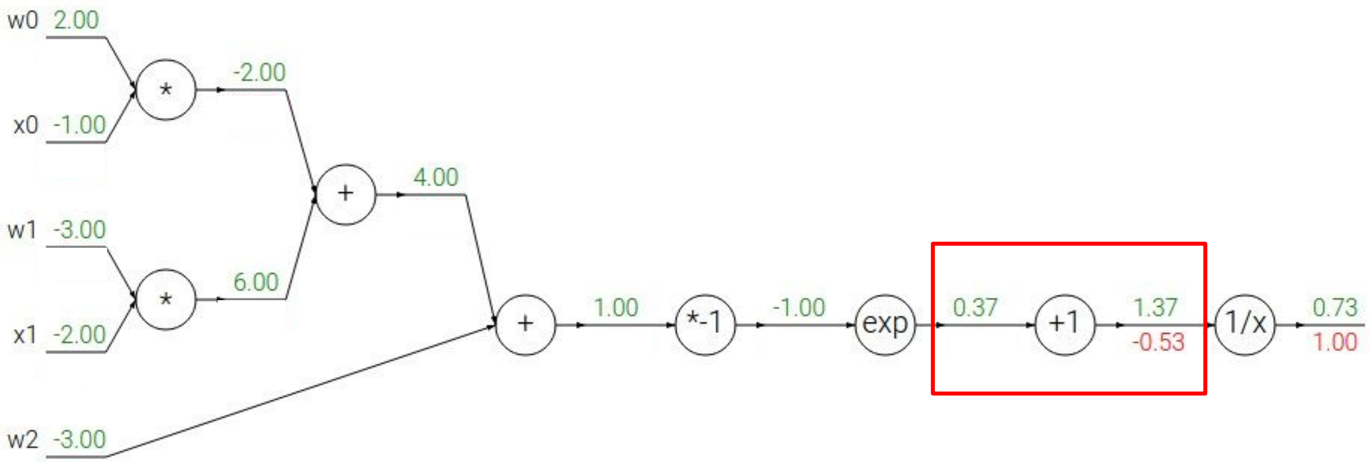

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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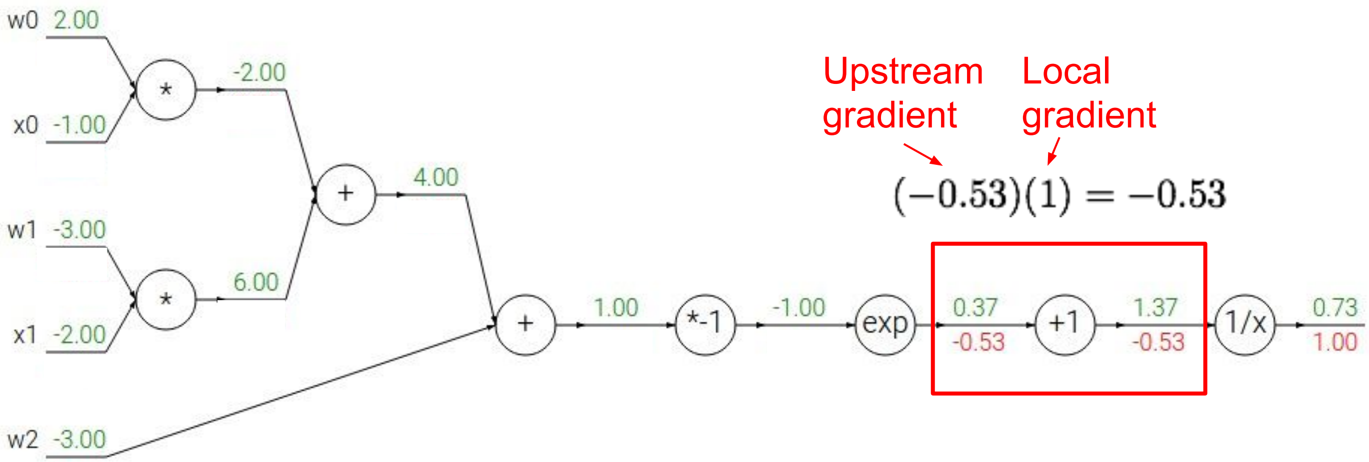

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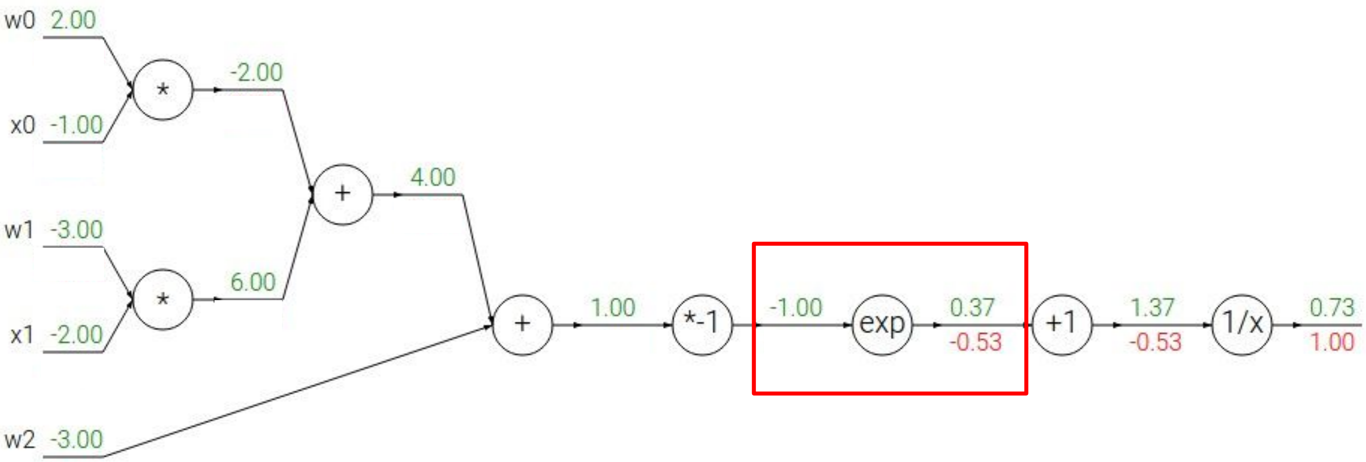

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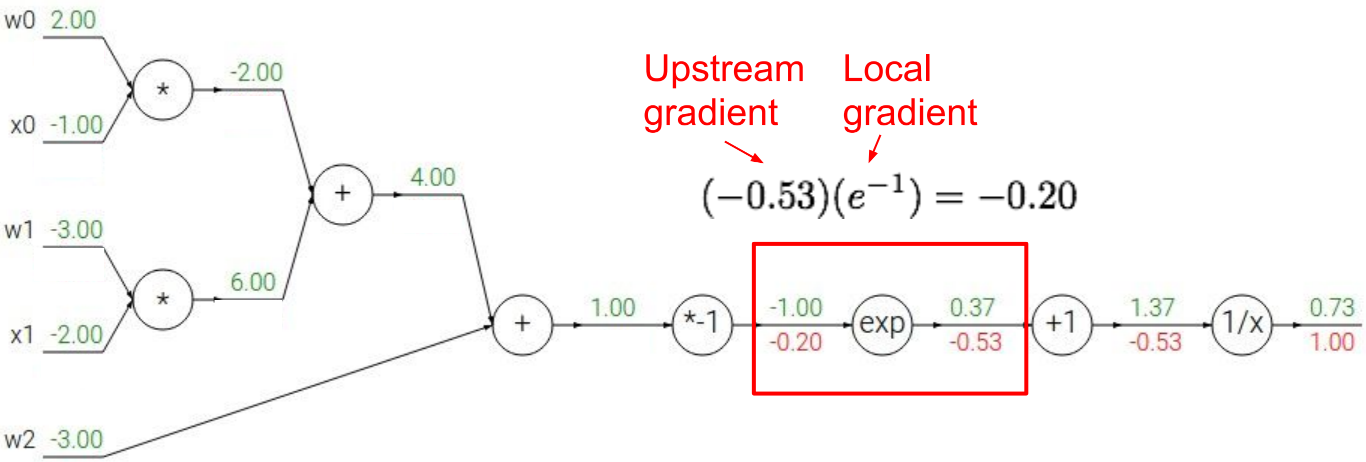

$$(-0.53)(e^{-1}) = -0.20$$

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

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

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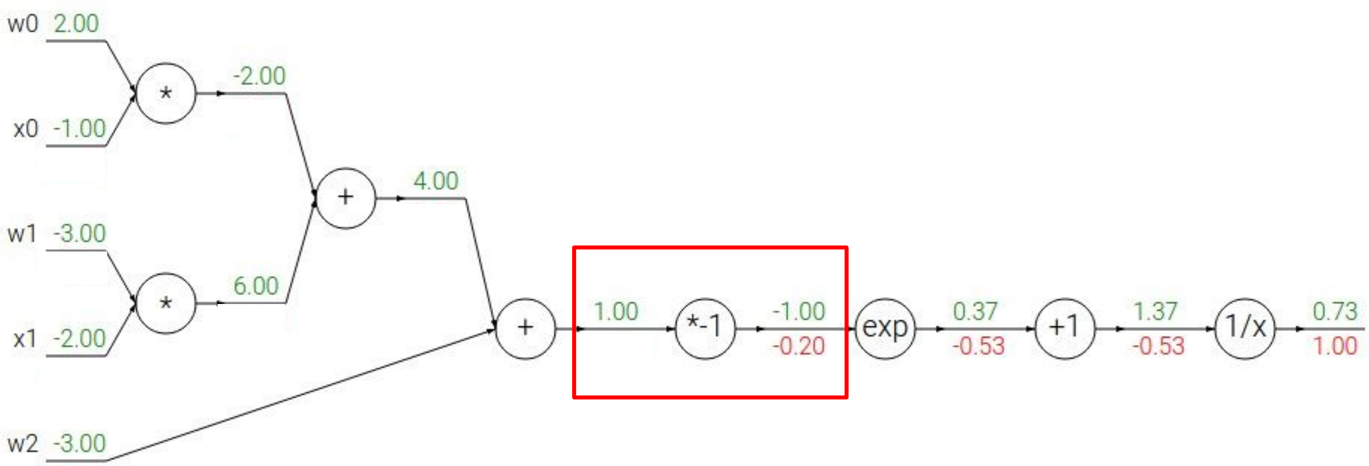

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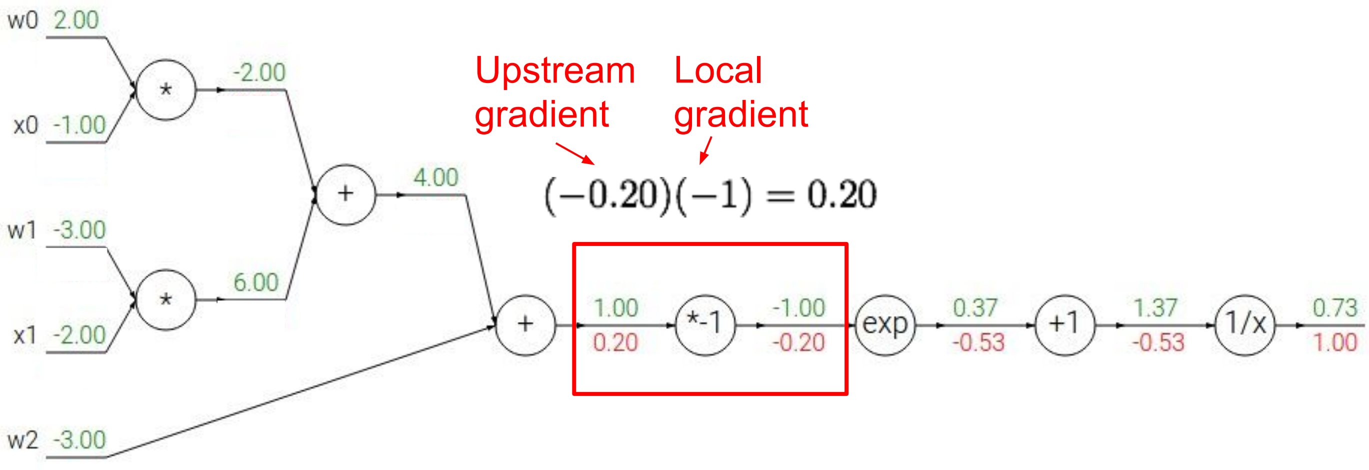

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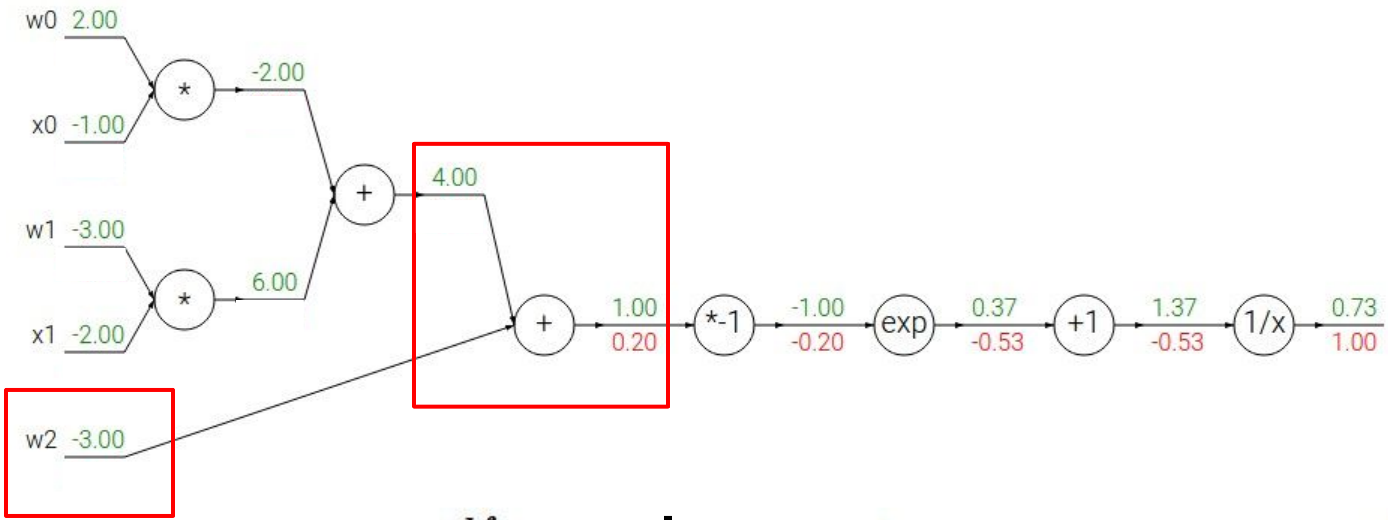

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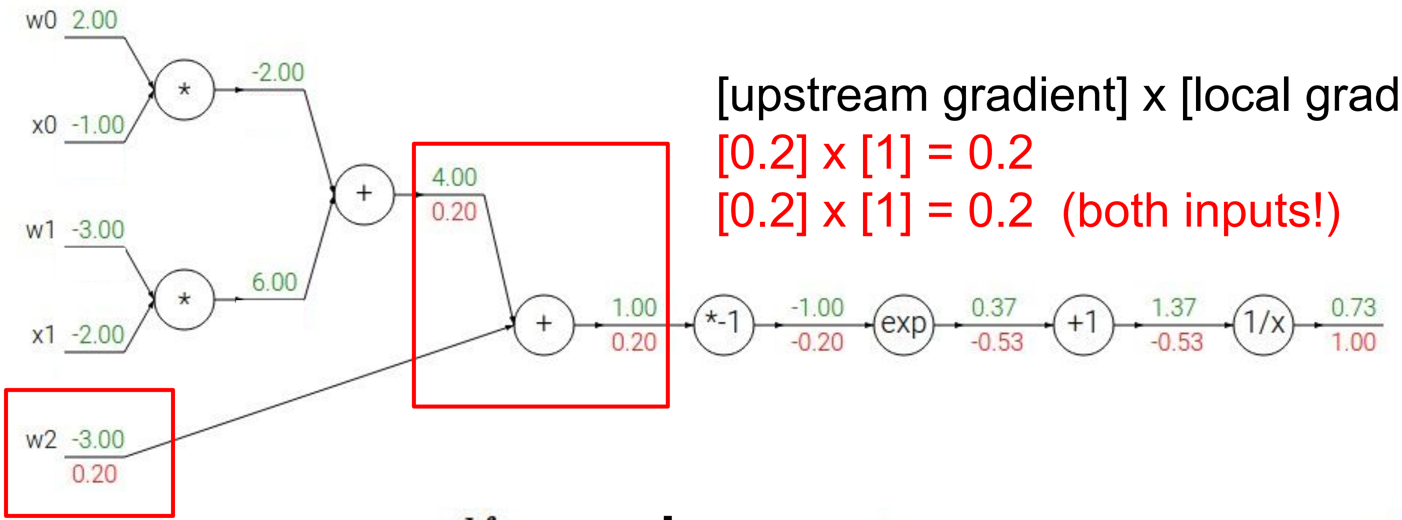

[upstream gradient] x [local gradient]
[0.2] x [1] = 0.2
[0.2] x [1] = 0.2 (both inputs!)

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

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

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

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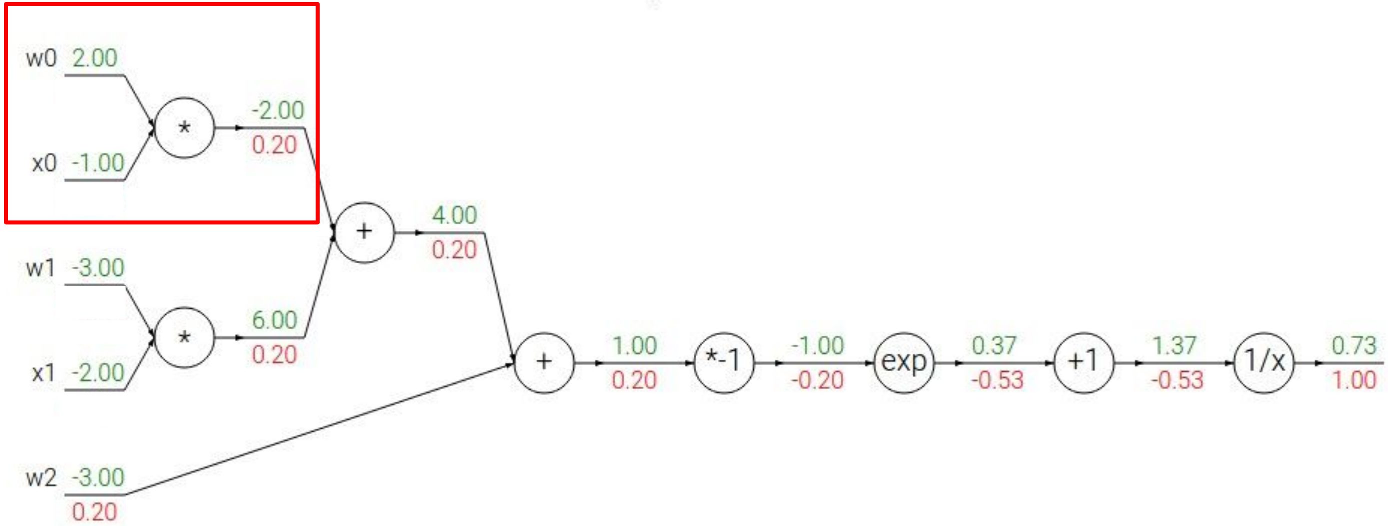

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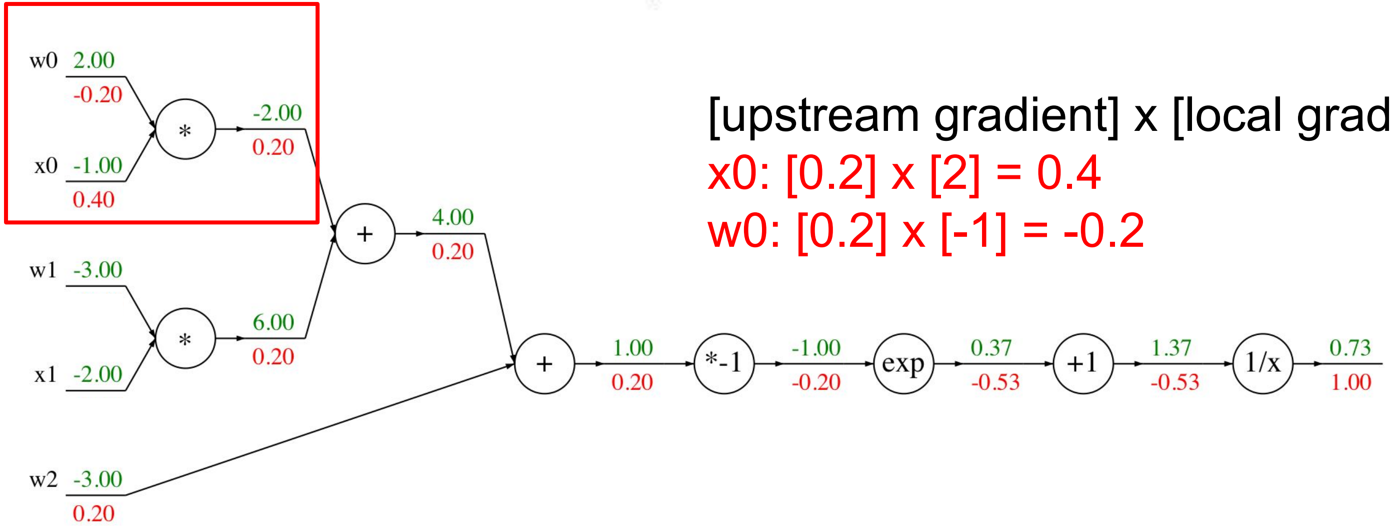

[upstream gradient] x [local gradient]

x0: [0.2] x [2] = 0.4

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

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

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

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

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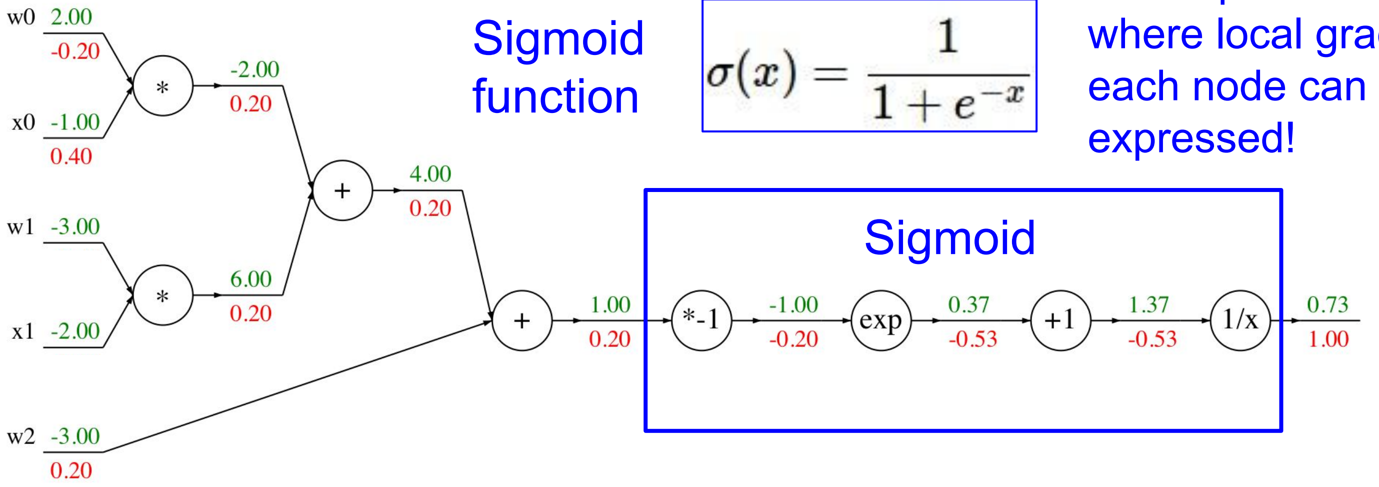
Another example:

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

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

Sigmoid function

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



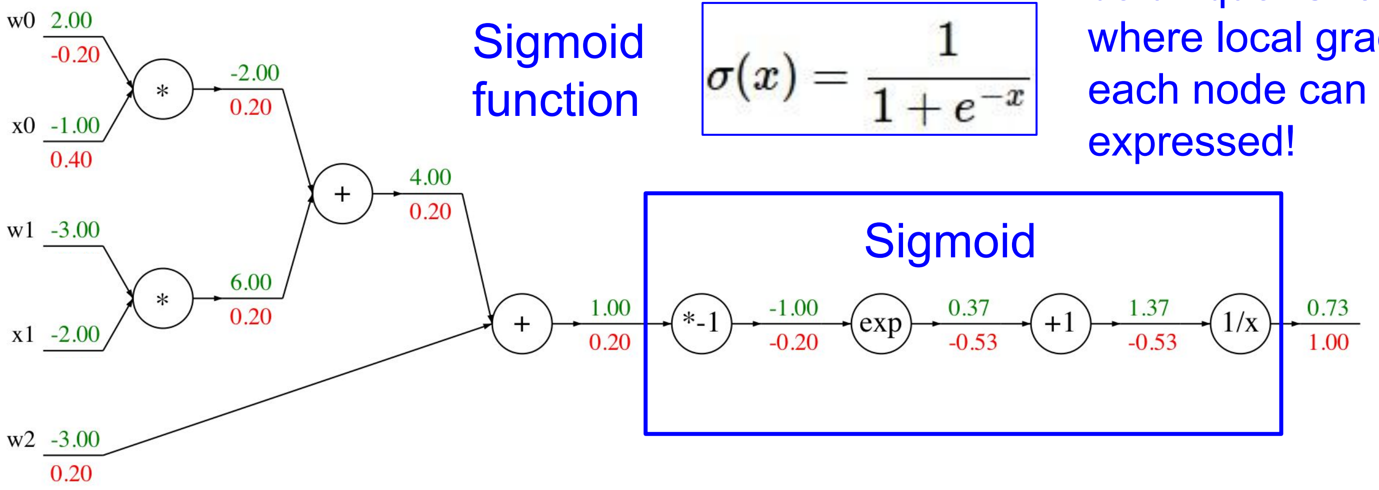
Another example:

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

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

Sigmoid function

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



Sigmoid local gradient:

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

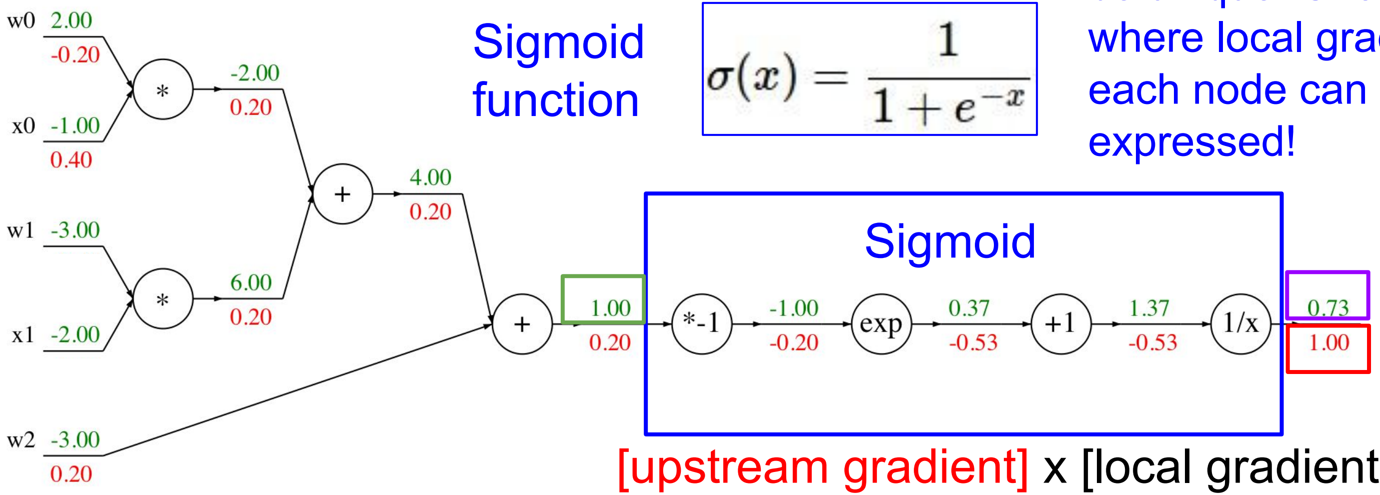
Another example:

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

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

Sigmoid function

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



[upstream gradient] x [local gradient]

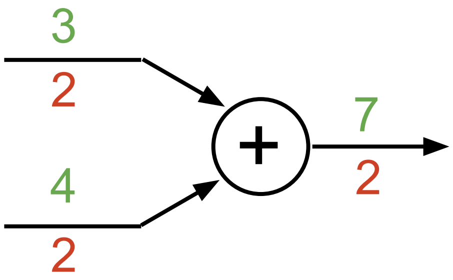
[1.00] x [(1 - 0.73) (0.73)] = 0.2

Sigmoid local gradient:

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

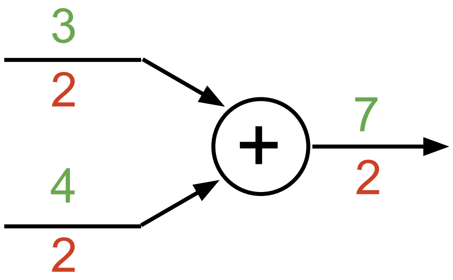
Patterns in gradient flow

add gate: gradient distributor

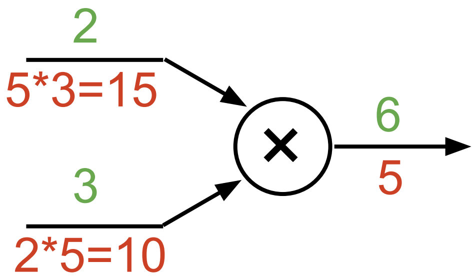


Patterns in gradient flow

add gate: gradient distributor

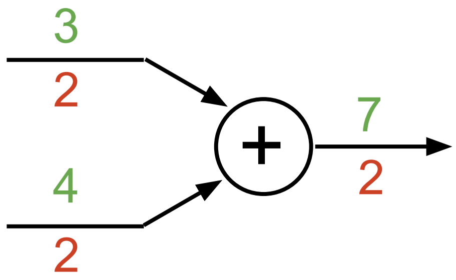


mul gate: “swap multiplier”

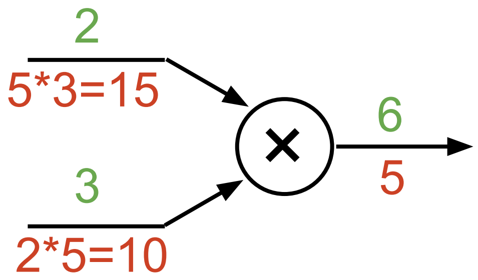


Patterns in gradient flow

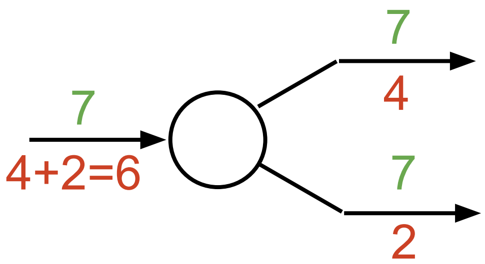
add gate: gradient distributor



mul gate: “swap multiplier”

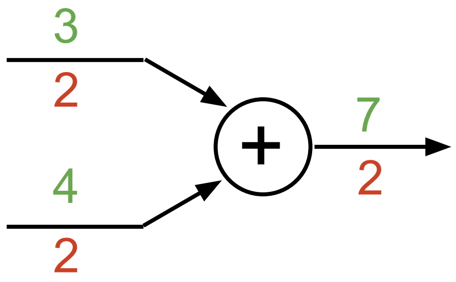


copy gate: gradient adder

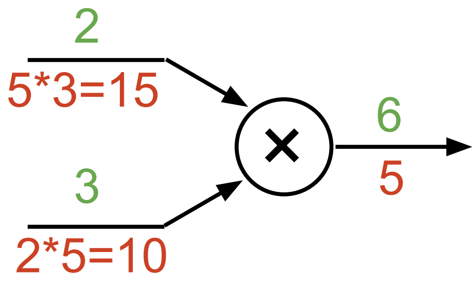


Patterns in gradient flow

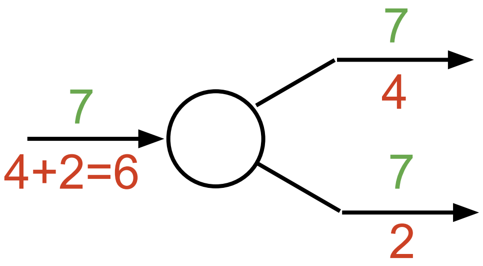
add gate: gradient distributor



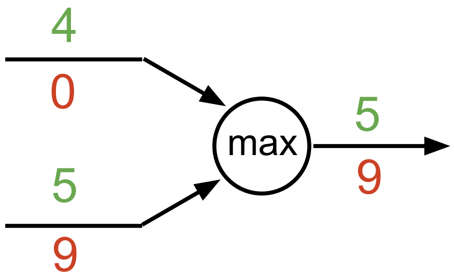
mul gate: “swap multiplier”



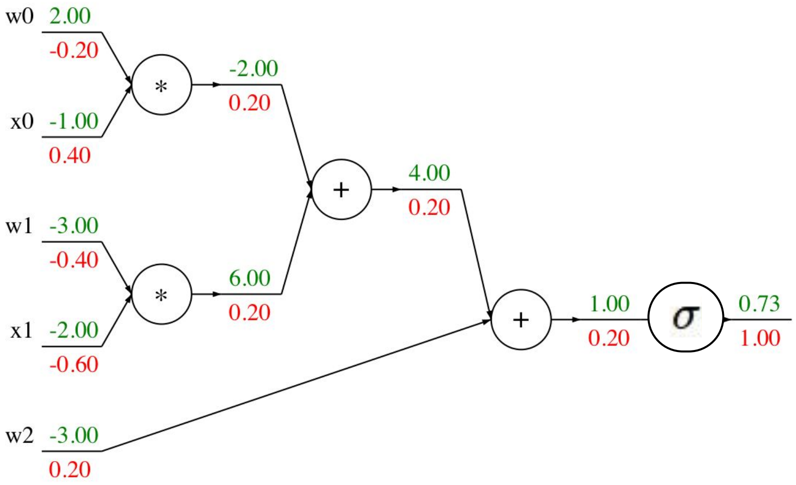
copy gate: gradient adder



max gate: gradient router



Backprop Implementation: "Flat" code



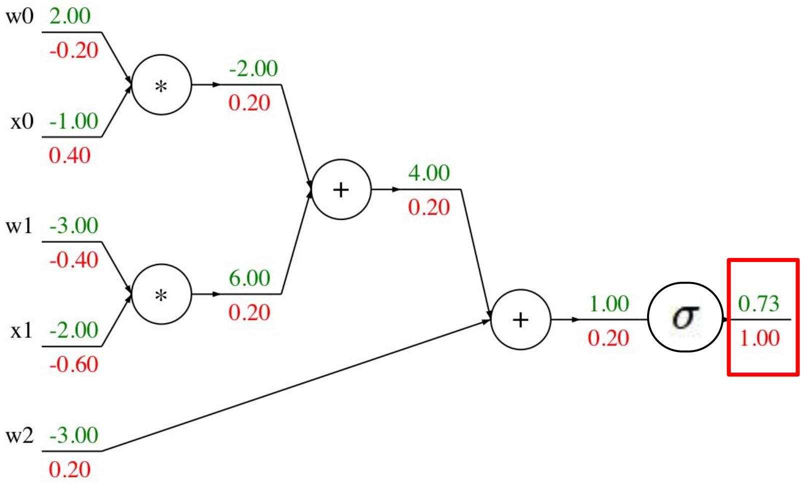
Forward pass:
Compute output

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

Backward pass:
Compute grads

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

Backprop Implementation: "Flat" code



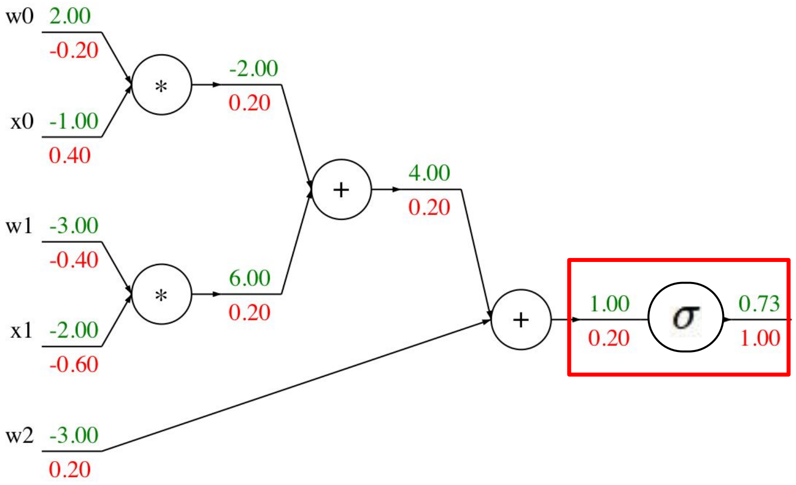
Forward pass:
Compute output

Base case

```
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



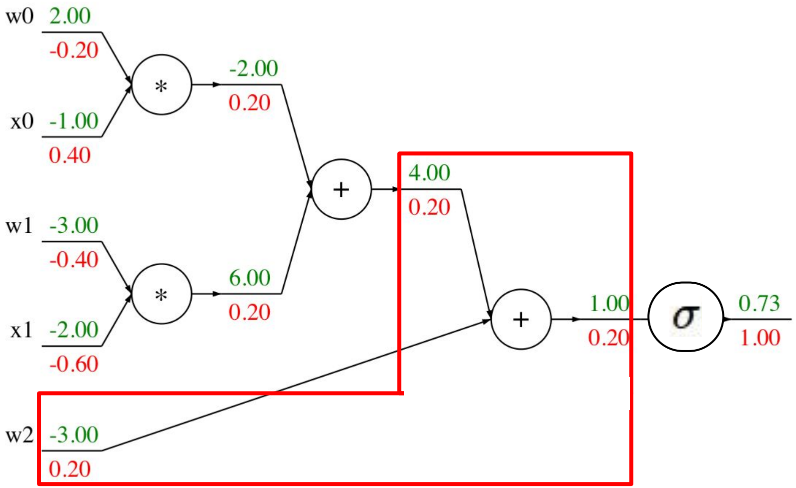
Forward pass:
Compute output

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

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



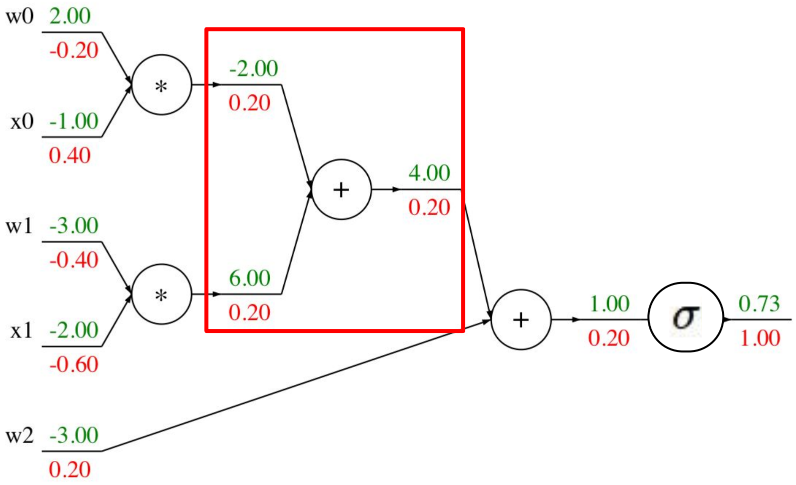
Forward pass:
Compute output

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

  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



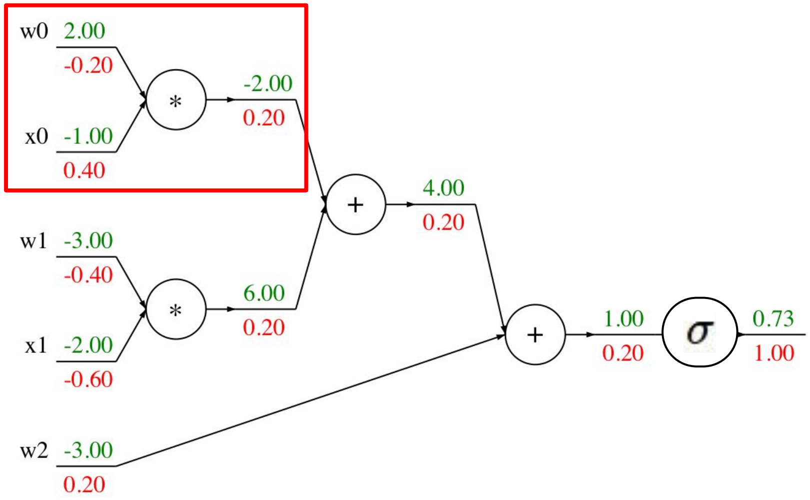
Forward pass:
Compute output

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



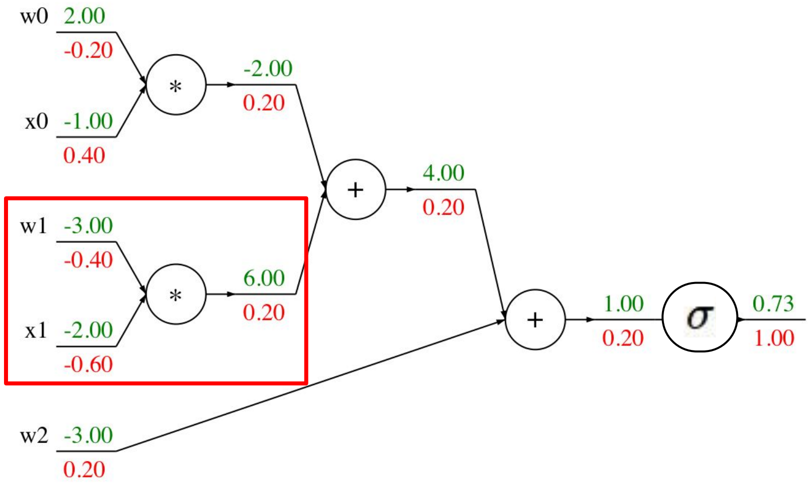
Forward pass: Compute output

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

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

Multiply gate

Backprop Implementation: "Flat" code



Forward pass: Compute output

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

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

Multiply gate

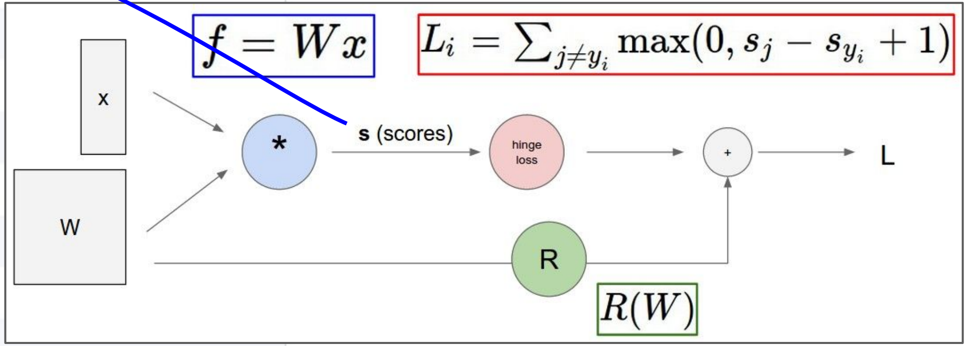
“Flat” Backprop: Do this for assignment 1!

Stage your forward/backward computation!

E.g. for the SVM:

```
# receive W (weights), X (data)
# forward pass (we have 8 lines)
scores = #...
margins = #...
data_loss = #...
reg_loss = #...
loss = data_loss + reg_loss
# backward pass (we have 5 lines)
dmargins = # ... (optionally, we go direct to dscores)
dscores = #...
dW = #...
```

margins

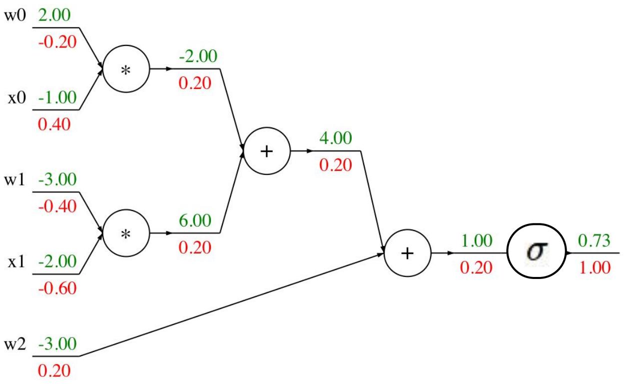


“Flat” Backprop: Do this for assignment 1!

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 = #...
```

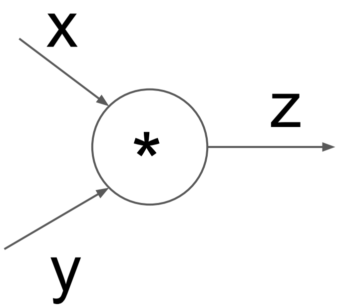
Backprop Implementation: Modularized API



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



(x,y,z are scalars)

Gate / Node / Function object: Actual PyTorch code

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

Need to stash some values for use in backward

Upstream gradient

Multiply upstream and local gradients

Example: PyTorch operators

pytorch / pytorch

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Tree: 517c7c9861 — pytorch / aten / src / THNN / generic /

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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
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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
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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
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SpatialMaxUnpooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialReflectionPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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VolumetricFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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VolumetricUpSamplingTrilinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
linear_upsampling.h	Implement nn.functional.interpolate based on upsample. (#8591)	9 months ago
pooling_shape.h	Use integer math to compute output size of pooling operations (#14405)	4 months ago
unfold.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago

PyTorch sigmoid layer

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

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

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

#endif
```

Forward

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

Source

PyTorch sigmoid layer

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

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

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

#endif
```

Forward

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

```cpp
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...

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

Source

PyTorch sigmoid layer

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

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

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

#endif
```

Forward

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

```
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...

Backward

$$\boxed{(1-\sigma(x))\,\sigma(x)}$$

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

Vector to Vector

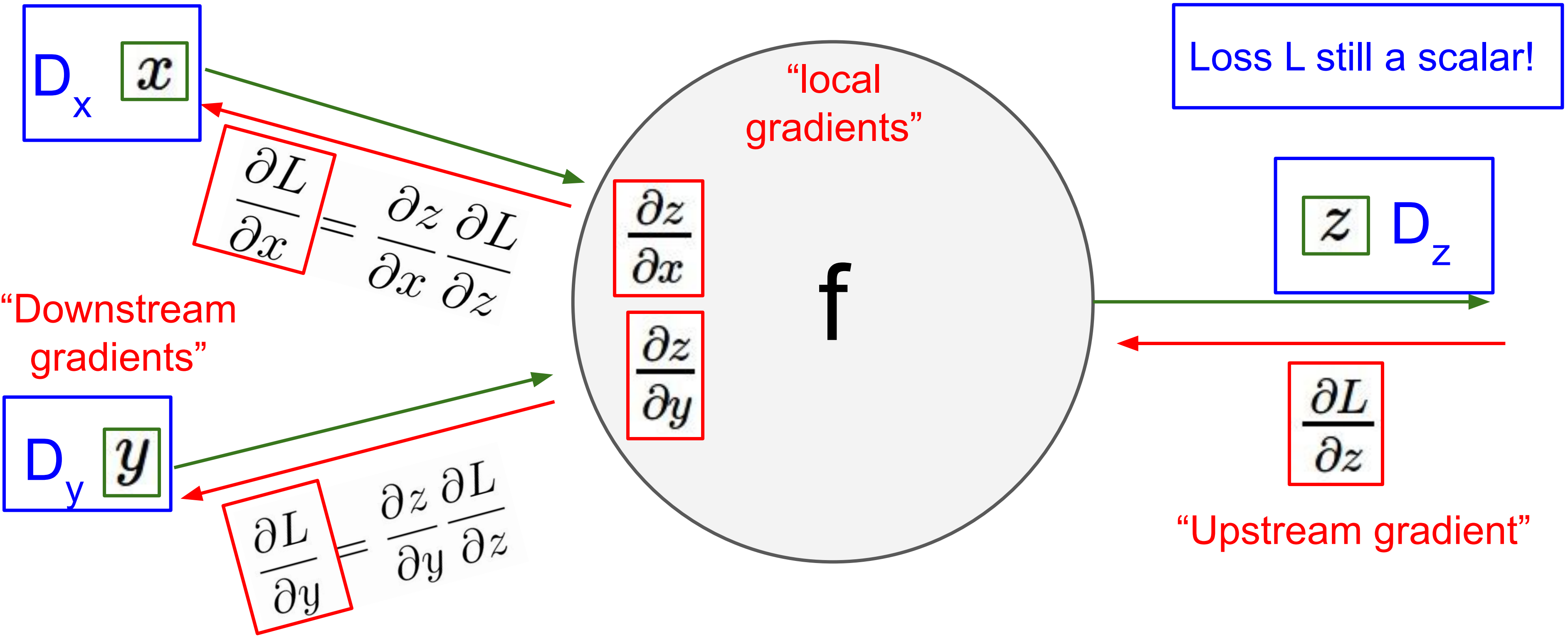
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

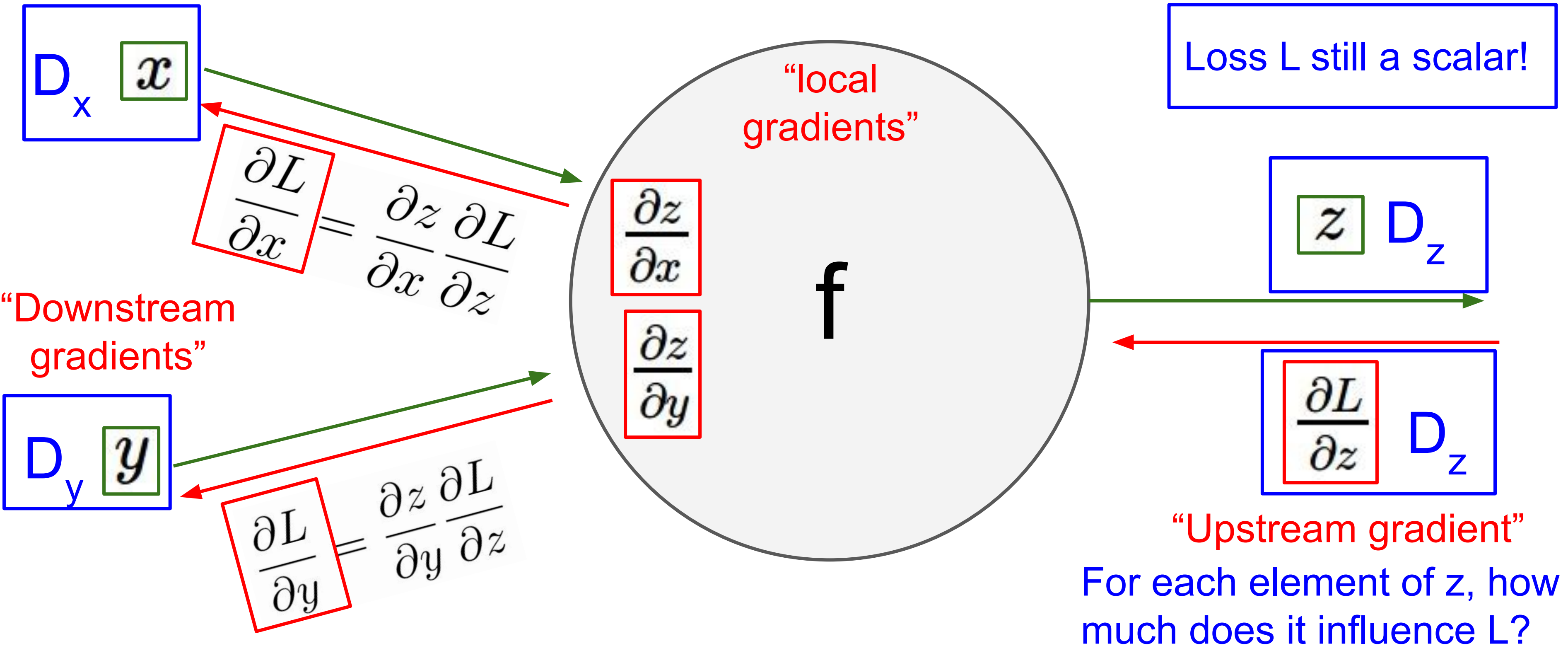
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x}\right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

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

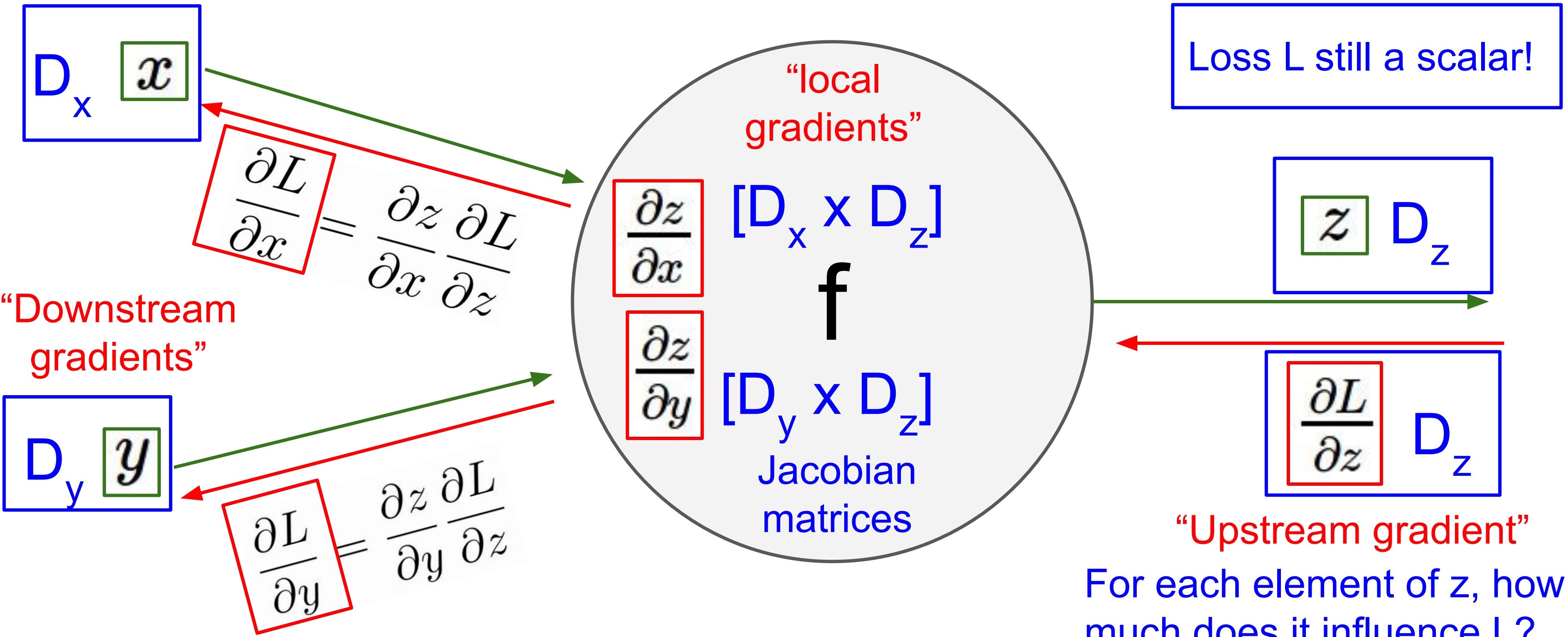
Backprop with Vectors



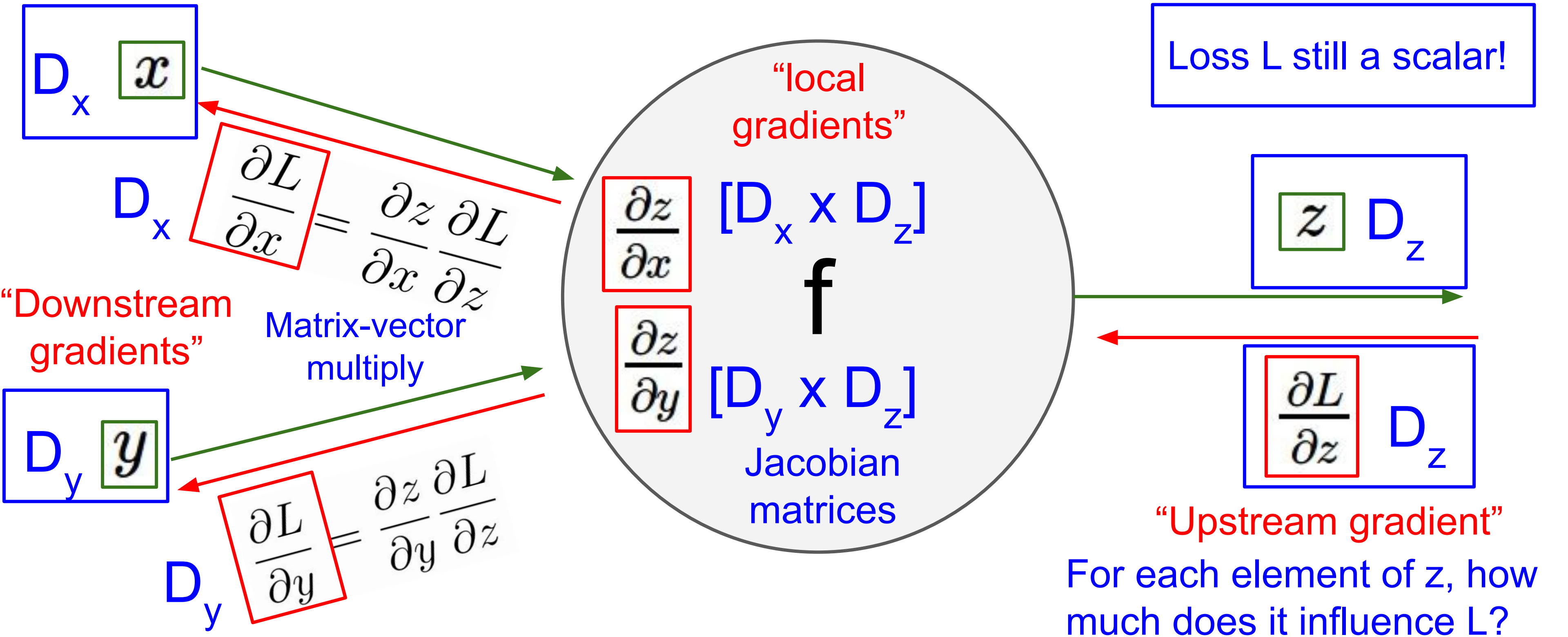
Backprop with Vectors



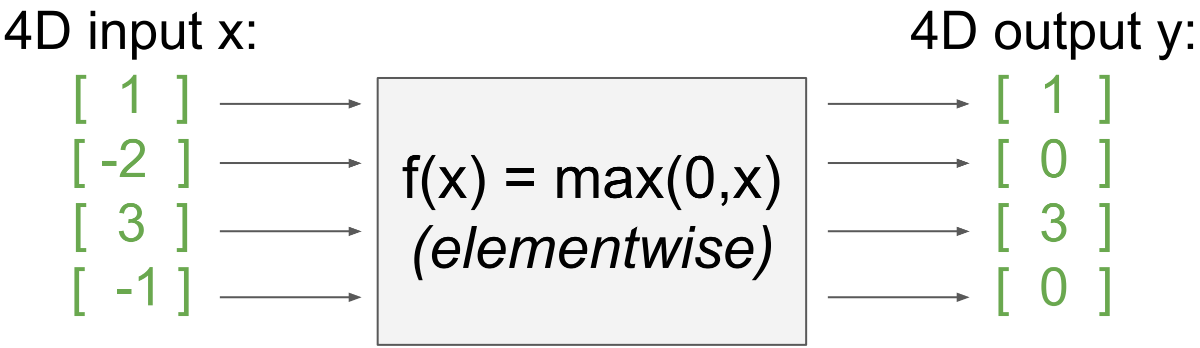
Backprop with Vectors



Backprop with Vectors



Backprop with Vectors



Backprop with Vectors

4D input x:

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

f(x) = max(0,x)
(elementwise)

4D output y:

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

4D dL/dy:

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

Upstream gradient

Backprop with Vectors

4D input x:

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

f(x) = max(0,x)
(elementwise)

4D output y:

[1]
[0]
[3]
[0]

Jacobian dy/dx

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

4D dL/dy:

[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Vectors

4D input x:

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

f(x) = max(0,x)
(elementwise)

4D output y:

[1]
[0]
[3]
[0]

[dy/dx] [dL/dy]

[1 0 0 0] [4]
[0 0 0 0] [-1]
[0 0 1 0] [5]
[0 0 0 0] [9]

4D dL/dy:

[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \rightarrow \boxed{\begin{matrix} f(x) = \max(0,x) \\ \textit{(elementwise)} \end{matrix}} \rightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D output y:

4D dL/dx: [dy/dx] [dL/dy] 4D dL/dy:

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

Upstream gradient

Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \rightarrow \boxed{\begin{array}{c} f(x) = \max(0,x) \\ \textit{(elementwise)} \end{array}} \rightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D output y:

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

4D dL/dx: [dy/dx] [dL/dy] 4D dL/dy:

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

Upstream gradient

Backprop with Vectors

4D input x:

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

f(x) = max(0,x)
(elementwise)

4D output y:

[1]
[0]
[3]
[0]

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

4D dL/dx:

[4]
[0]
[5]
[0]

[dy/dx] [dL/dy]

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

4D dL/dy:

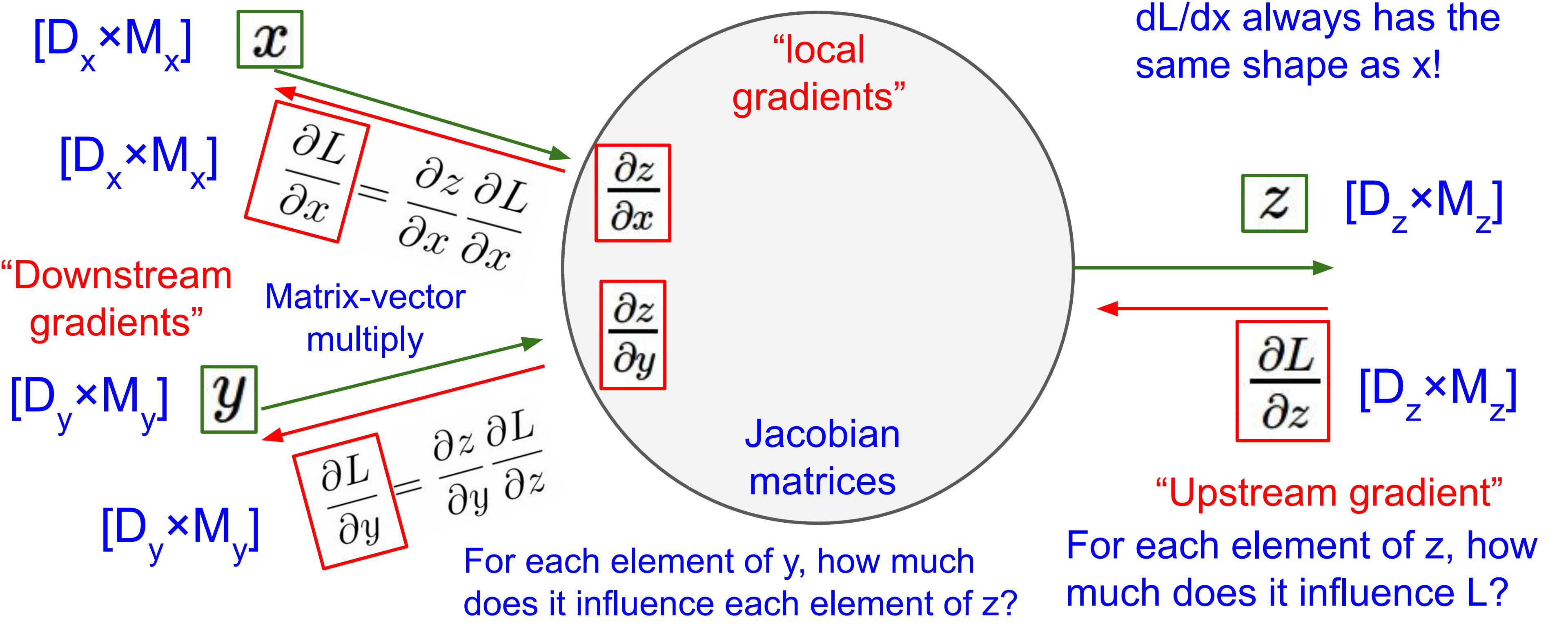
[4]
[-1]
[5]
[9]

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)

$\boxed{\text{Loss L still a scalar!}}$

dL/dx always has the same shape as x!

$[D_x \times M_x]$ x

$[D_x \times M_x]$ $\boxed{\frac{\partial L}{\partial x}} = \frac{\partial z}{\partial x}\frac{\partial L}{\partial z}$

"Downstream gradients"

Matrix-vector multiply

$[D_y \times M_y]$ y

$[D_y \times M_y]$ $\boxed{\frac{\partial L}{\partial y}} = \frac{\partial z}{\partial y}\frac{\partial L}{\partial z}$

"local gradients"

$\boxed{\frac{\partial z}{\partial x}}$ $[(D_x \times M_x) \times (D_z \times M_z)]$

$\boxed{\frac{\partial z}{\partial y}}$ $[(D_y \times M_y) \times (D_z \times M_z)]$

Jacobian matrices

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

z $[D_z \times M_z]$

$\boxed{\frac{\partial L}{\partial z}}$ $[D_z \times M_z]$

"Upstream gradient"

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

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

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

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 in the course notes:
http://cs231n.stanford.edu/handouts/linear-backprop.pdf

Backprop with Matrices

x: [N×D]
[2 1 -3]
[-3 4 2]

w: [D×M]
[3 2 1 -1]
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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]

Jacobians:
dy/dx: [(N×D)×(N×M)]
dy/dw: [(D×M)×(N×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]

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

w: [D×M]

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

Matrix Multiply

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

y: [N×M]

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

dL/dy: [N×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?

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

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

y: [N×M]

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

dL/dy: [N×M]

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

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

A: $\boxed{x_{n,d}}$ 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×D]

[2 $\boxed{1}$ -3]
[-3 4 2]

w: [D×M]

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

Matrix Multiply

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

y: [N×M]

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

dL/dy: [N×M]

[2 3 -3 9]
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Q: What parts of y are affected by one element of x?

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

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

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

Backprop with Matrices

x: [N×D]
[2 1 -3]
[-3 4 2]

w: [D×M]
[3 2 1 -1]
[2 1 3 2]
[3 2 1 -2]

Matrix Multiply

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

y: [N×M]
[13 9 -2 -6]
[5 2 17 1]

dL/dy: [N×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 $y_{n,m}$?

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]

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Matrix Multiply

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

y: [N×M]

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

dL/dy: [N×M]

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

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

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

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

A: $\boxed{w_{d,m}}$

[N×D] [N×M] [M×D]

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

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

Backprop with Matrices

x: [N×D]

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

w: [D×M]

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

Matrix Multiply

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

y: [N×M]

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

dL/dy: [N×M]

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

By similar logic:

[N×D] [N×M] [M×D]

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

[D×M] [D×N] [N×M]

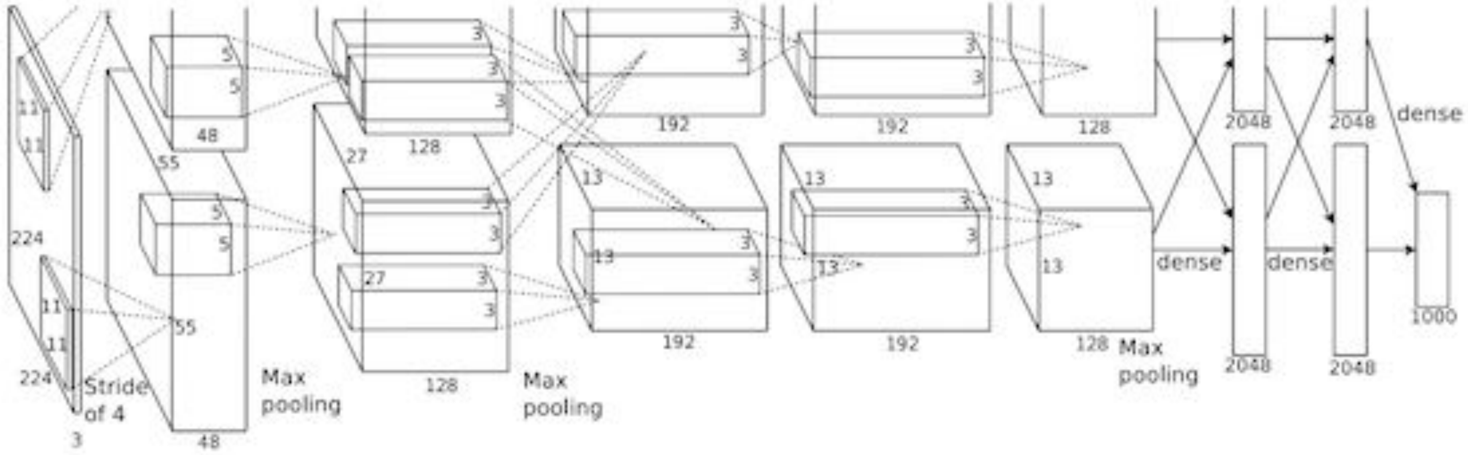
$$\boxed{\frac{\partial L}{\partial w} = x^T \left(\frac{\partial L}{\partial y}\right)}$$

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

Summary for today:

- **(Fully-connected) Neural Networks** are stacks of linear functions and nonlinear activation functions; they have much more representational power than linear classifiers
- **backpropagation** = recursive application of the chain rule along a computational graph to compute the gradients of all inputs/parameters/intermediates
- implementations maintain a graph structure, where the nodes implement the **forward**() / **backward**() API
- **forward**: compute result of an operation and save any intermediates needed for gradient computation in memory
- **backward**: apply the chain rule to compute the gradient of the loss function with respect to the inputs

Next Time: Convolutional Networks!

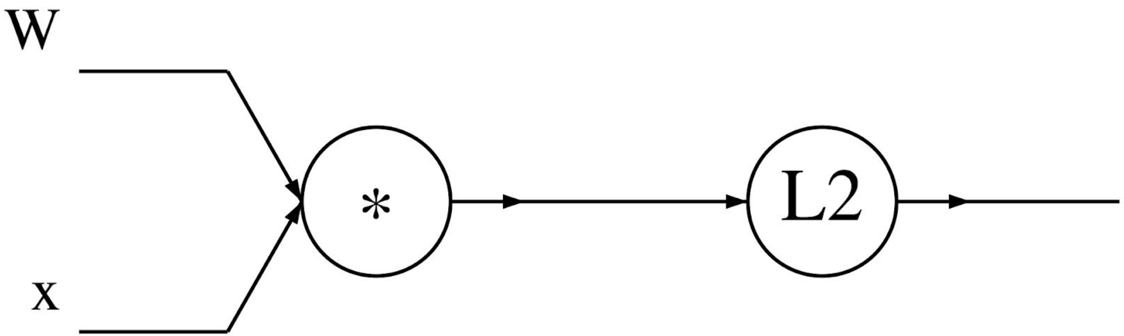


A vectorized example: $f(x,W) = ||W \cdot x||^2 = \sum_{i=1}^{n} (W \cdot x)_i^2$

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

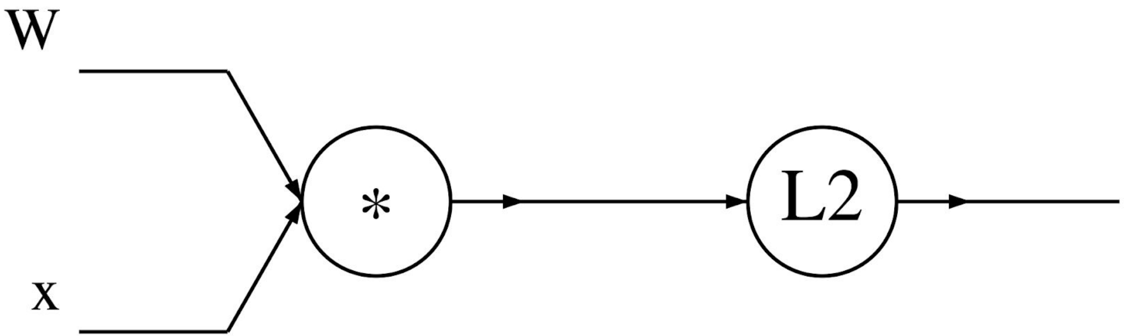
$\in \mathbb{R}^n \quad \in \mathbb{R}^{n \times n}$

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



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

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

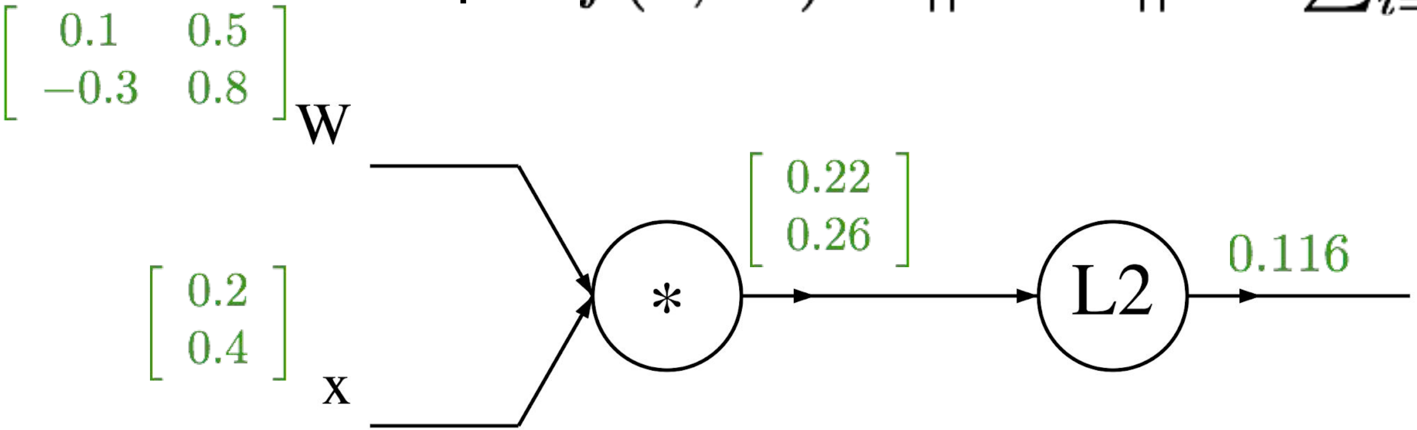


$$\begin{bmatrix} 0.2 \\ 0.4 \end{bmatrix}$$

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

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

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



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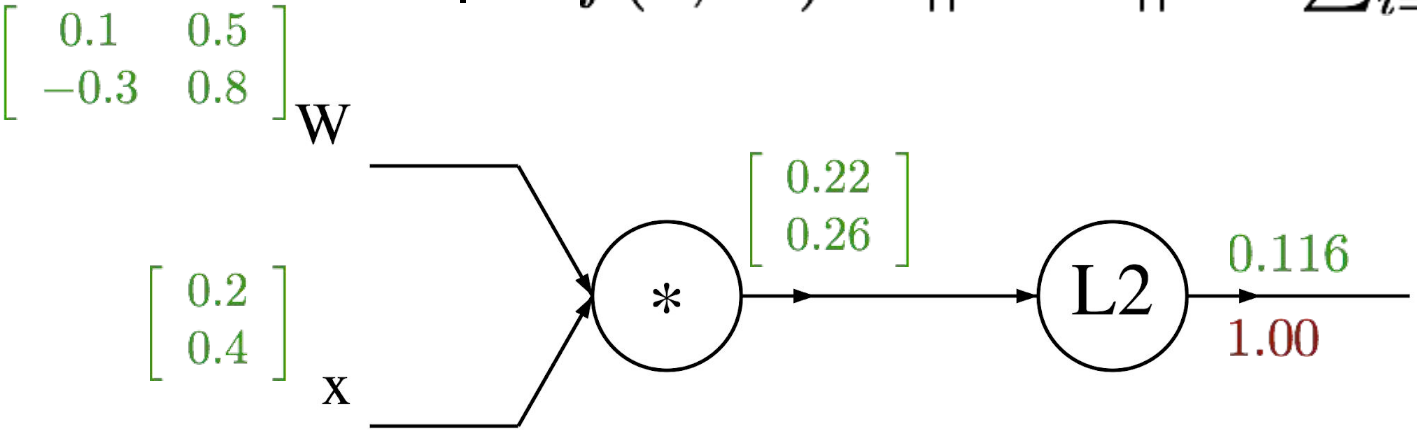

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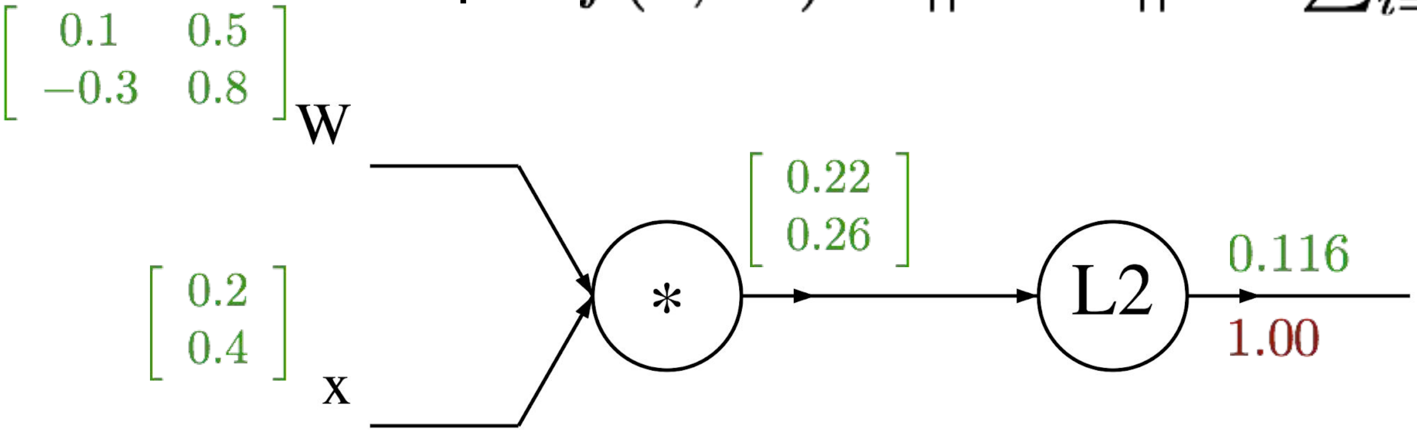

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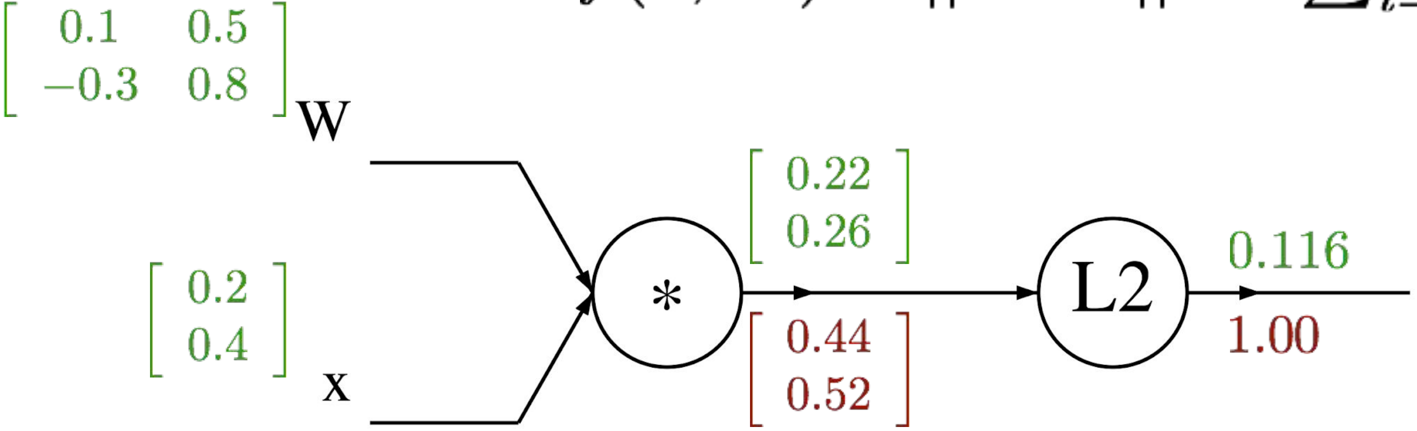
$$f(q) = ||q||^2 = q_1^2 + \cdots + q_n^2$$

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

$$\boxed{\nabla_q f = 2q}$$

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



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

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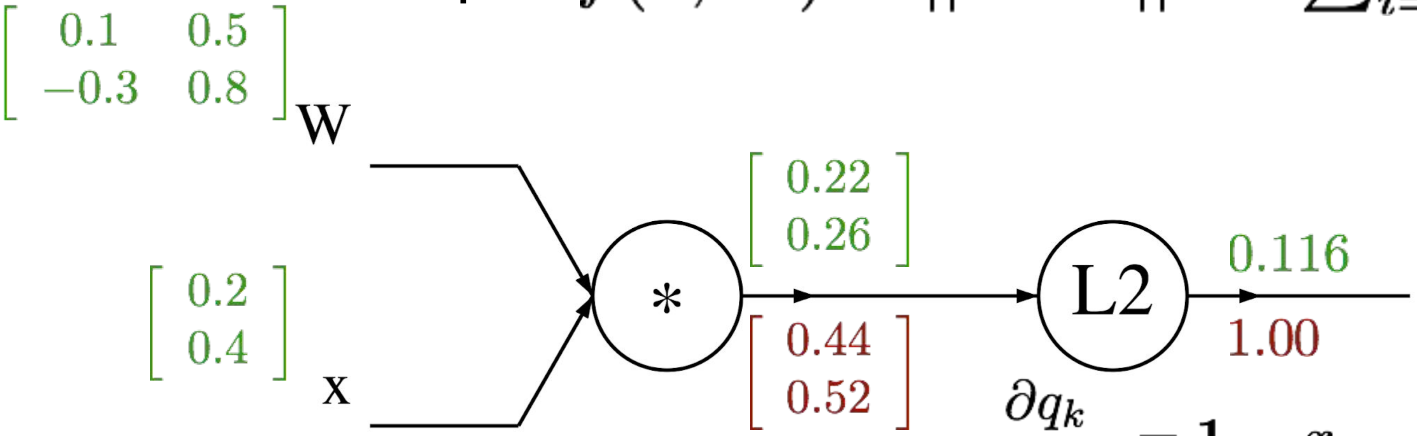
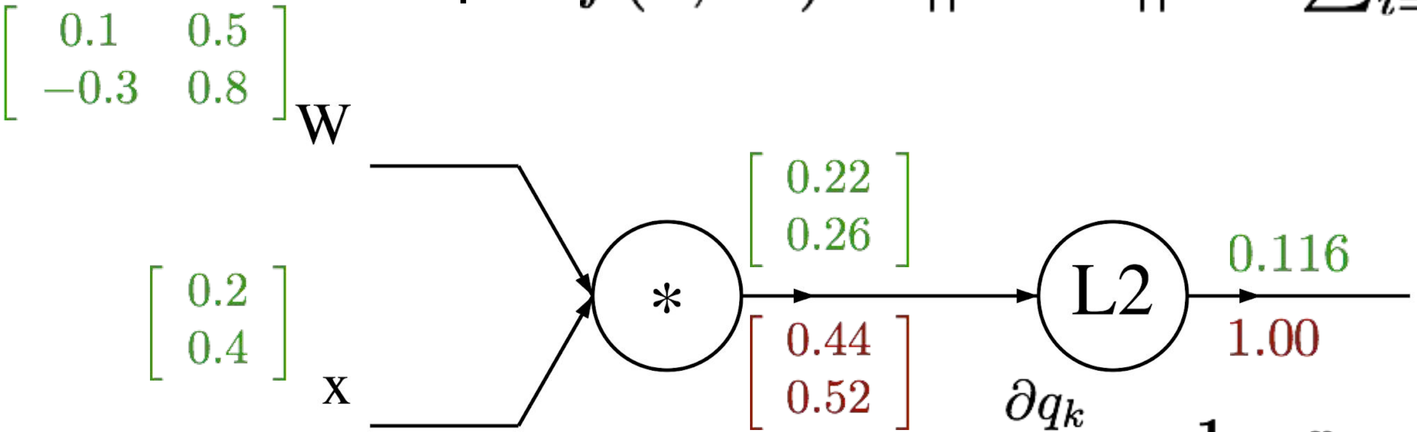


$$\frac{\partial q_k}{\partial W_{i,j}} = \mathbf{1}_{k=i} x_j$$

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

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

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



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

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

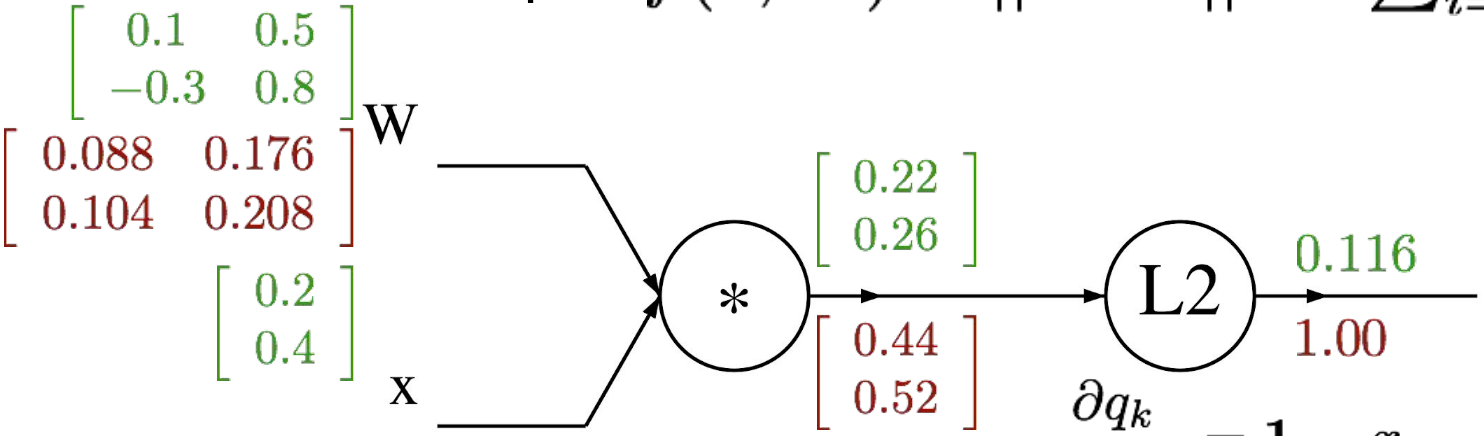
$$= \sum_k (2q_k)(\mathbf{1}_{k=i} x_j)$$

$$= 2q_i x_j$$

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

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

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



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

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

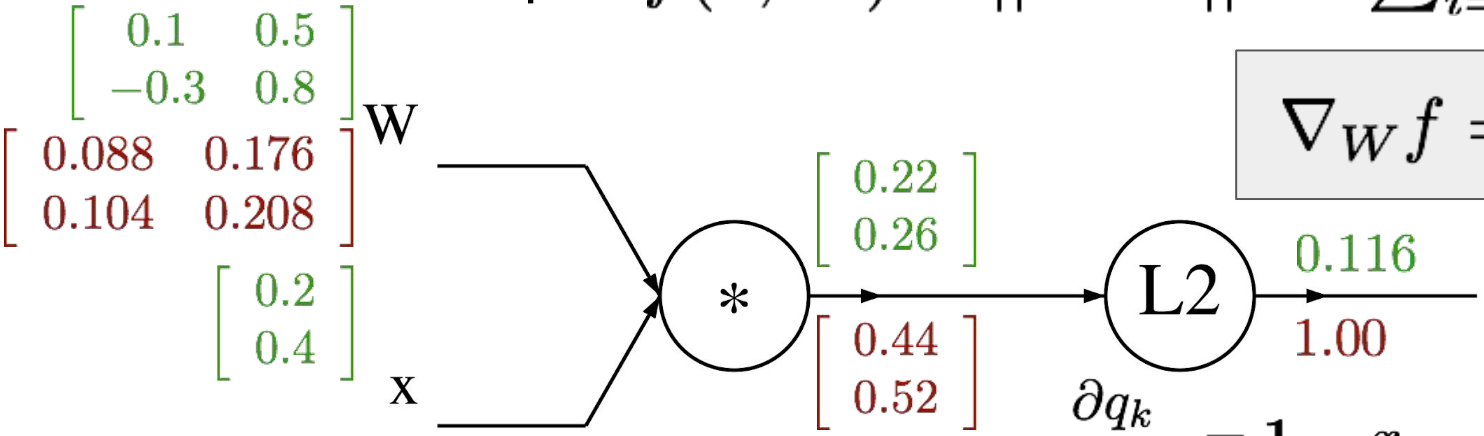
$$= \sum_k (2q_k)(\mathbf{1}_{k=i} x_j)$$

$$= 2q_i x_j$$

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

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

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



$$\boxed{\nabla_W f = 2q \cdot x^T}$$

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

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

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

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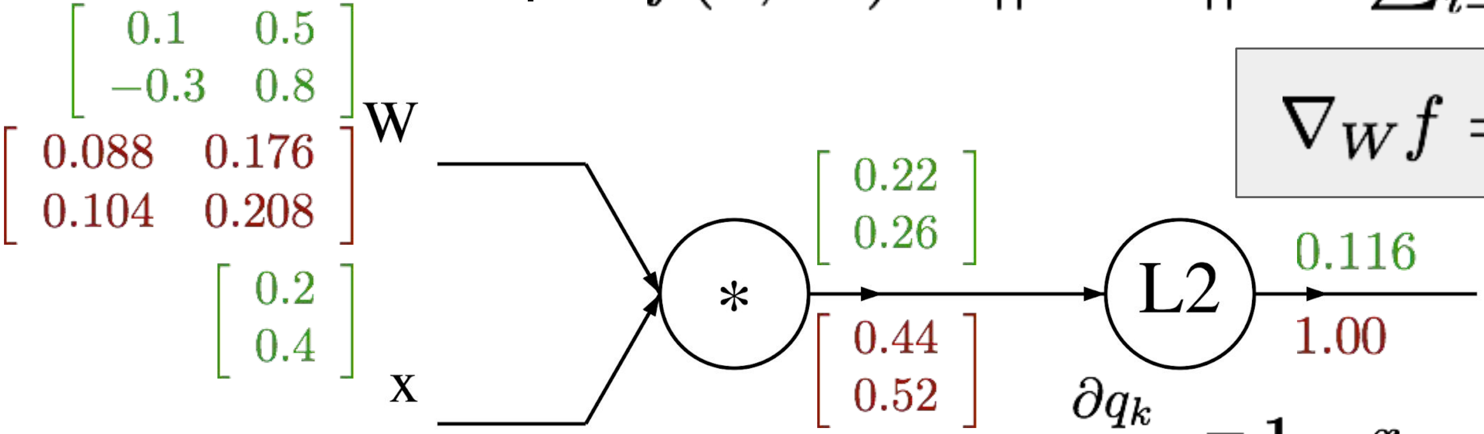

$$\boxed{\nabla_W f = 2q \cdot x^T}$$

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

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

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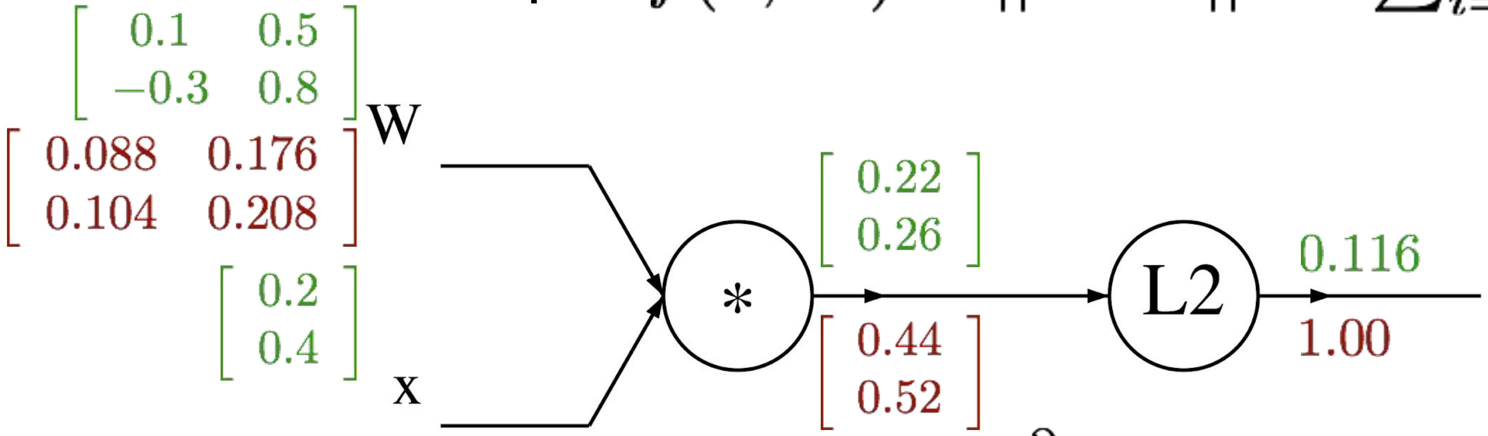

$$\frac{\partial q_k}{\partial x_i} = W_{k,i}$$

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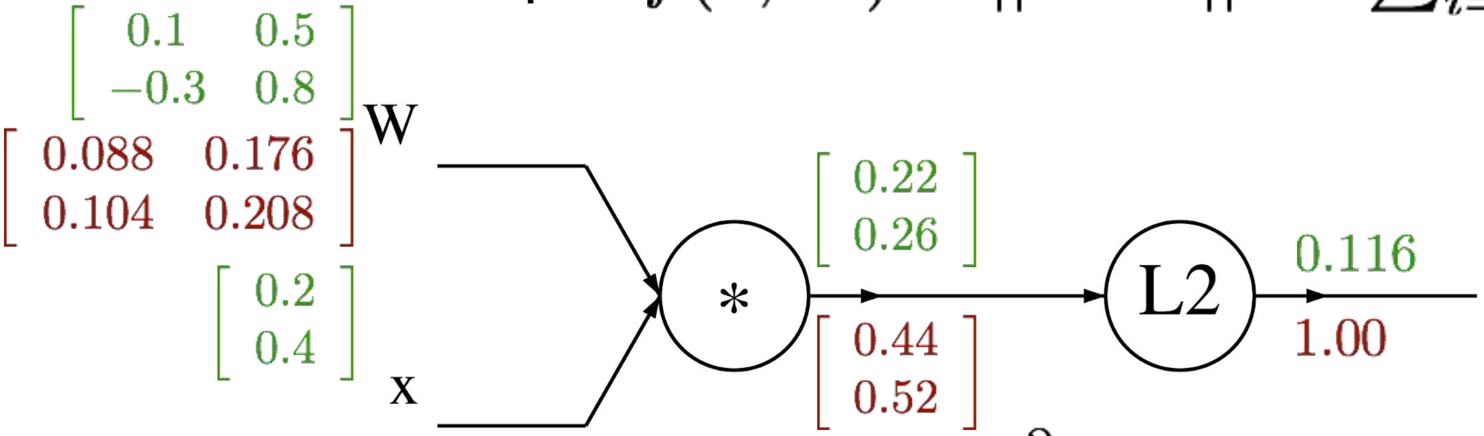

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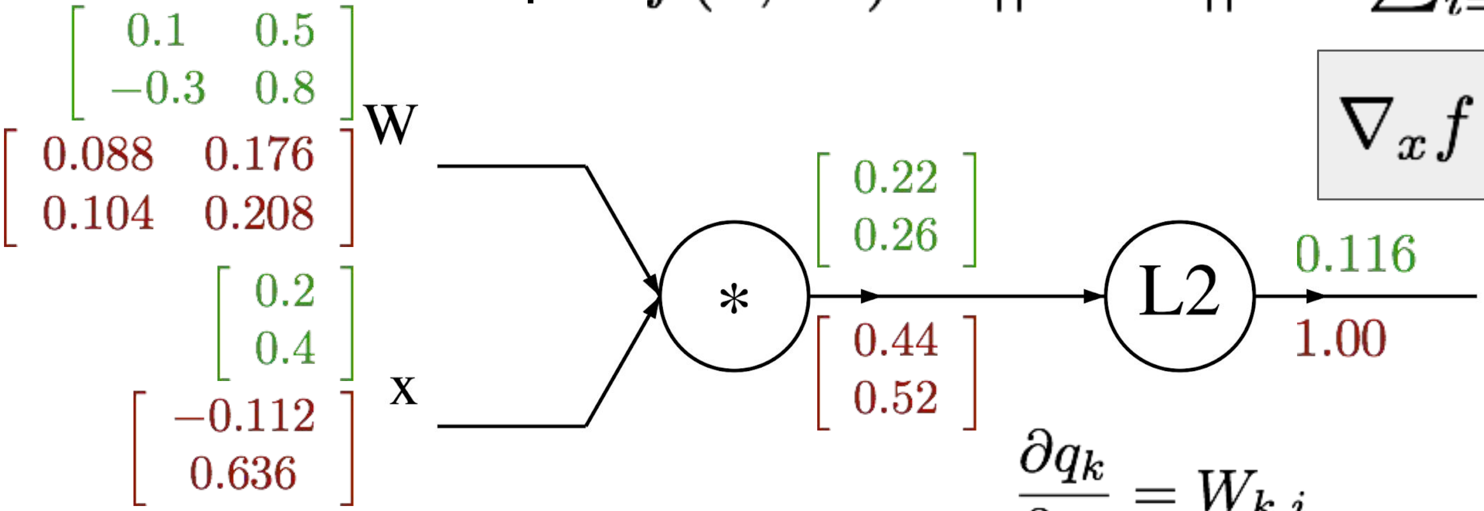

$$\boxed{\nabla_x f = 2W^T \cdot q}$$

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

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

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

In discussion section: A matrix example...

$$z_1 = XW_1$$

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

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

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

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

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