

# Lecture 4:

# Neural Networks and Backpropagation

# Administrative: Assignment 1

Due 4/16 11:59pm

- K-Nearest Neighbor
- Linear classifiers: SVM, Softmax

# Administrative: EdStem

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

# Administrative: Fridays

This Friday 9:30-10:30am and again 12:30-1:30pm

**Project Design & Backprop**

**Come to office hours to talk about your ideas**

# Administrative: Course Project

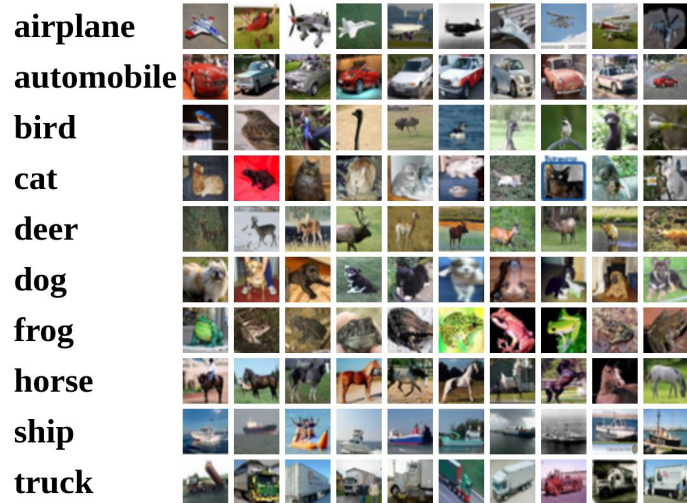
Project proposal due 4/29 11:59pm

“Is X a valid project for 493G1?”

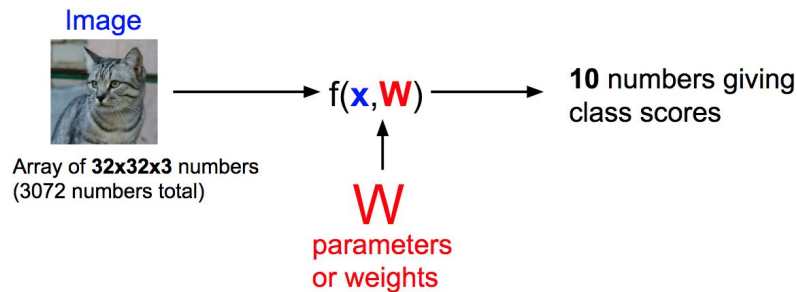
- Anything related to deep learning or computer vision
- Maximum of 3 students per team
- Make a EdStem private post or come to TA Office Hours

More info on the website

# Recap: from last time



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



# Recap: loss functions

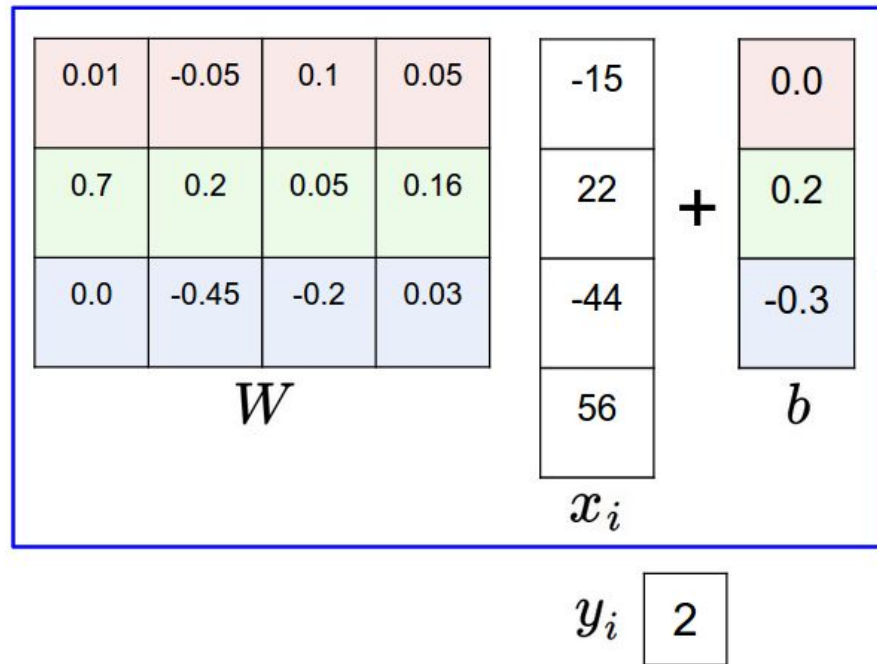
$$s = f(x; W) = Wx \quad \text{Linear score function}$$

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

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

# Recap: Softmax vs. SVM

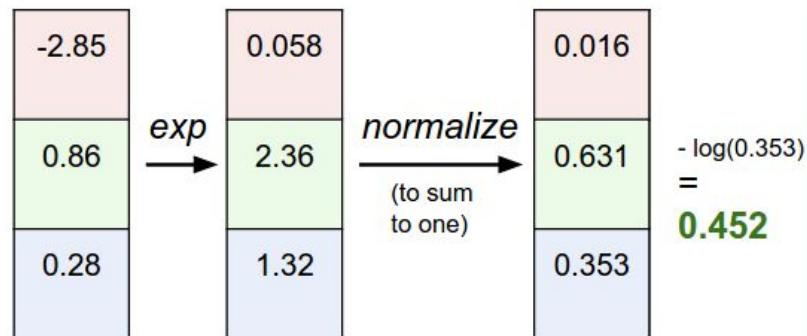
matrix multiply + bias offset



hinge loss (SVM)

$$\begin{aligned} &\max(0, -2.85 - 0.28 + 1) + \\ &\max(0, 0.86 - 0.28 + 1) \\ &= \\ &\mathbf{1.58} \end{aligned}$$

cross-entropy loss (Softmax)





# Optimization



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





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

# Strategy #1: A first very bad idea solution: **Random search**

```
# assume X_train is the data where each column is an example (e.g. 3073 x 50,000)
# assume Y_train are the labels (e.g. 1D array of 50,000)
# assume the function L evaluates the loss function

bestloss = float("inf") # Python assigns the highest possible float value
for num in xrange(1000):
    W = np.random.randn(10, 3073) * 0.0001 # generate random parameters
    loss = L(X_train, Y_train, W) # get the loss over the entire training set
    if loss < bestloss: # keep track of the best solution
        bestloss = loss
        bestW = W
    print 'in attempt %d the loss was %f, best %f' % (num, loss, bestloss)

# prints:
# in attempt 0 the loss was 9.401632, best 9.401632
# in attempt 1 the loss was 8.959668, best 8.959668
# in attempt 2 the loss was 9.044034, best 8.959668
# in attempt 3 the loss was 9.278948, best 8.959668
# in attempt 4 the loss was 8.857370, best 8.857370
# in attempt 5 the loss was 8.943151, best 8.857370
# in attempt 6 the loss was 8.605604, best 8.605604
# ... (truncated: continues for 1000 lines)
```

Lets see how well this works on the test set...

```
# Assume X_test is [3073 x 10000], Y_test [10000 x 1]  
scores = Wbest.dot(Xte_cols) # 10 x 10000, the class scores for all test examples  
# find the index with max score in each column (the predicted class)  
Yte_predict = np.argmax(scores, axis = 0)  
# and calculate accuracy (fraction of predictions that are correct)  
np.mean(Yte_predict == Yte)  
# returns 0.1555
```

15.5% accuracy! not bad!  
(SOTA is ~99.7%)



## Strategy #2: Follow the slope



## Strategy #2: **Follow the slope**

In 1-dimension, the derivative of a function:

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

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

The slope in any direction is the **dot product** of the direction with the gradient  
The direction of steepest descent is the **negative gradient**

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**gradient dW:**

[?,  
?,  
?,  
?,  
?,  
?,  
?,  
?,  
?,...]



**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**W + h (first dim):**

[0.34 + **0.0001**,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25322**

**gradient dW:**

[?,  
?,  
?,  
?,  
?,  
?,  
?,  
?,  
?,...]

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**W + h (first dim):**

[0.34 + **0.0001**,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25322**

**gradient dW:**

**[-2.5,**  
?,  
?,

$(1.25322 - 1.25347)/0.0001$   
 $= -2.5$

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

?,  
?,...]

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**W + h (second dim):**

[0.34,  
-1.11 + **0.0001**,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25353**

**gradient dW:**

[-2.5,  
?,  
?,  
?,  
?,  
?,  
?,  
?,  
?,...]

current **W**:

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**W + h** (second dim):

[0.34,  
-1.11 + **0.0001**,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25353**

gradient **dW**:

[-2.5,  
**0.6**,  
?,  
?,

$$(1.25353 - 1.25347)/0.0001 = 0.6$$

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

?,...]

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**W + h (third dim):**

[0.34,  
-1.11,  
0.78 + **0.0001**,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**gradient dW:**

[-2.5,  
0.6,  
?,  
?,  
?,  
?,  
?,  
?,  
?,...]

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

[0.34,  
-1.11,  
0.78 + **0.0001**,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

[-2.5,  
0.6,  
**0**,  
?,  
0

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

□, □, □, □, □

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**W + h (third dim):**

[0.34,  
-1.11,  
0.78 + **0.0001**,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**gradient dW:**

[-2.5,  
0.6,  
**0**,  
?,  
0,  
?,  
?,...,]

### Numeric Gradient

- Slow! Need to loop over all dimensions
- Approximate

?,...,]

This is silly. The loss is just a function of  $W$ :

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

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

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

want  $\nabla_W L$



This is silly. The loss is just a function of  $W$ :

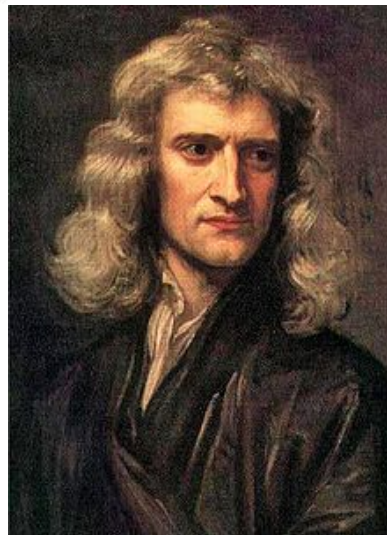
$$L = \frac{1}{N} \sum_{i=1}^N L_i + \sum_k W_k^2$$

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

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

want  $\nabla_W L$

Use calculus to compute an  
**analytic gradient**



[This image](#) is in the public domain




[This image](#) is in the public domain

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

$dW = \dots$   
(some function  
data and W)



**gradient dW:**

[-2.5,  
0.6,  
0,  
0.2,  
0.7,  
-0.5,  
1.1,  
1.3,  
-2.1,...]

## In summary:

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

=>

In practice: Always use analytic gradient, but check implementation with numerical gradient. This is called a **gradient check**.

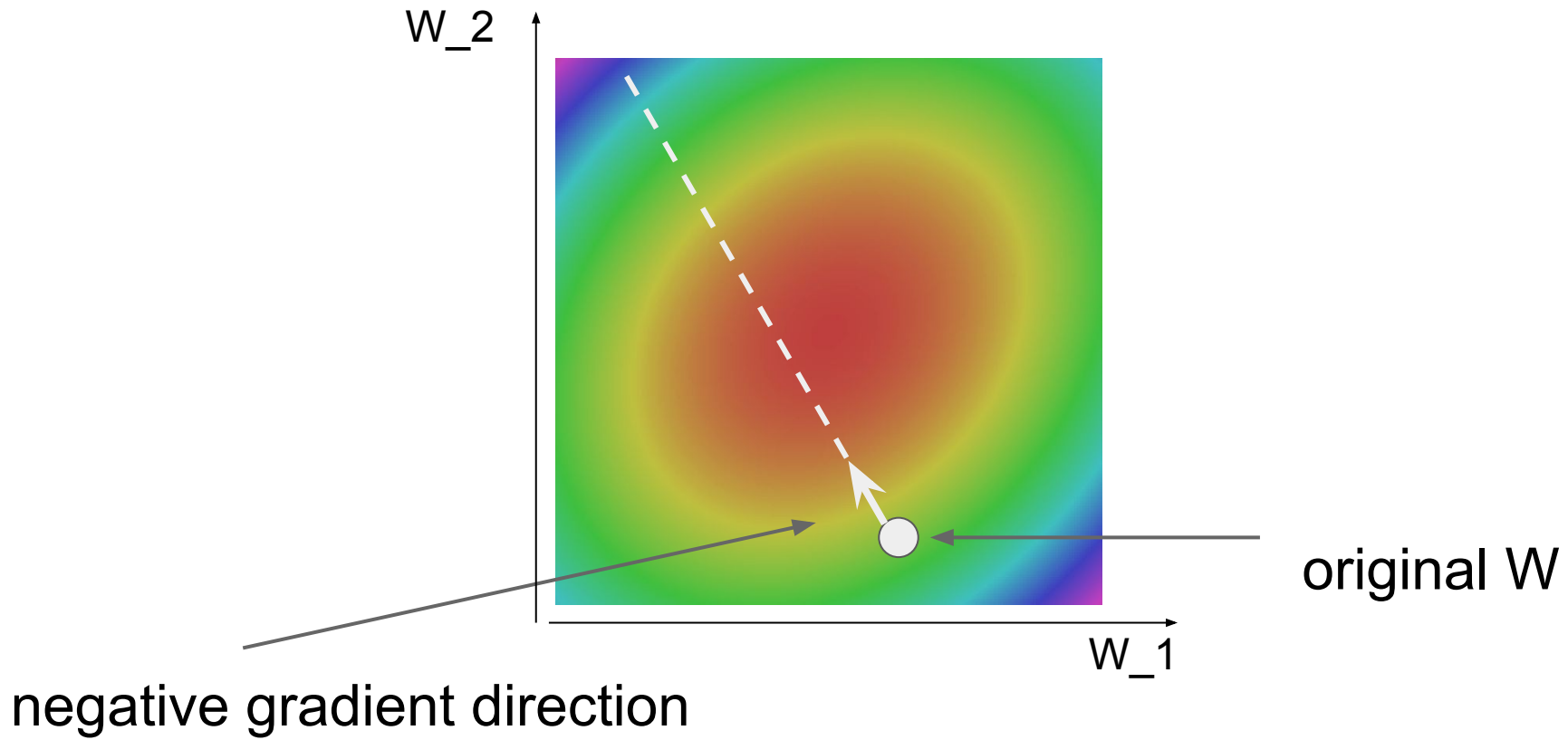
# Gradient Descent

```
# Vanilla Gradient Descent
```

```
while True:
```

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

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



# Stochastic Gradient Descent (SGD)

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

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

Full sum expensive  
when N is large!

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

```
# Vanilla Minibatch Gradient Descent
```

```
while True:
```

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

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

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

# Calculating the analytical gradient requires calculus!

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

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

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

How to find the best  $W$ ?

$$\nabla_W L$$

Before we discuss how to calculate  
gradients analytically,

let's introduce **neural networks**



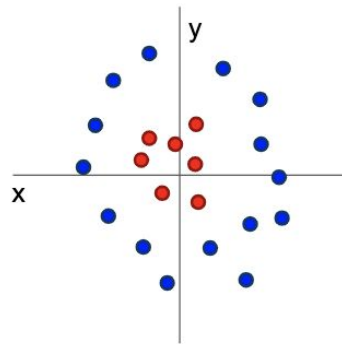
# Problem: Linear Classifiers are not very powerful

## Visual Viewpoint



Linear classifiers learn  
one template per class

## Geometric Viewpoint



Linear classifiers  
can only draw linear  
decision boundaries

# Pixel Features

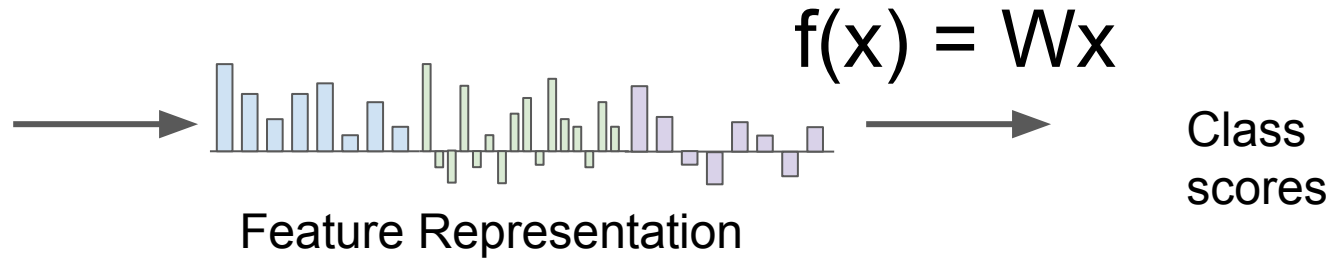


$$f(x) = Wx$$

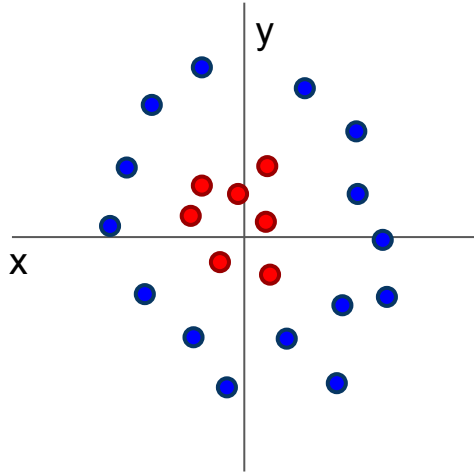
Class  
scores



# Image Features

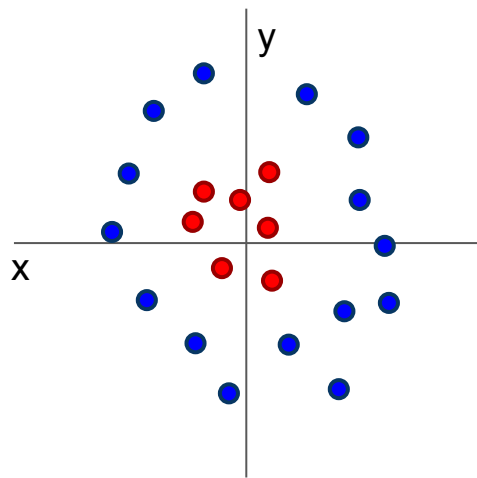


# Image Features: Motivation



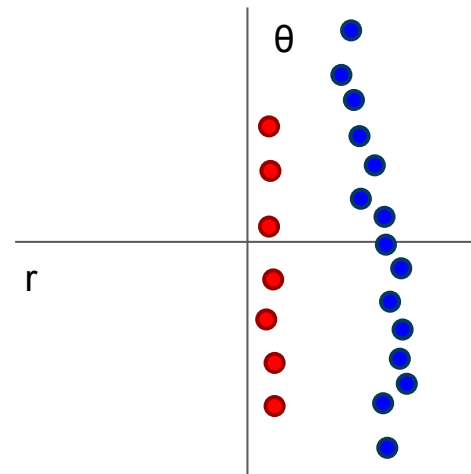
Cannot separate red  
and blue points with  
linear classifier

# Features become linearly separable through a non-linear transformation



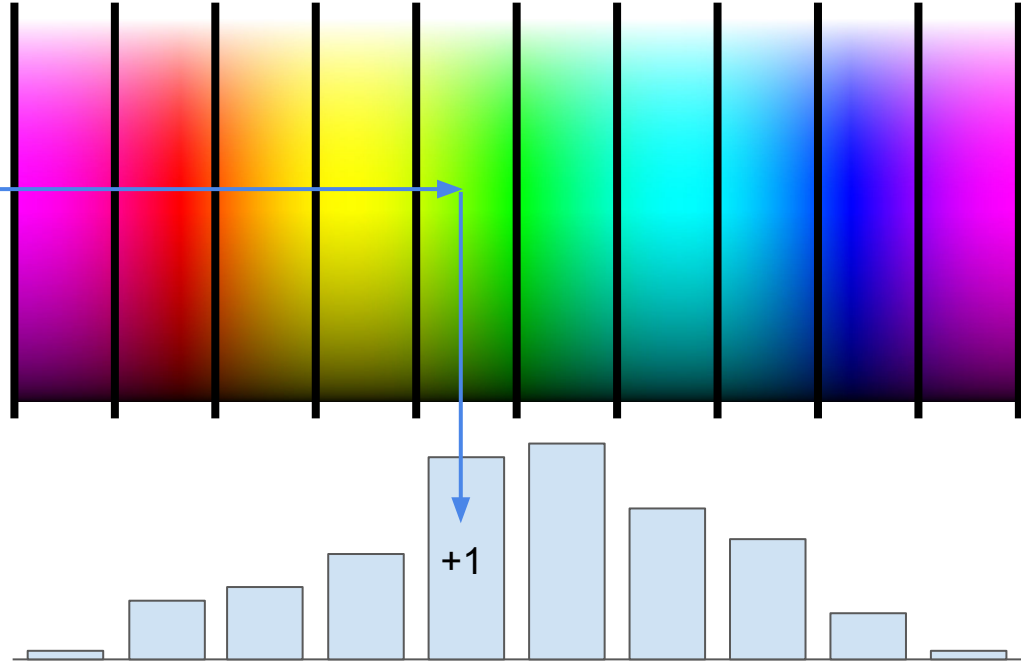
Cannot separate red and blue points with linear classifier

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



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

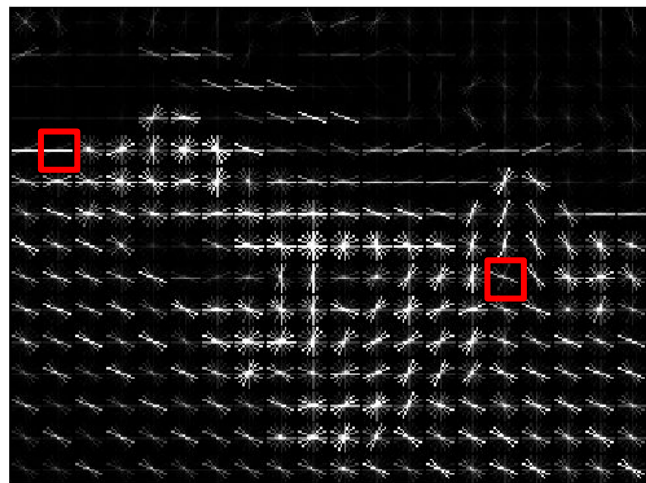
# Example: Color Histogram



# Example: Histogram of Oriented Gradients (HoG)



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



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

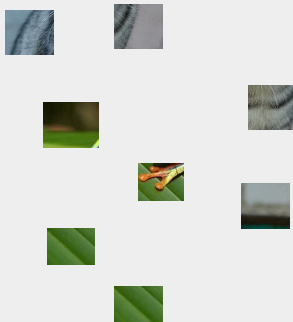
Lowe, "Object recognition from local scale-invariant features", ICCV 1999  
Dalal and Triggs, "Histograms of oriented gradients for human detection," CVPR 2005

# Example: Bag of Words

## Step 1: Build codebook



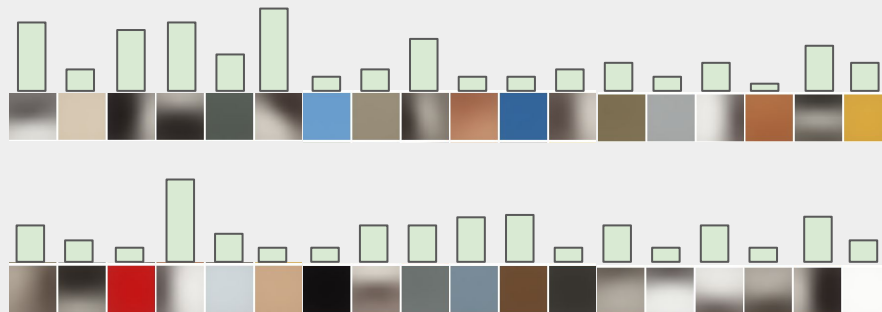
Extract random  
patches



Cluster patches to  
form “codebook”  
of “visual words”



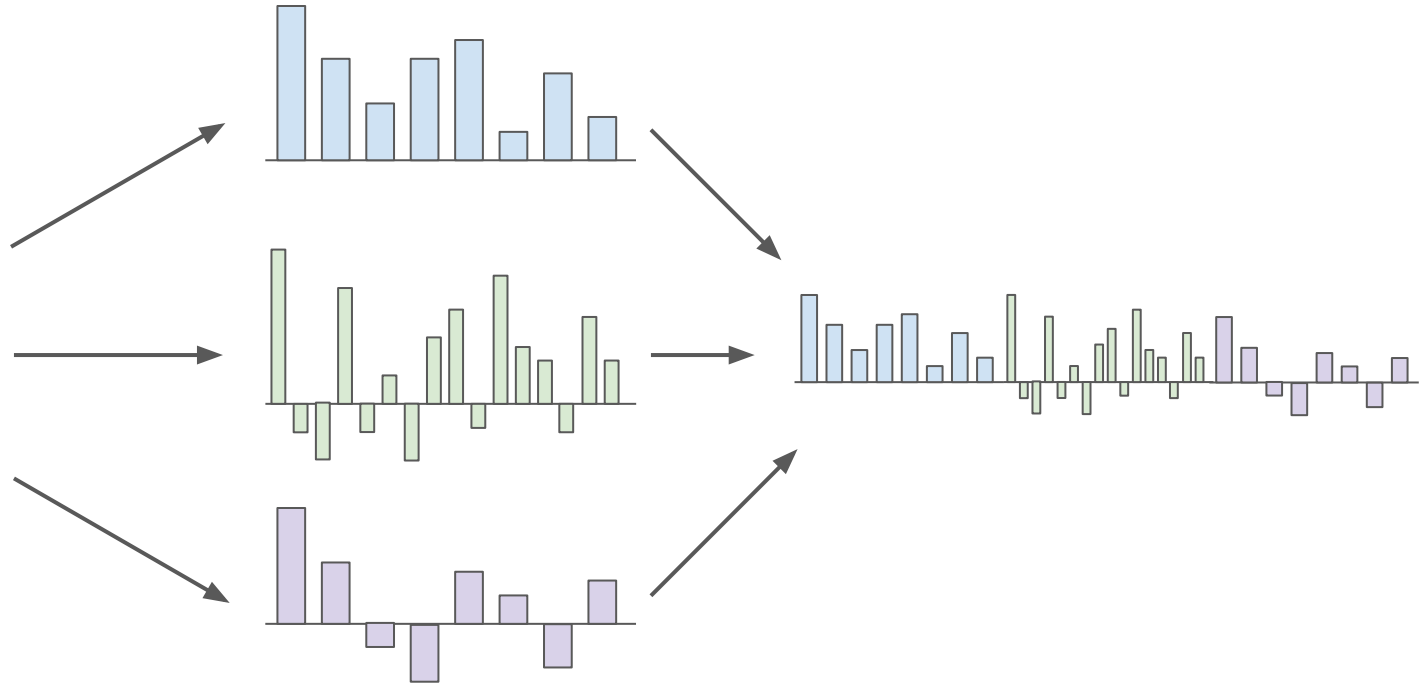
## Step 2: Encode images



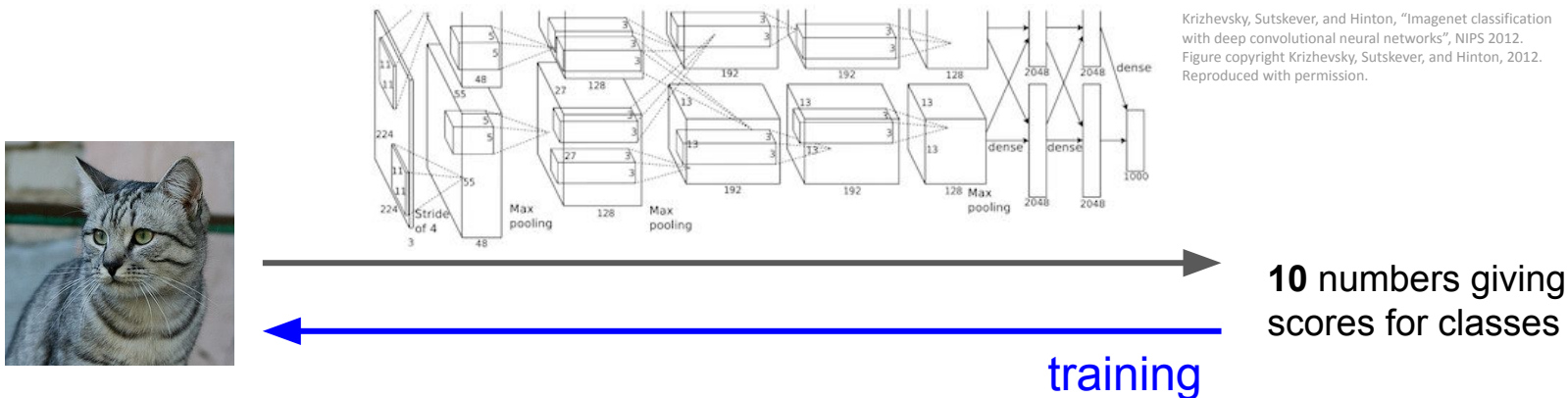
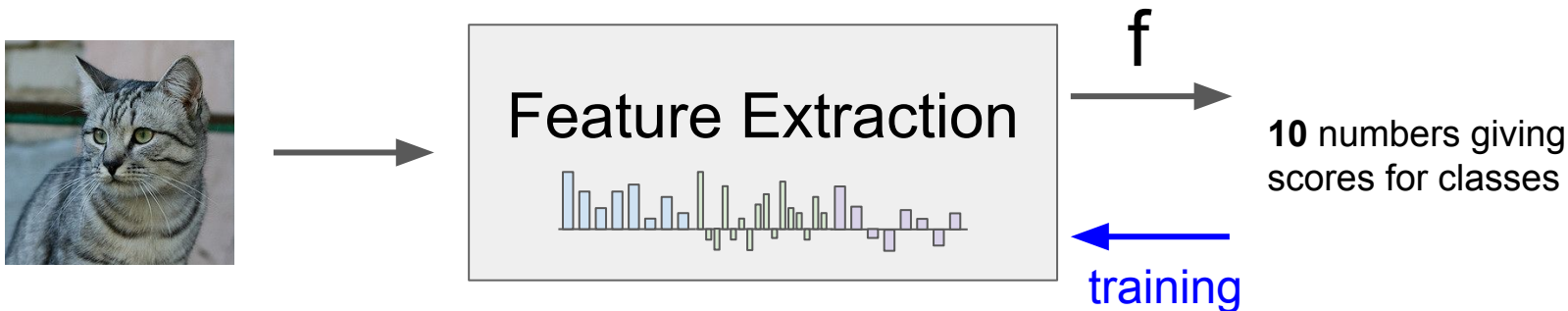
Fei-Fei and Perona, “A bayesian hierarchical model for learning natural scene categories”, CVPR 2005



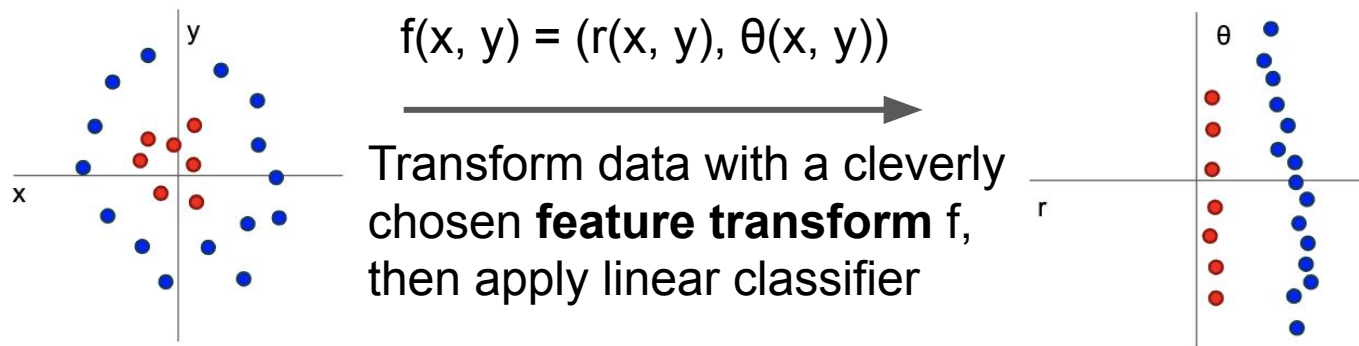
# Combine many different features if unsure which features are better



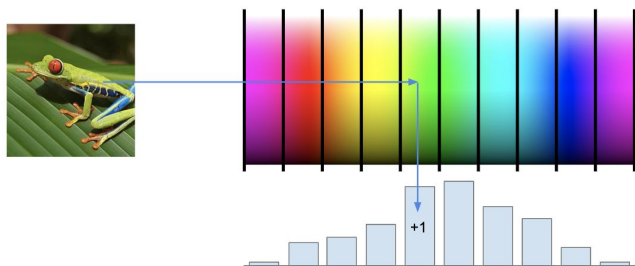
# Image features vs neural networks



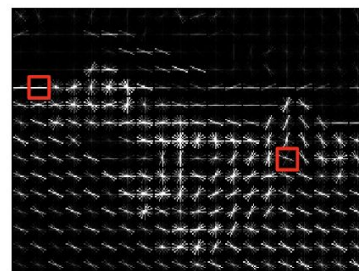
# One Solution: Non-linear feature transformation



Color Histogram



Histogram of Oriented Gradients (HoG)



# Neural Networks

# Neural networks: the original linear classifier

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

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

# Neural networks: 2 layers

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

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

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

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

# Neural networks: also called fully connected network

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

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

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

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

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

# Neural networks: 3 layers

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

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

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

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

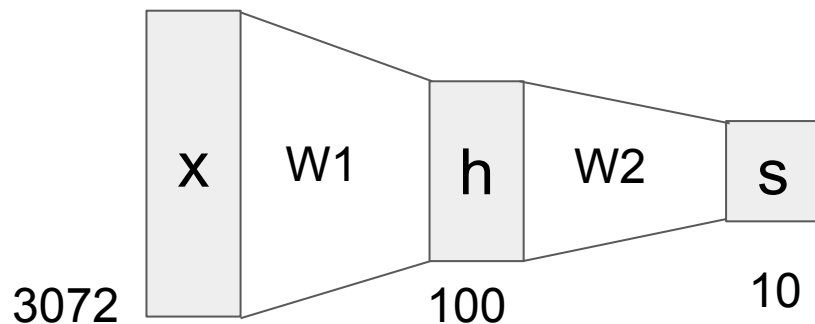
(In practice we will usually add a learnable bias at each layer as well)



# Neural networks: hierarchical computation

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

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

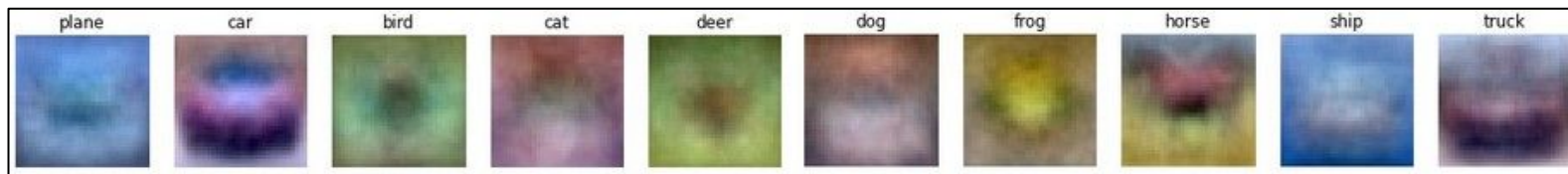
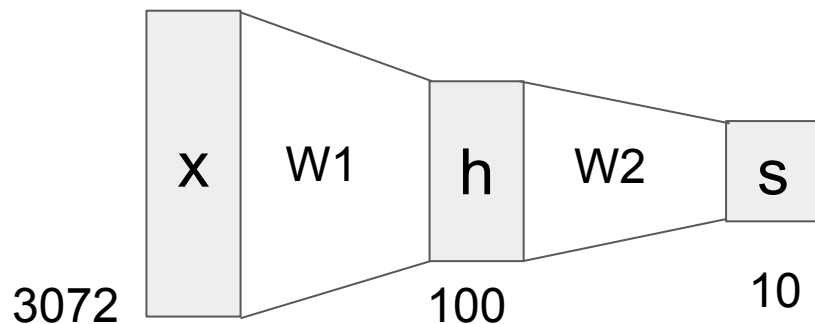


$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

# Neural networks: learning 100s of templates

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

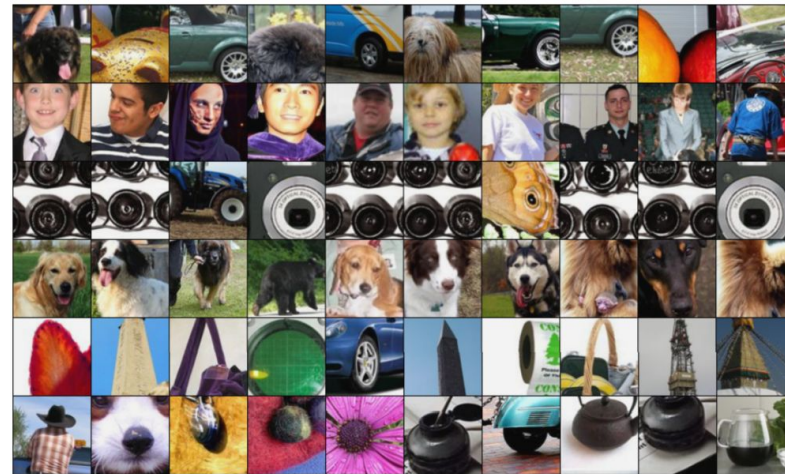
(**Now**) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$



Learn 100 templates instead of 10.

Share templates between classes

# Examples of templates from real neural networks



Springenberg et al, "Striving for Simplicity: The All Convolutional Net", ICLR Workshop 2015  
Figure copyright Jost Tobias Springenberg, Alexey Dosovitskiy, Thomas Brox, Martin Riedmiller, 2015; reproduced with permission.

# Neural networks: why is max operator important?

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

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

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

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

$$f = W_2 W_1 x$$

# Neural networks: why is max operator important?

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

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

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

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

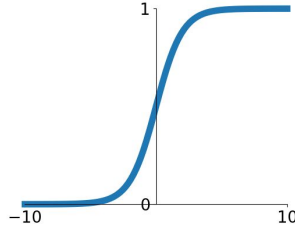
$$f = W_2 W_1 x \quad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

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

# Activation functions

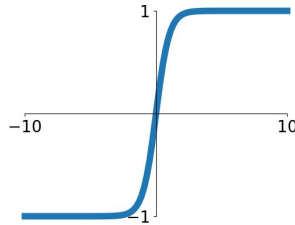
## Sigmoid

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



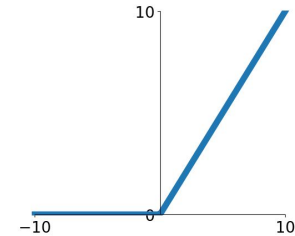
## tanh

$$\tanh(x)$$



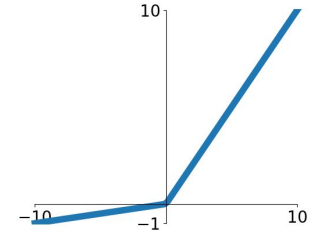
## ReLU

$$\max(0, x)$$



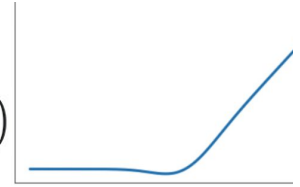
## Leaky ReLU

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



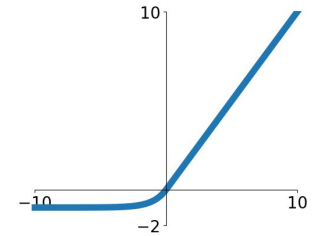
## GeLU

$$0.5x \left( 1 + \tanh \left[ \sqrt{2/\pi} (x + 0.044715x^3) \right] \right)$$



## ELU

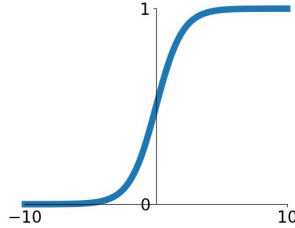
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



# Activation functions

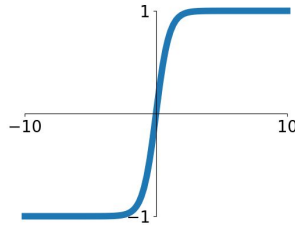
## Sigmoid

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



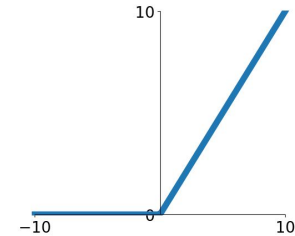
## tanh

$$\tanh(x)$$



## ReLU

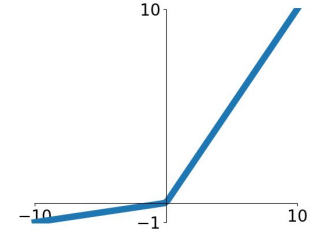
$$\max(0, x)$$



ReLU is a good default choice for most problems

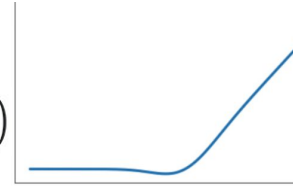
## Leaky ReLU

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



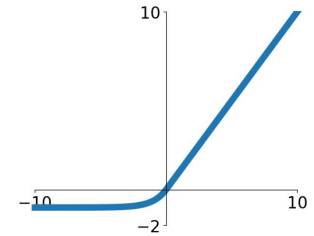
## GeLU

$$0.5x \left( 1 + \tanh \left[ \sqrt{2/\pi} (x + 0.044715x^3) \right] \right)$$



## ELU

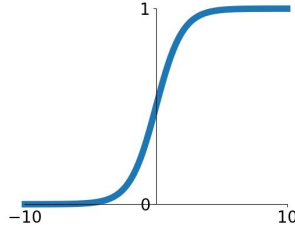
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



# Activation functions

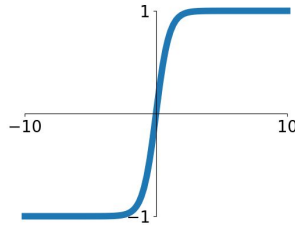
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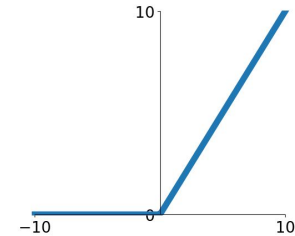
## tanh

$$\tanh(x)$$



## ReLU

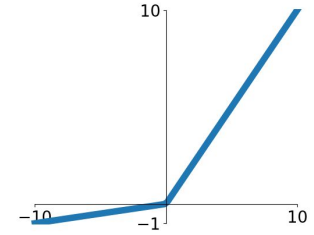
$$\max(0, x)$$



GeLU is the default choice  
for transformers

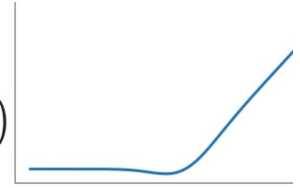
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$$\max(0.1x, x)$$



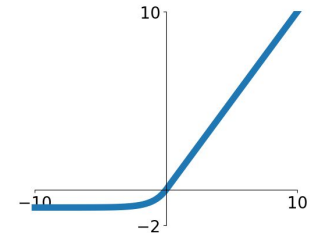
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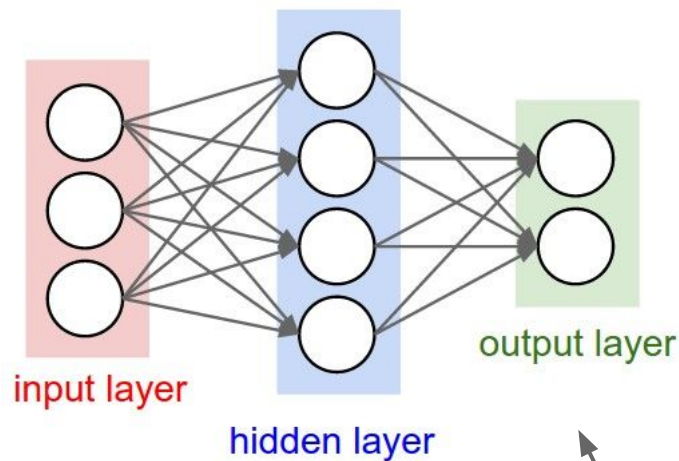
## ELU

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

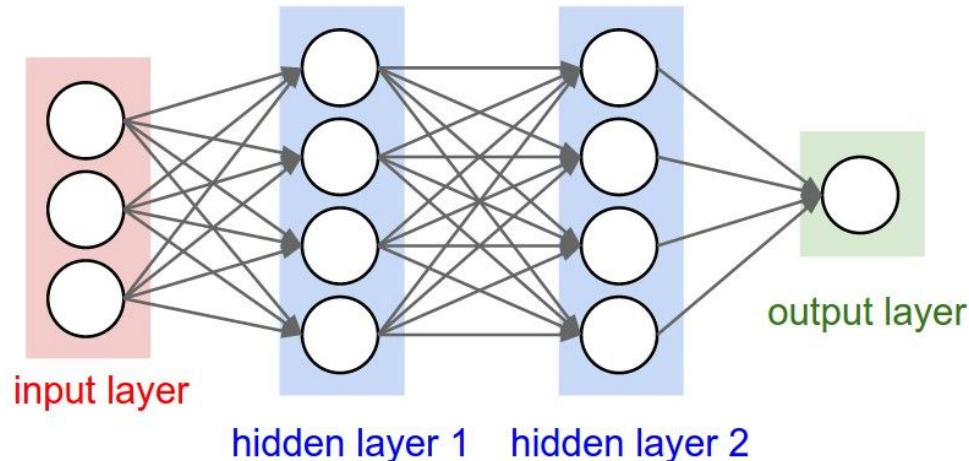




# Neural networks: Architectures



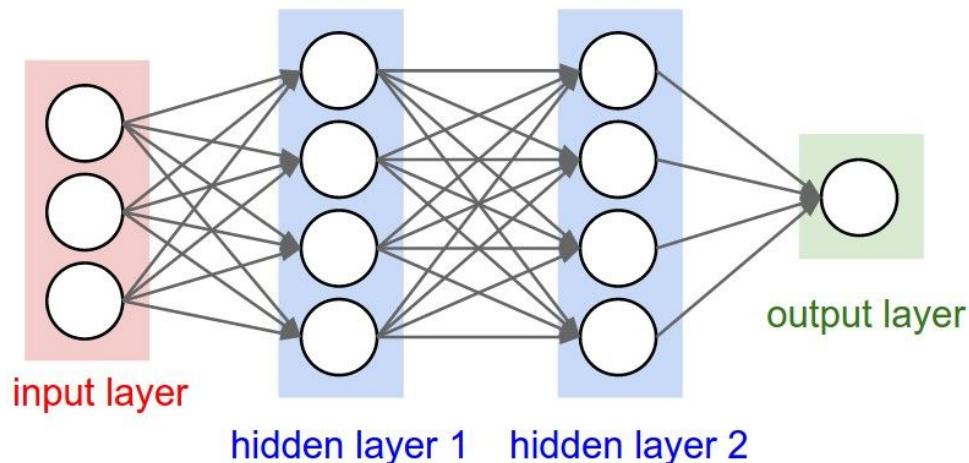
"2-layer Neural Net", or  
"1-hidden-layer Neural Net"



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

**"Fully-connected" layers**

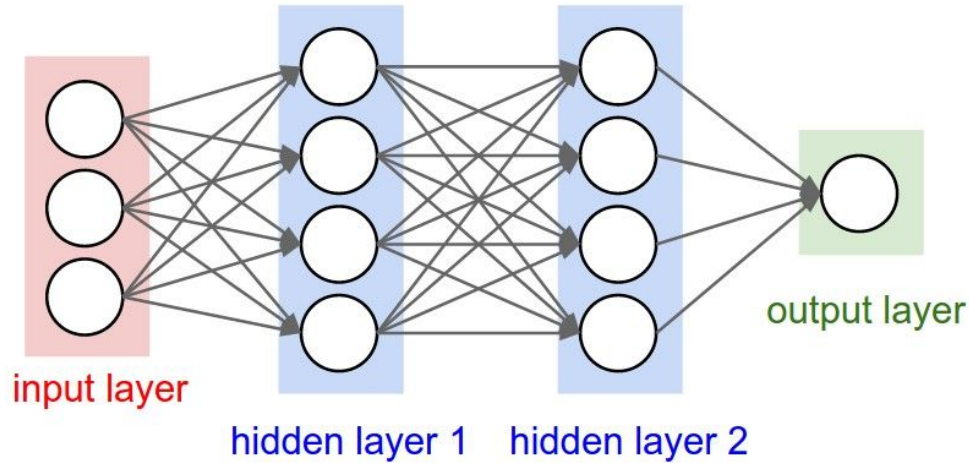
# Example feed-forward computation of a neural network



*# forward-pass of a 3-layer neural network:*

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

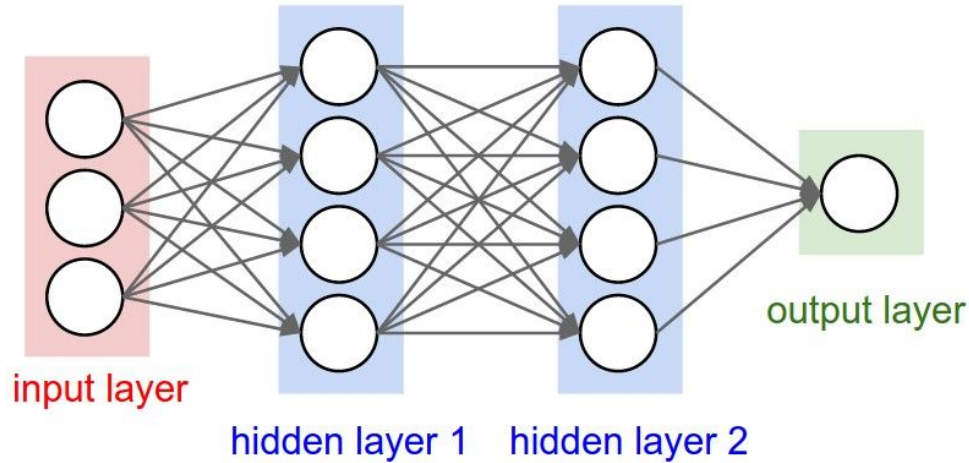
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```
# forward-pass of a 3-layer neural network:
```

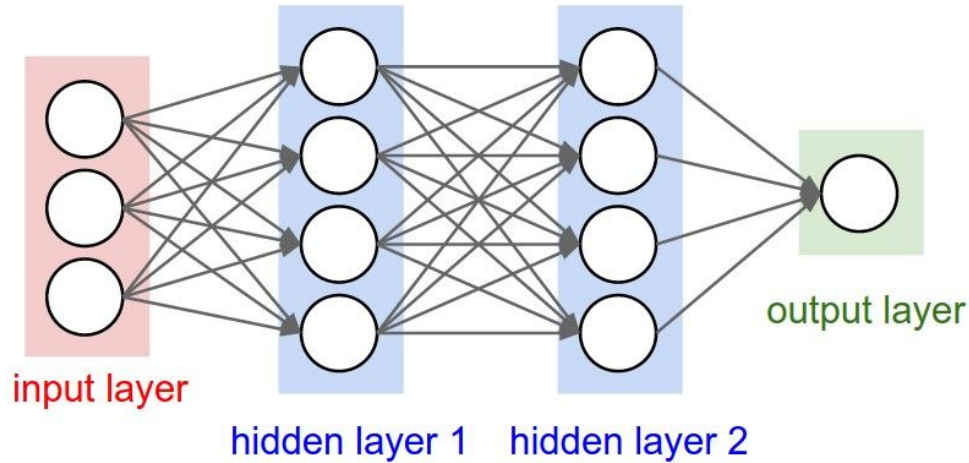
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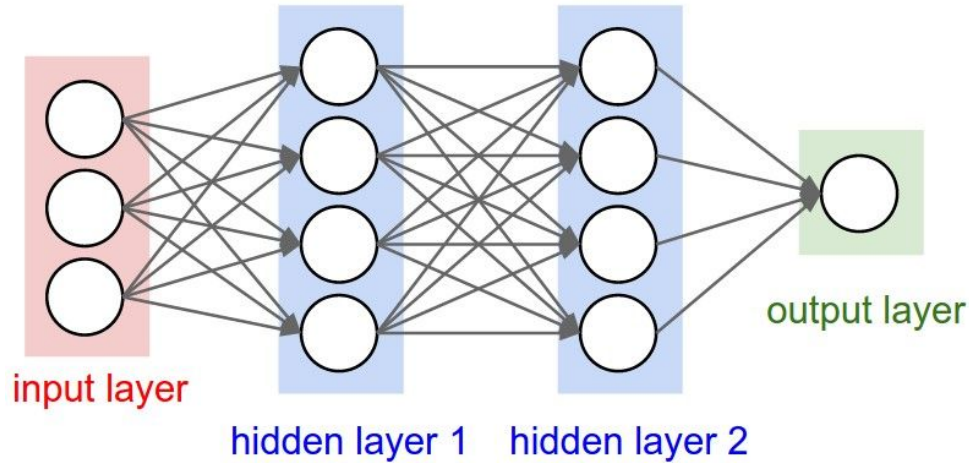
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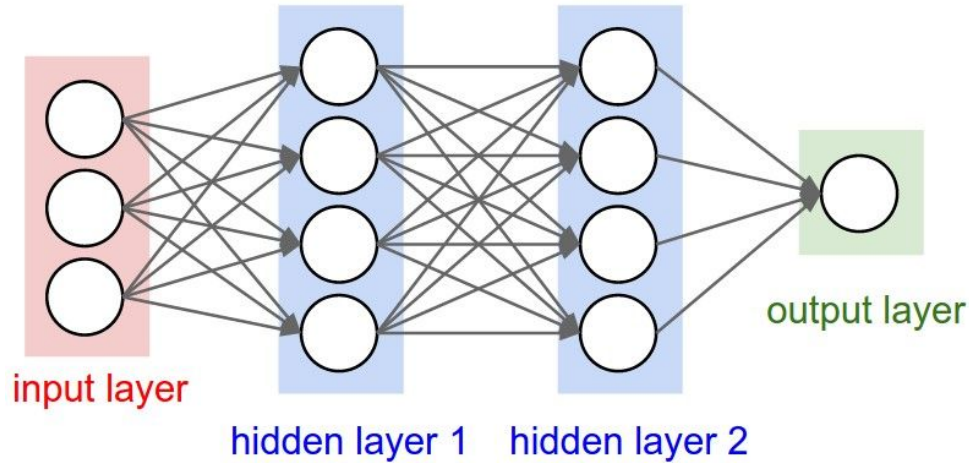


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```

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

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

Forward pass

Calculate the analytical gradients

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```

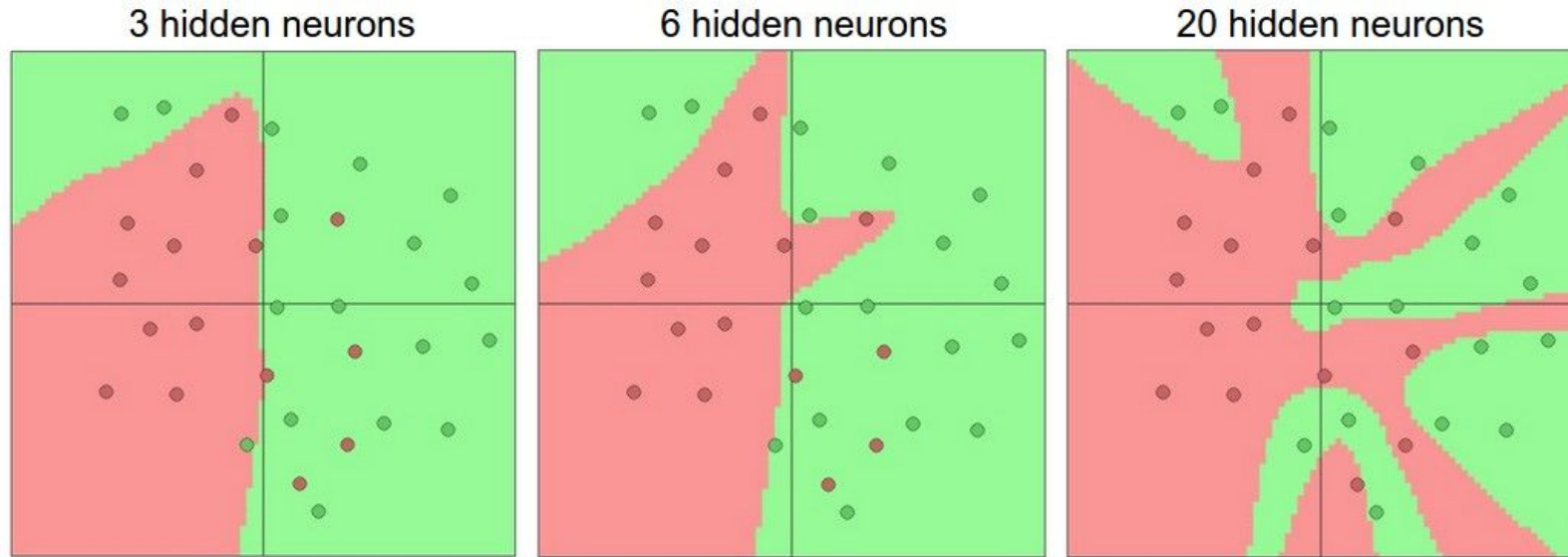
Define the network

Forward pass

Calculate the analytical gradients

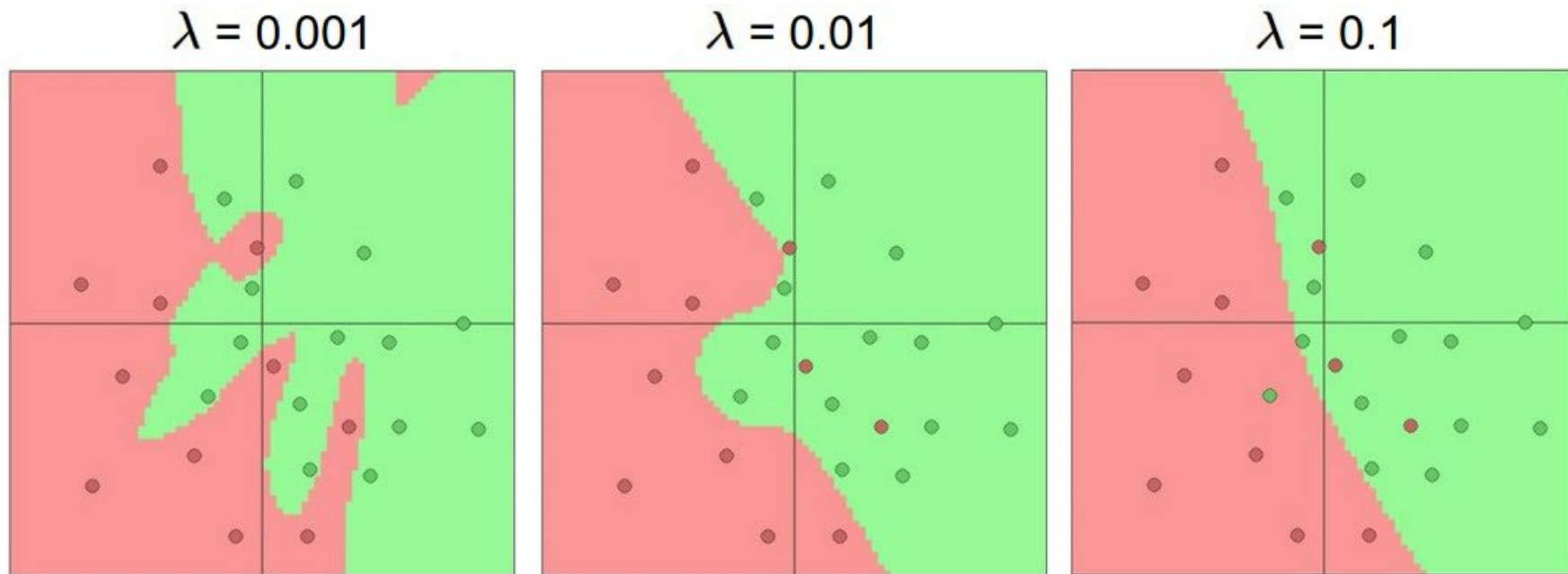
Gradient descent

# Setting the number of layers and their sizes

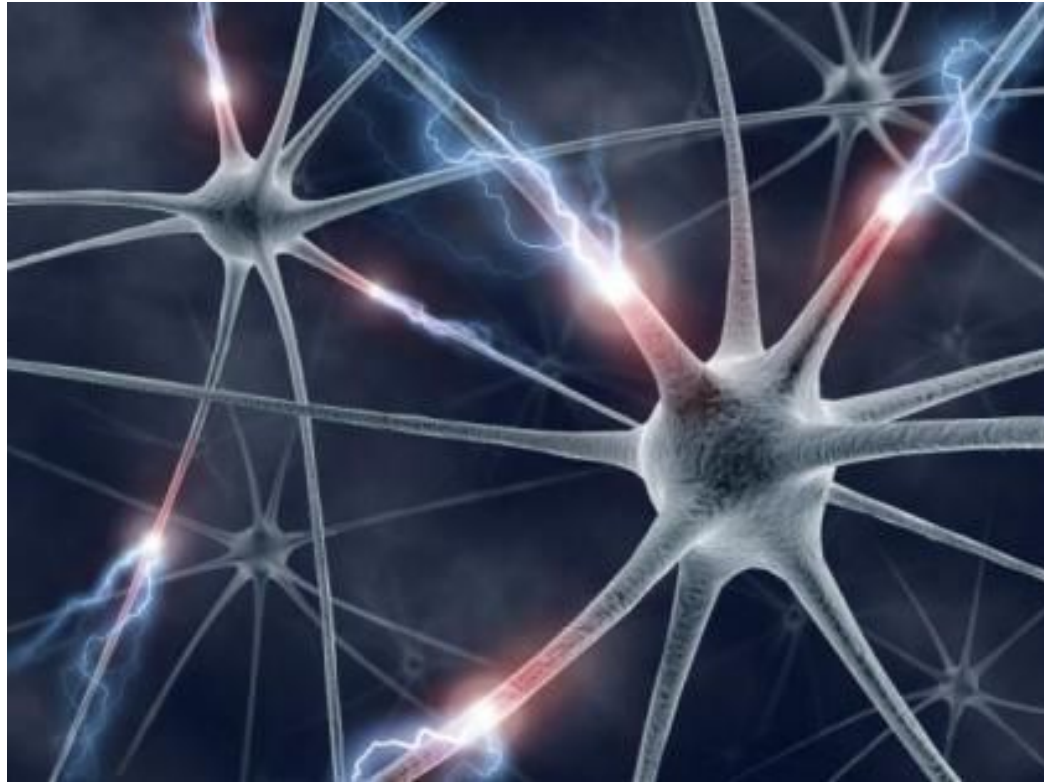


↑  
more neurons = more capacity

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

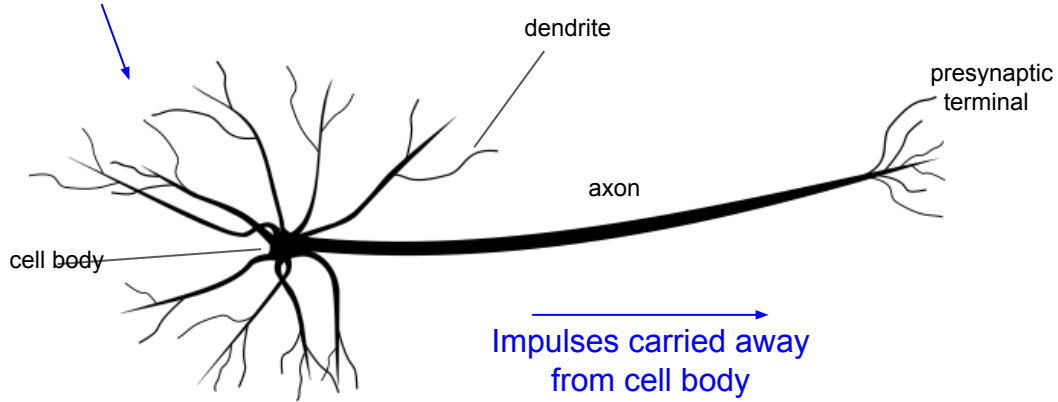


$$L(W) = \frac{1}{N} \sum_{i=1}^N L_i(f(x_i, W), y_i) + \lambda R(W)$$



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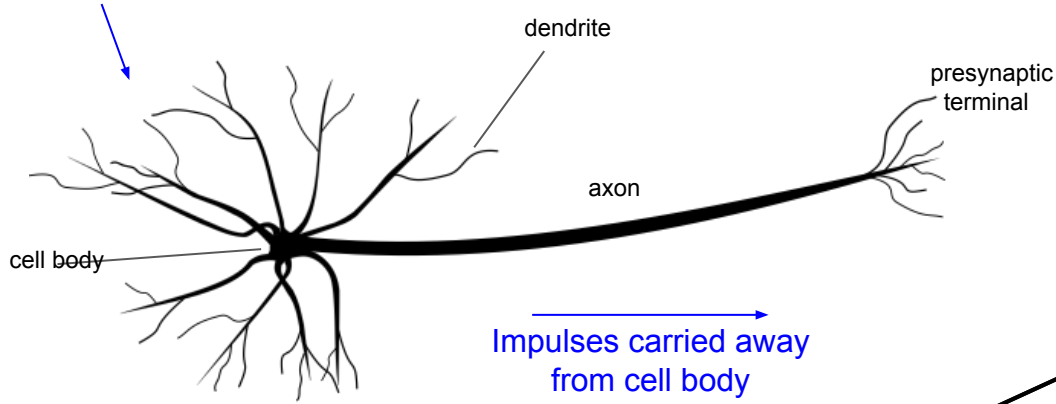
Impulses carried toward cell body



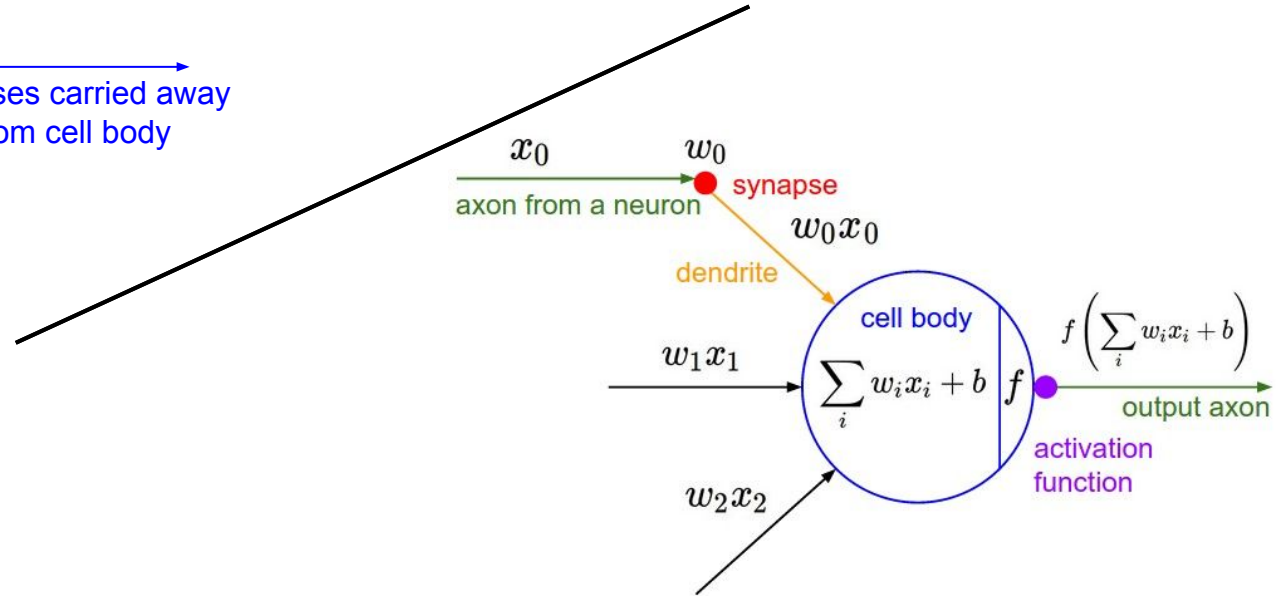
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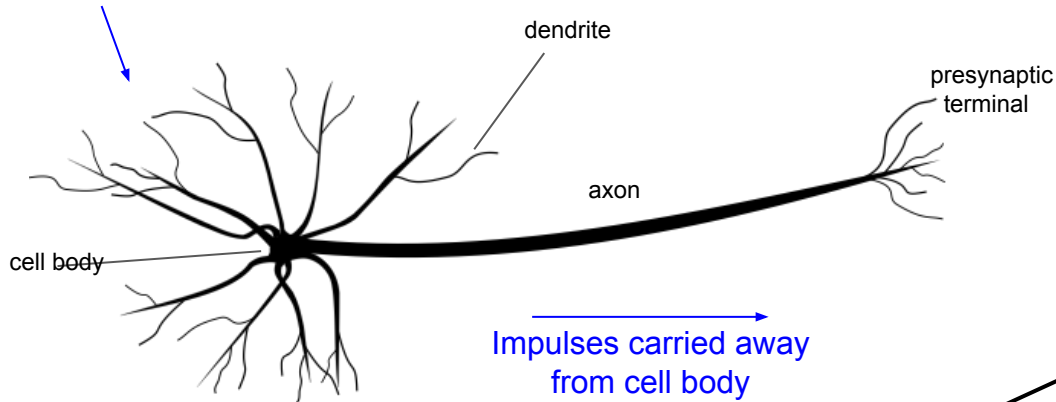
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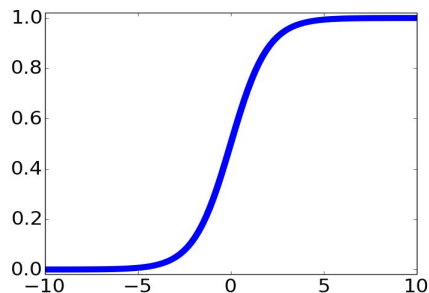
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Impulses carried toward cell body

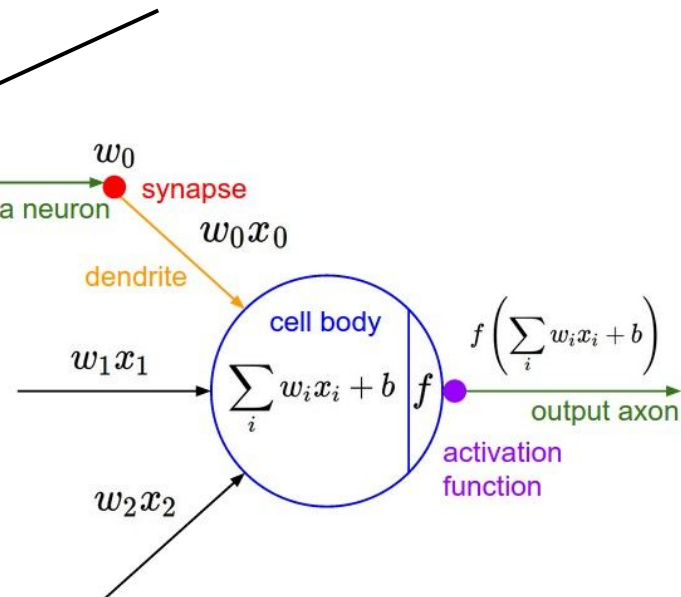


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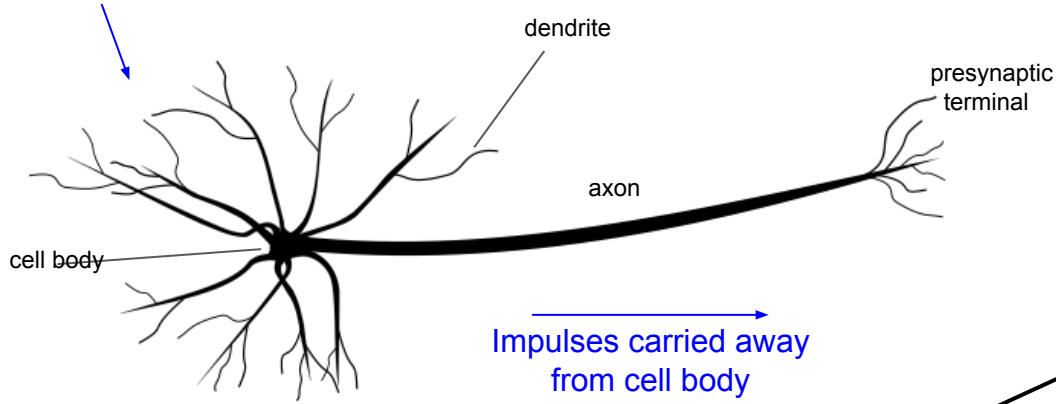


sigmoid activation function

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

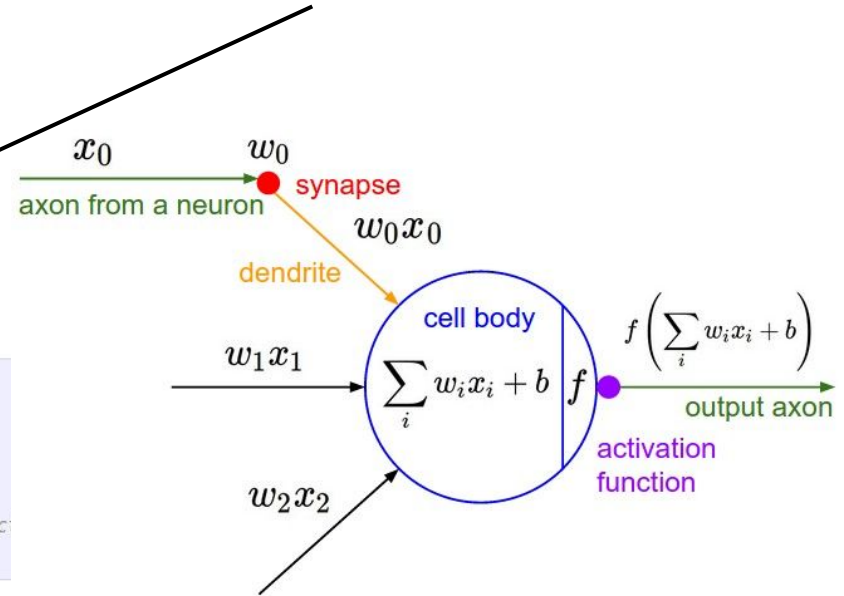


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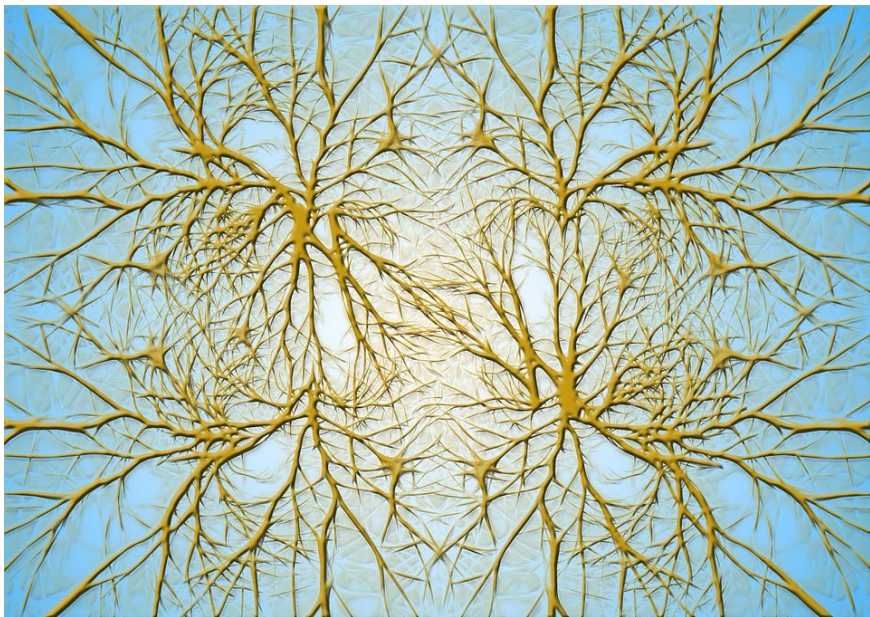


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is licensed under [CC-BY 3.0](https://creativecommons.org/licenses/by/3.0/)

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

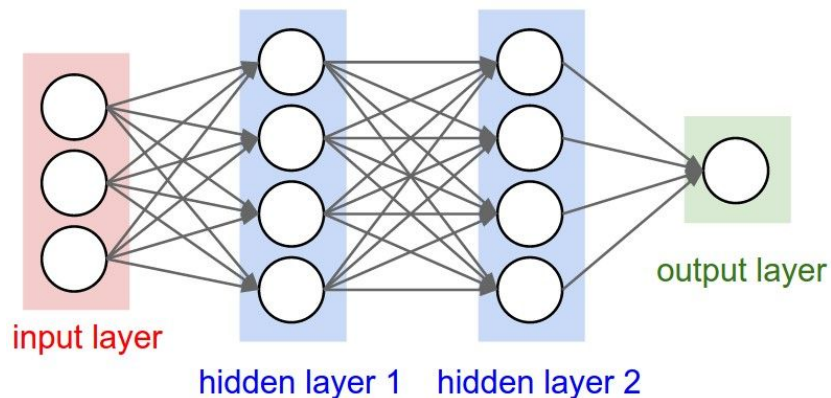


## Biological Neurons: Complex connectivity patterns



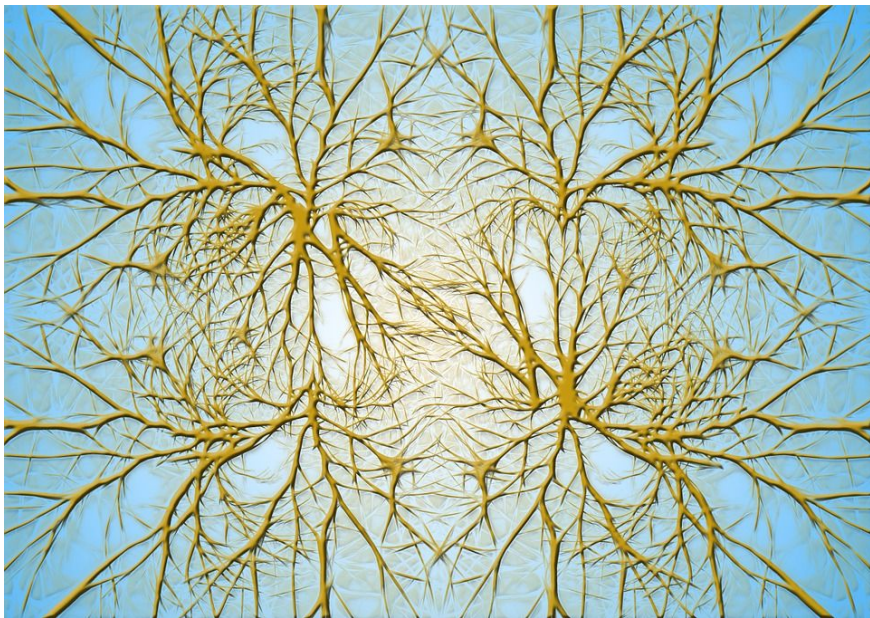
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## Neurons in a neural network: Organized into regular layers for computational efficiency



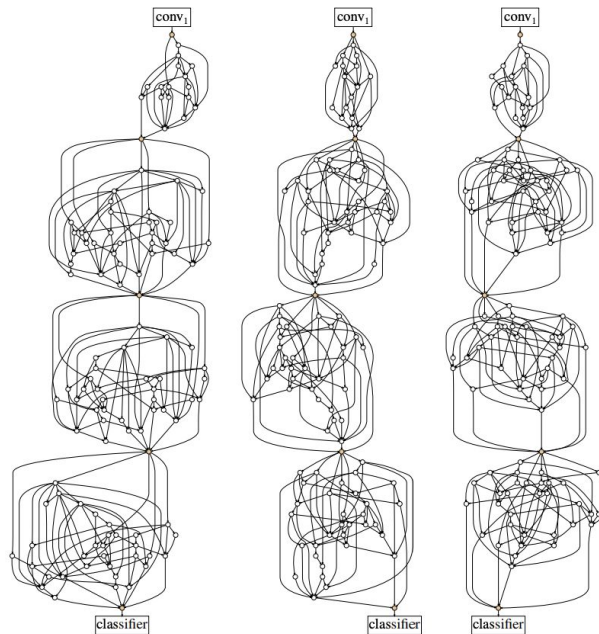


## Biological Neurons: Complex connectivity patterns



[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 Hausser]

Now let's calculate the  
analytical gradients

# Plugging in neural networks with loss functions

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

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

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

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



# Problem: How to compute gradients?

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

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

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

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

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

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

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

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

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

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

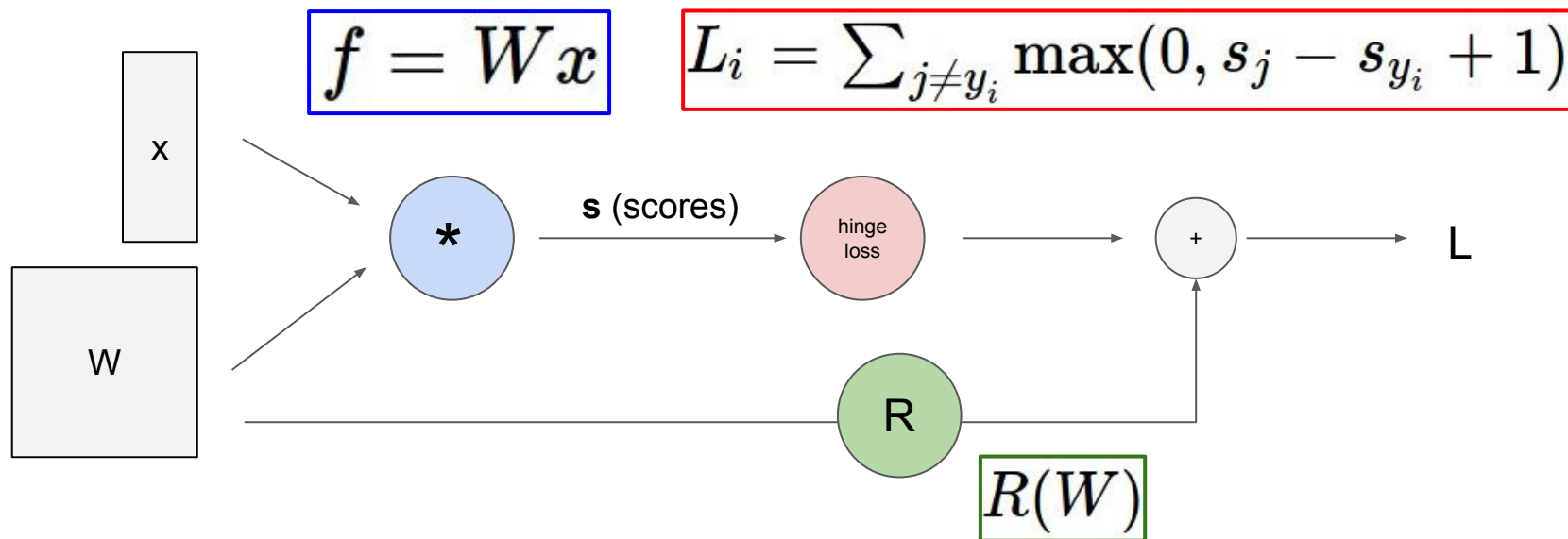
$$\nabla_W L = \nabla_W \left( \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

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

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

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

# Better Idea: Computational graphs + Backpropagation



# Convolutional network (AlexNet)

input image

weights

loss

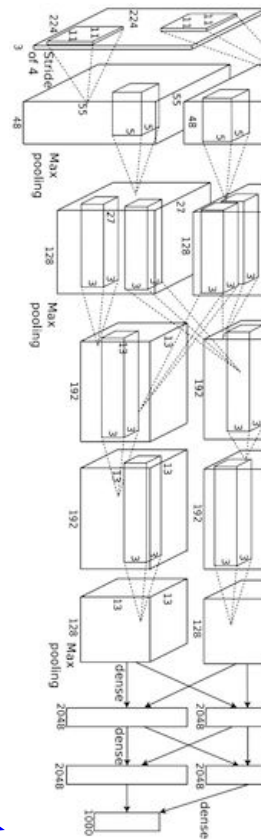


Figure copyright Alex Krizhevsky, Ilya Sutskever, and Geoffrey Hinton, 2012. Reproduced with permission.

# Really complex neural networks!!

input image

loss

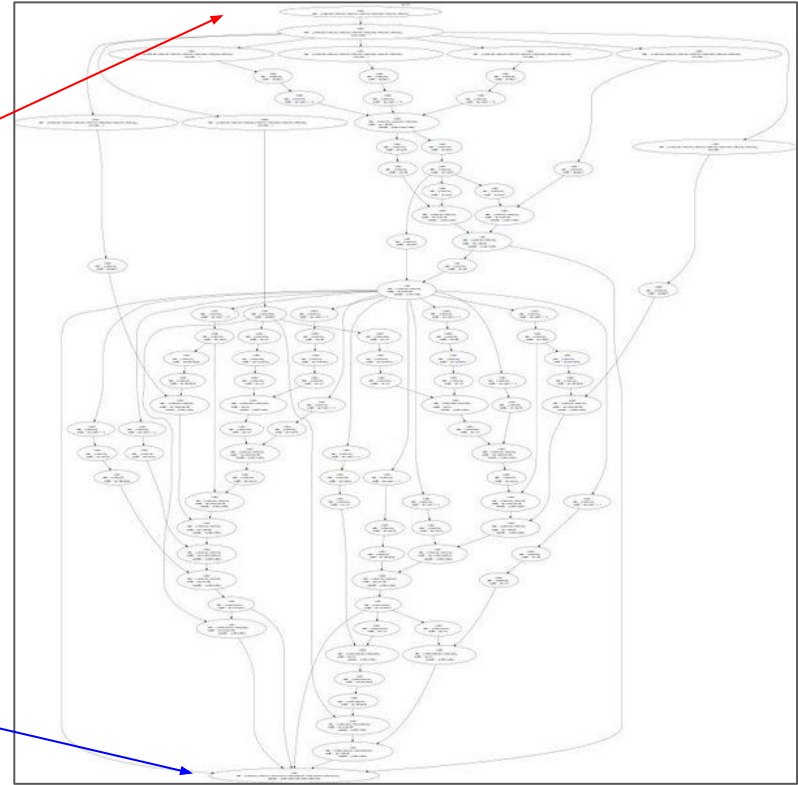


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

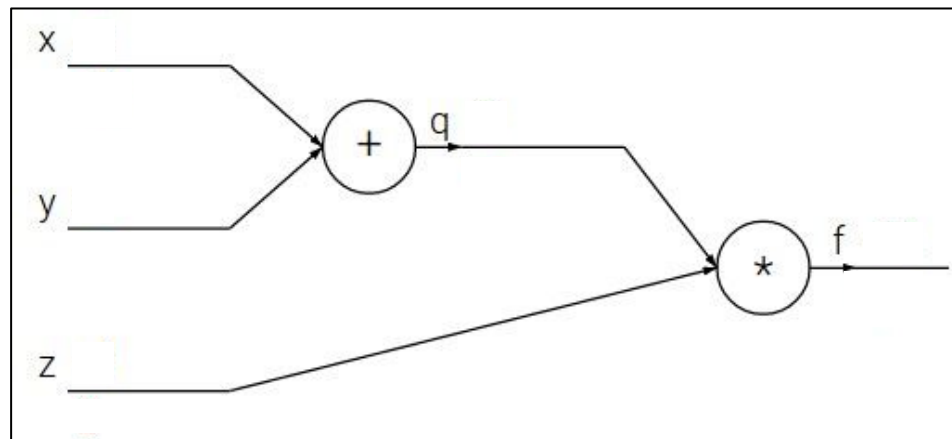
# Solution: Backpropagation

## Backpropagation: a simple example

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

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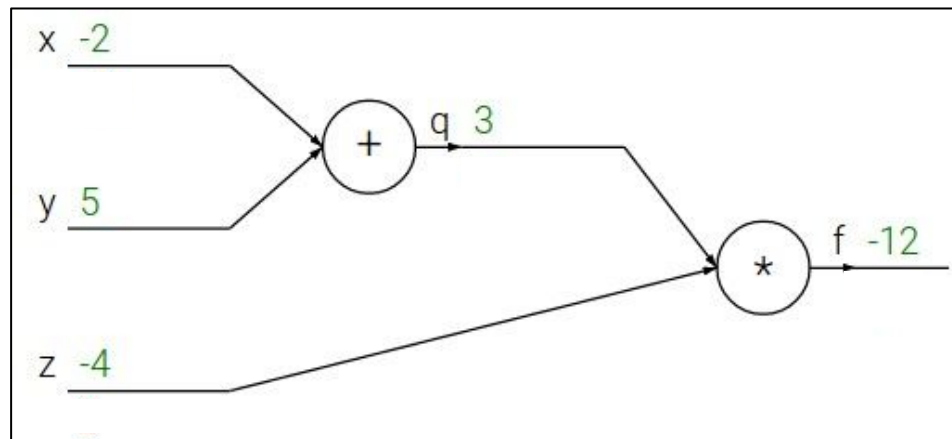




## Backpropagation: a simple example

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

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

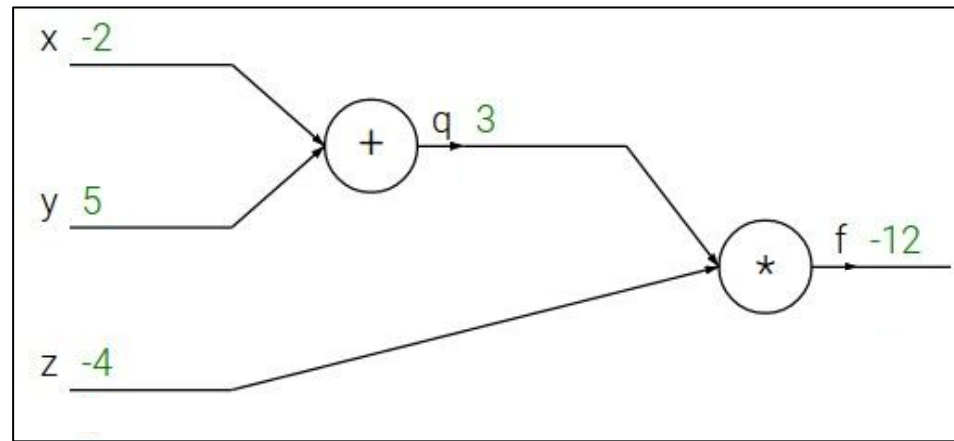


## Backpropagation: a simple example

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

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

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



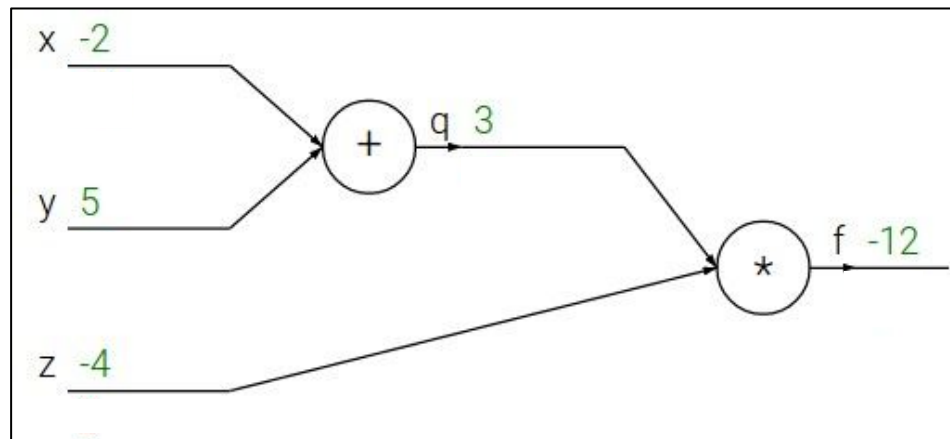
## Backpropagation: a simple example

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

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

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

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



## Backpropagation: a simple example

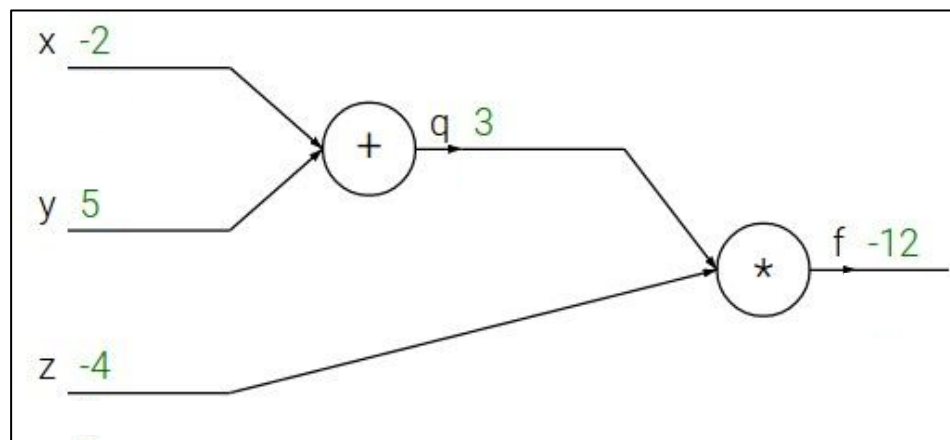
$$f(x, y, z) = (x + y)z$$

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

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

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

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



## Backpropagation: a simple example

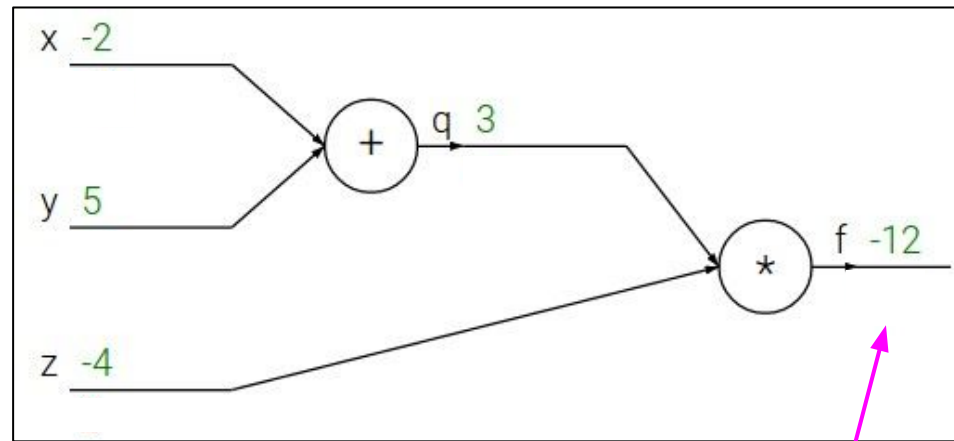
$$f(x, y, z) = (x + y)z$$

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

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

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

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



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

## Backpropagation: a simple example

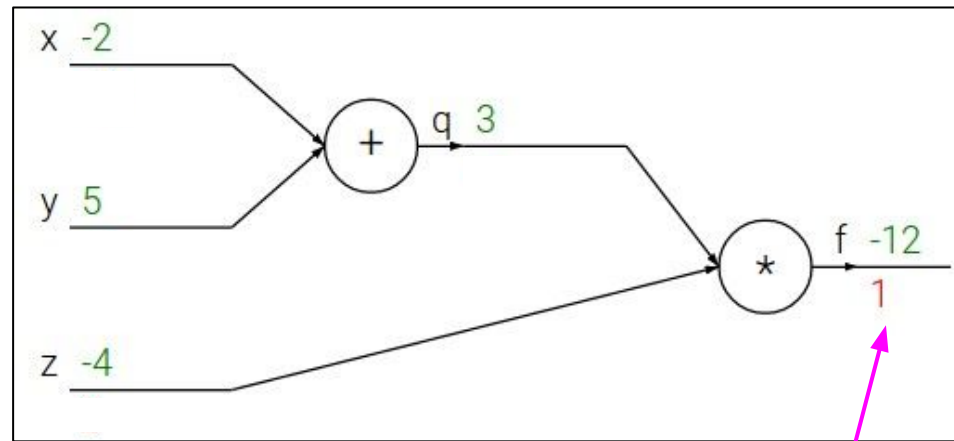
$$f(x, y, z) = (x + y)z$$

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

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

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

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



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

## Backpropagation: a simple example

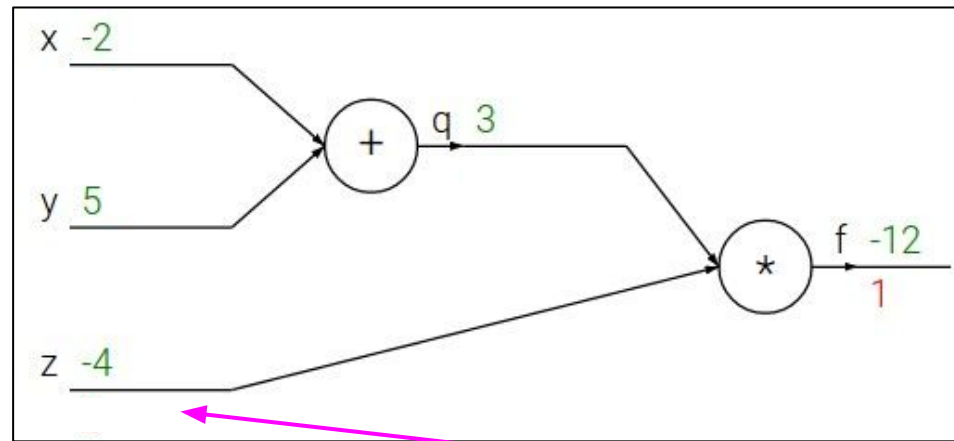
$$f(x, y, z) = (x + y)z$$

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

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

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

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



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

## Backpropagation: a simple example

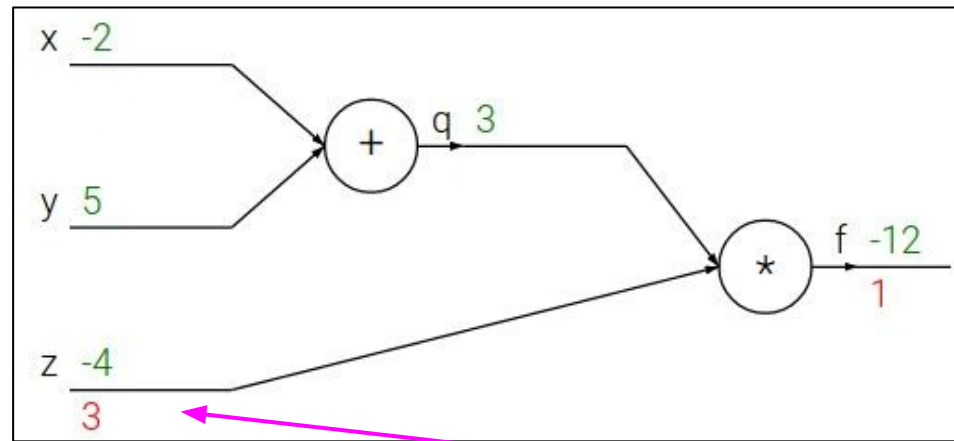
$$f(x, y, z) = (x + y)z$$

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

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

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

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



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



## Backpropagation: a simple example

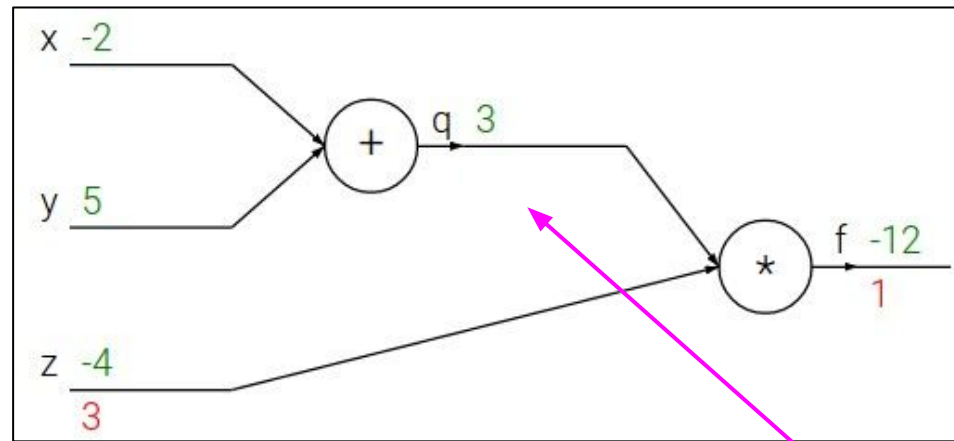
$$f(x, y, z) = (x + y)z$$

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

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

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

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



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

## Backpropagation: a simple example

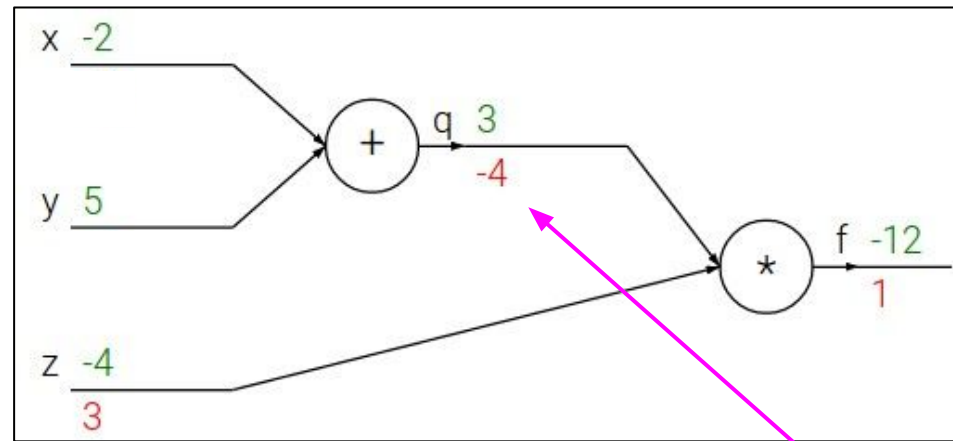
$$f(x, y, z) = (x + y)z$$

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

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



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

# Backpropagation: a simple example

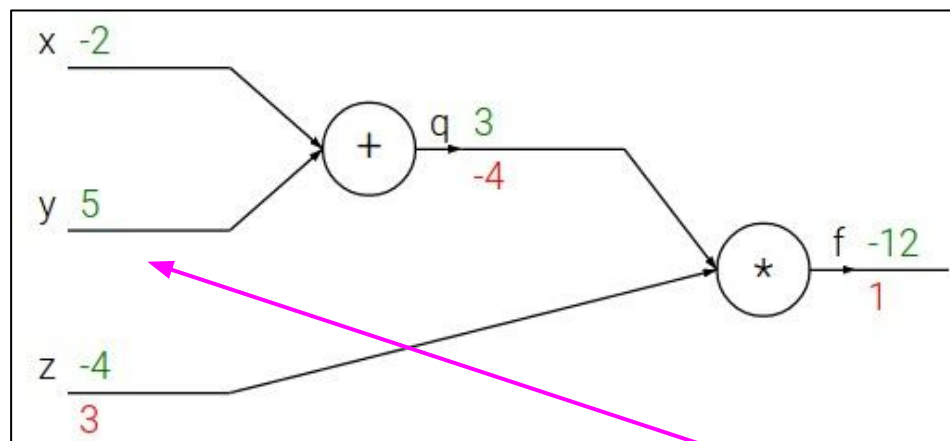
$$f(x, y, z) = (x + y)z$$

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

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

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

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



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

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

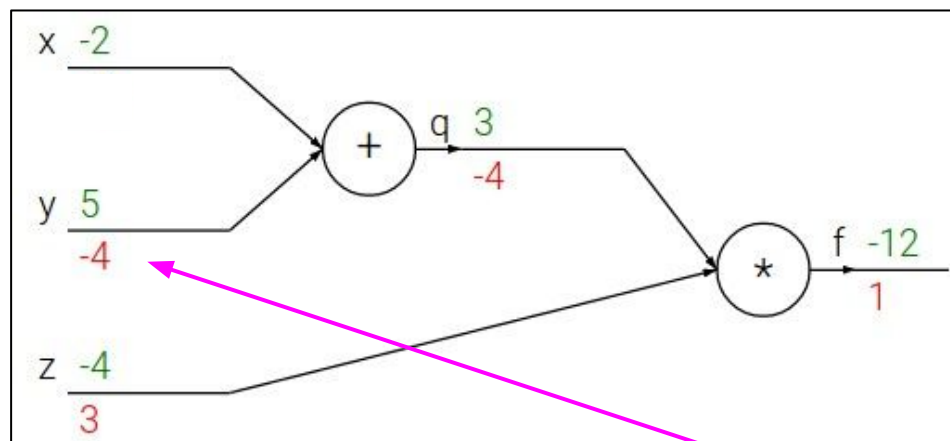
$$f(x, y, z) = (x + y)z$$

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

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

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



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

Chain rule:

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

Upstream  
gradient

Local  
gradient

## Backpropagation: a simple example

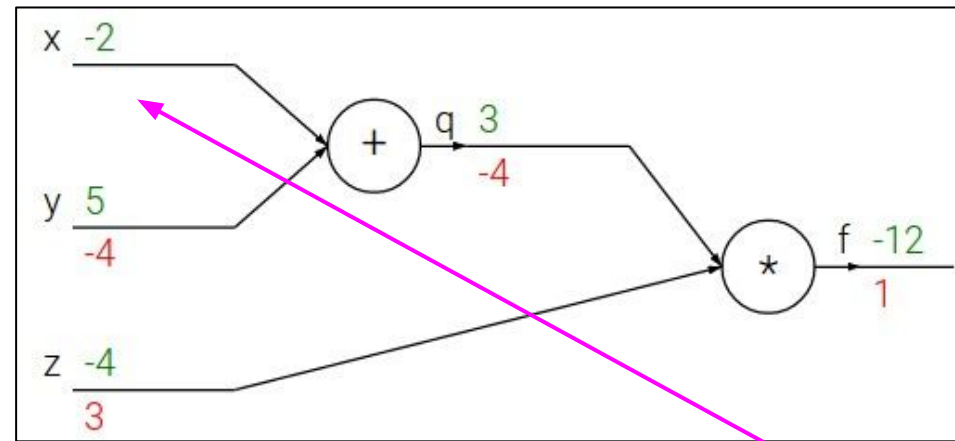
$$f(x, y, z) = (x + y)z$$

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

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

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

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



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

Chain rule:

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

Upstream  
gradient

Local  
gradient

## Backpropagation: a simple example

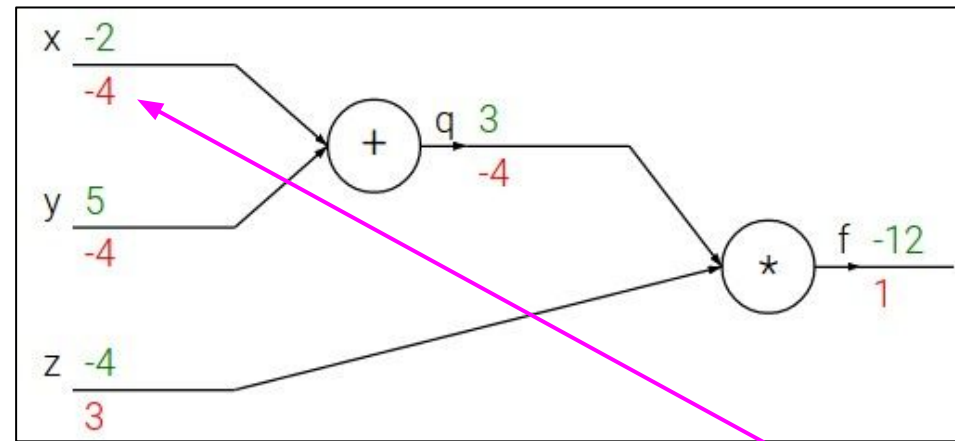
$$f(x, y, z) = (x + y)z$$

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

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

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

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



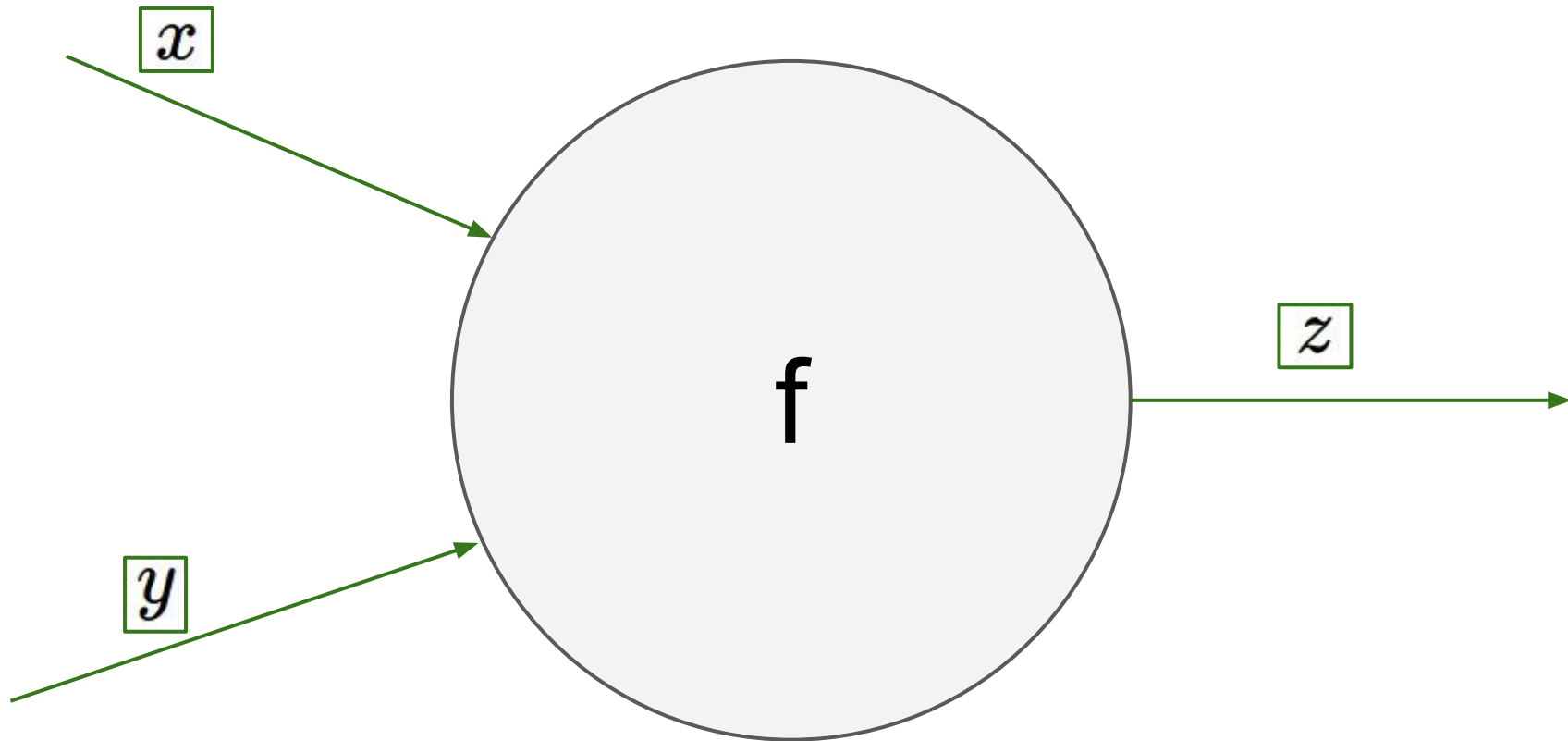
$$\frac{\partial f}{\partial x}$$

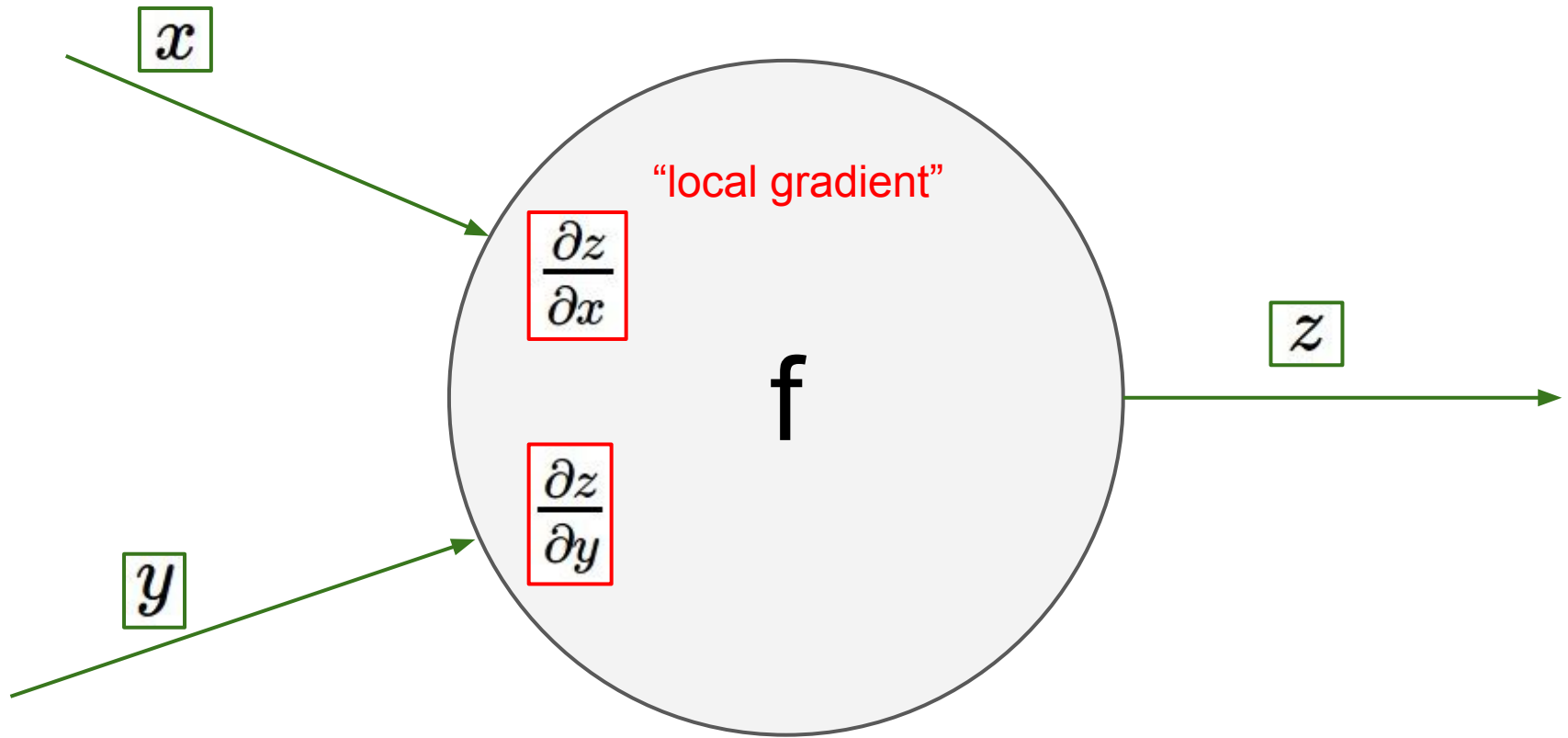
Chain rule:

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

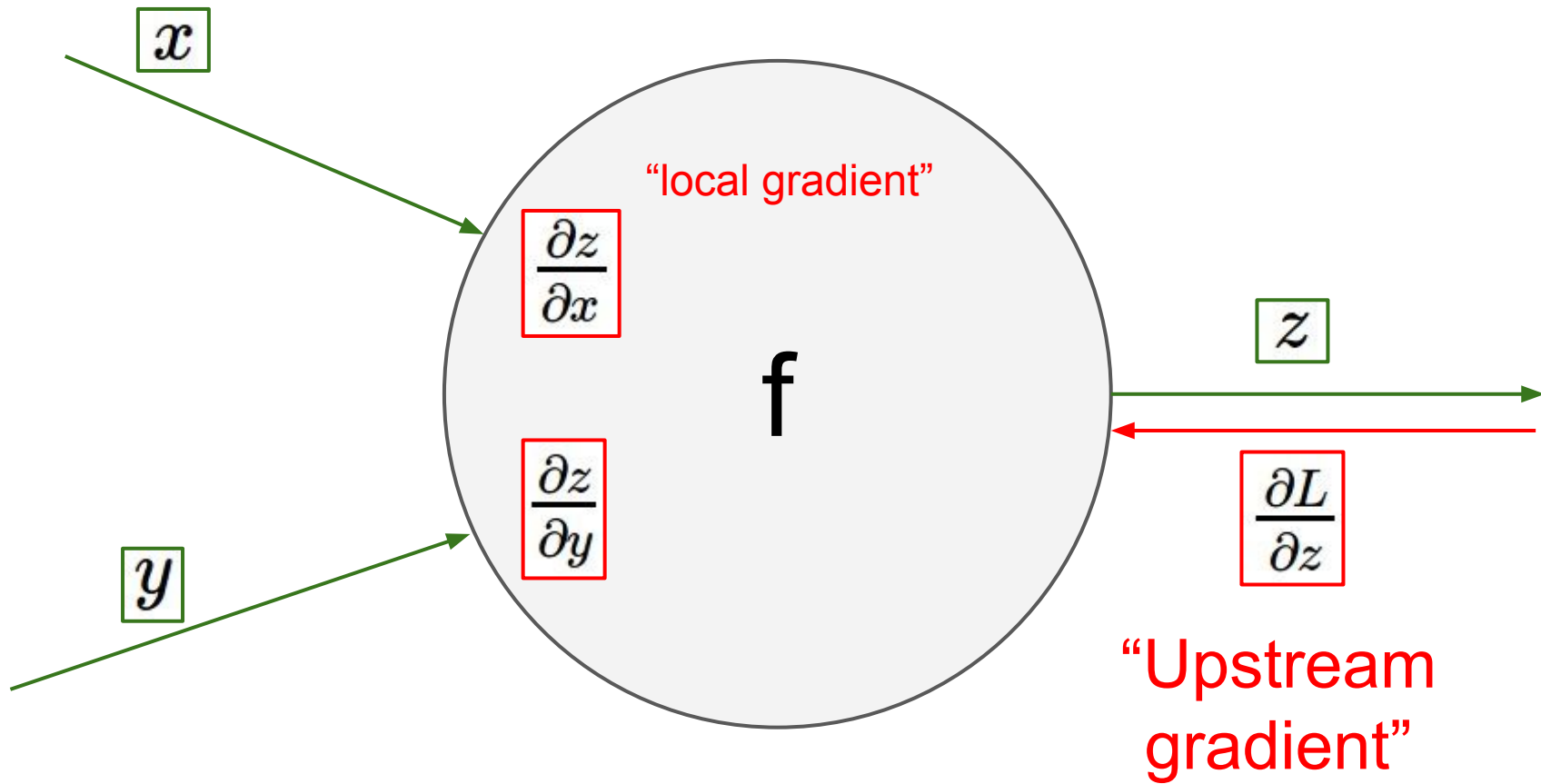
Upstream  
gradient

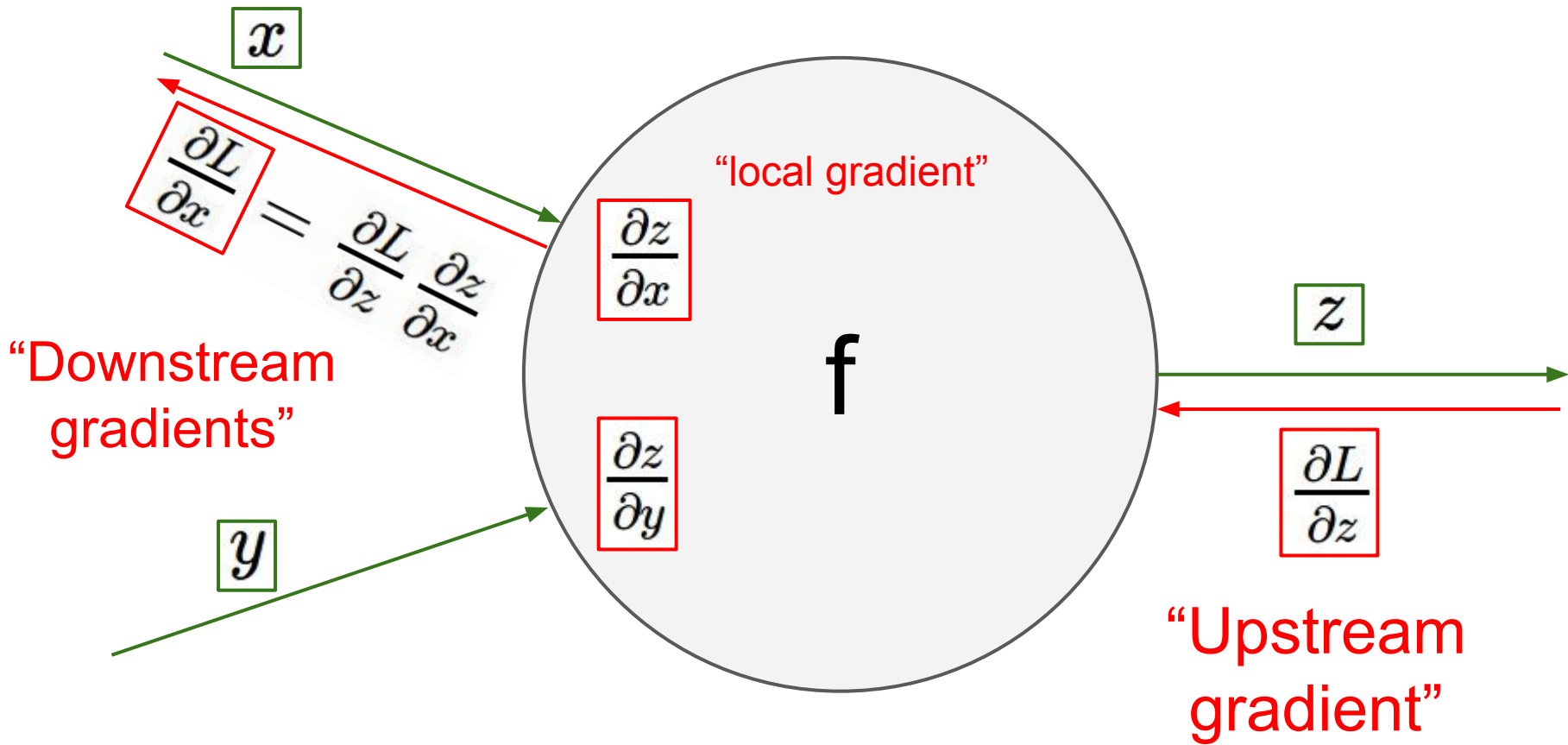
Local  
gradient

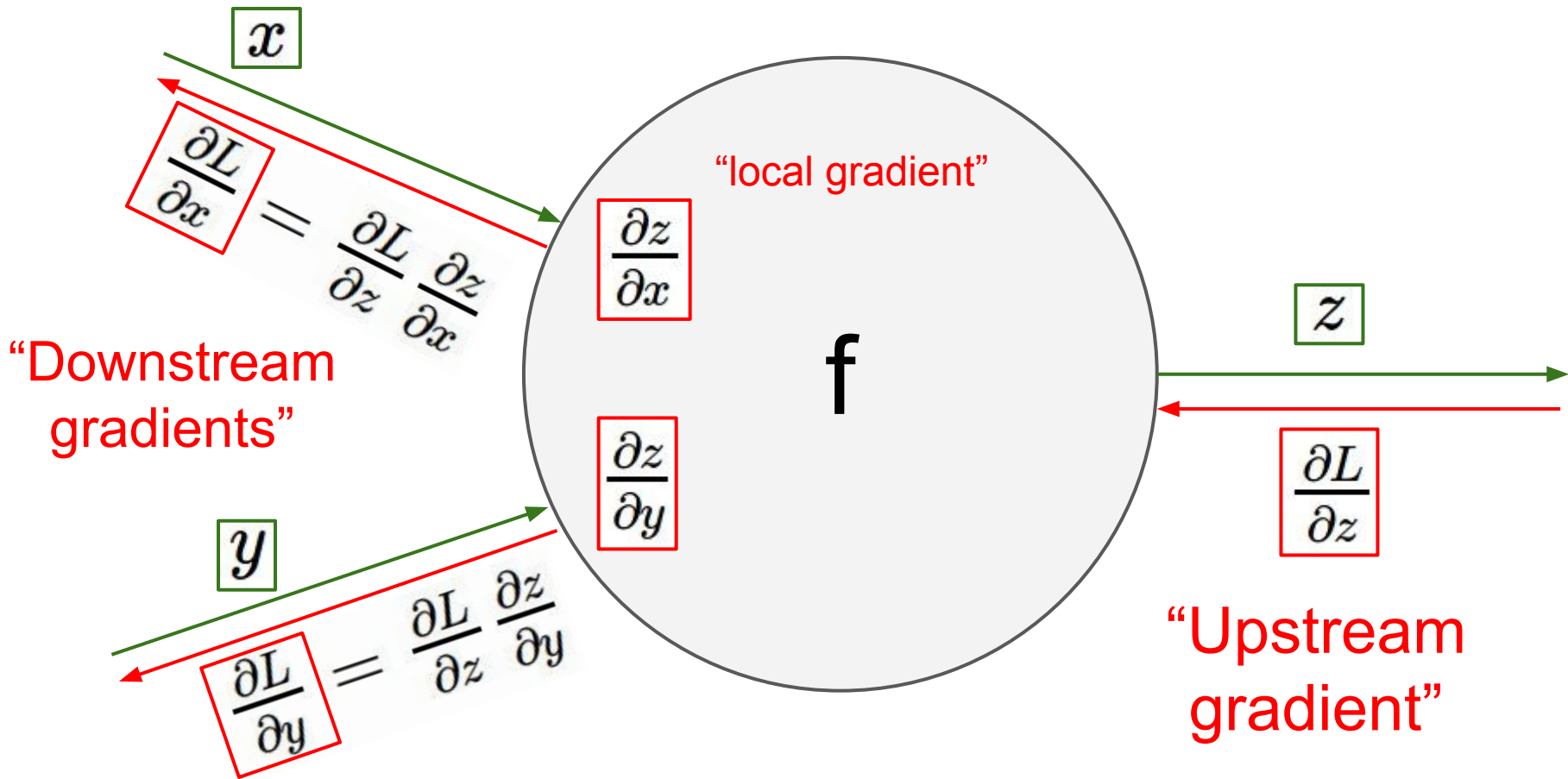


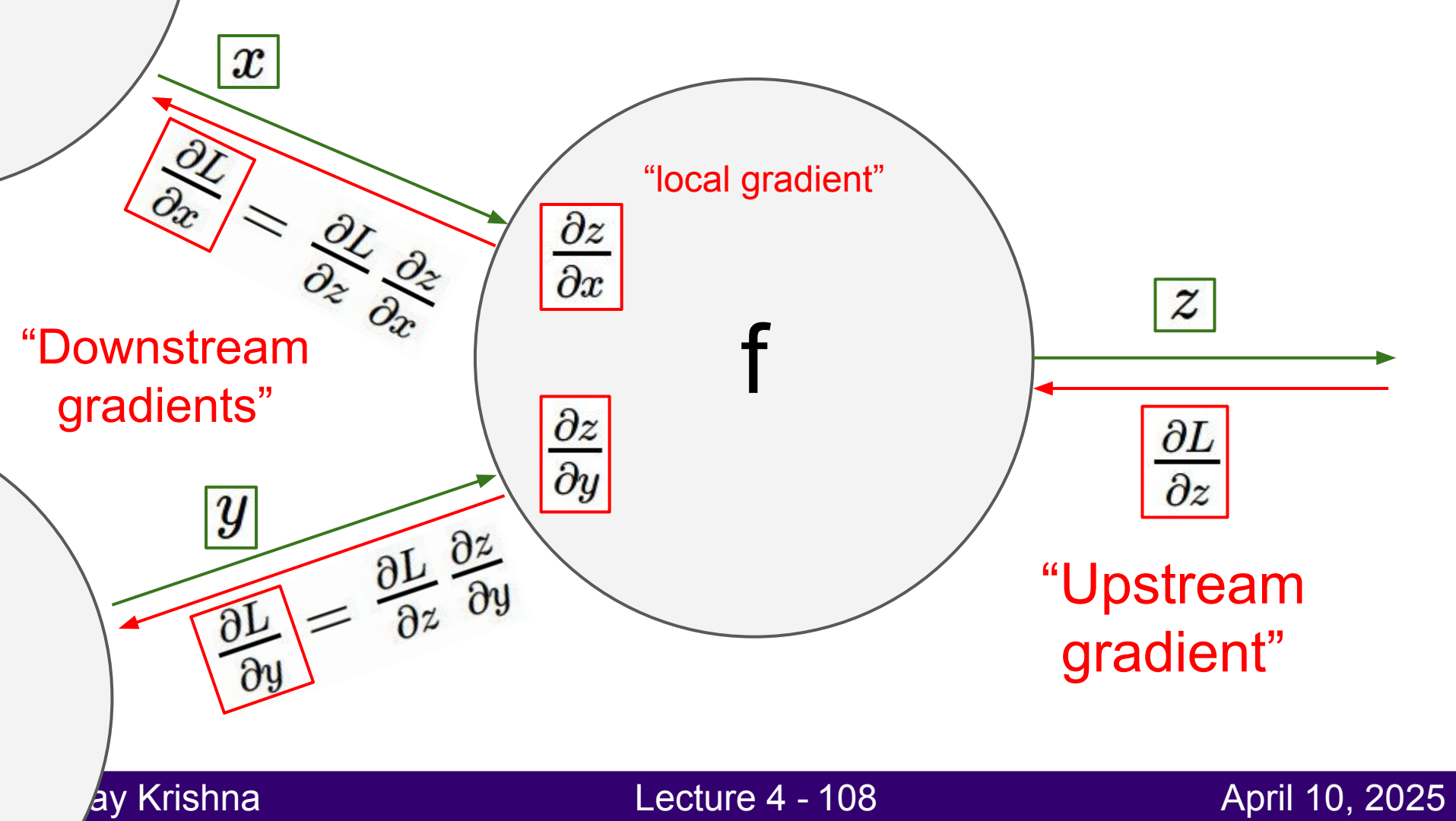




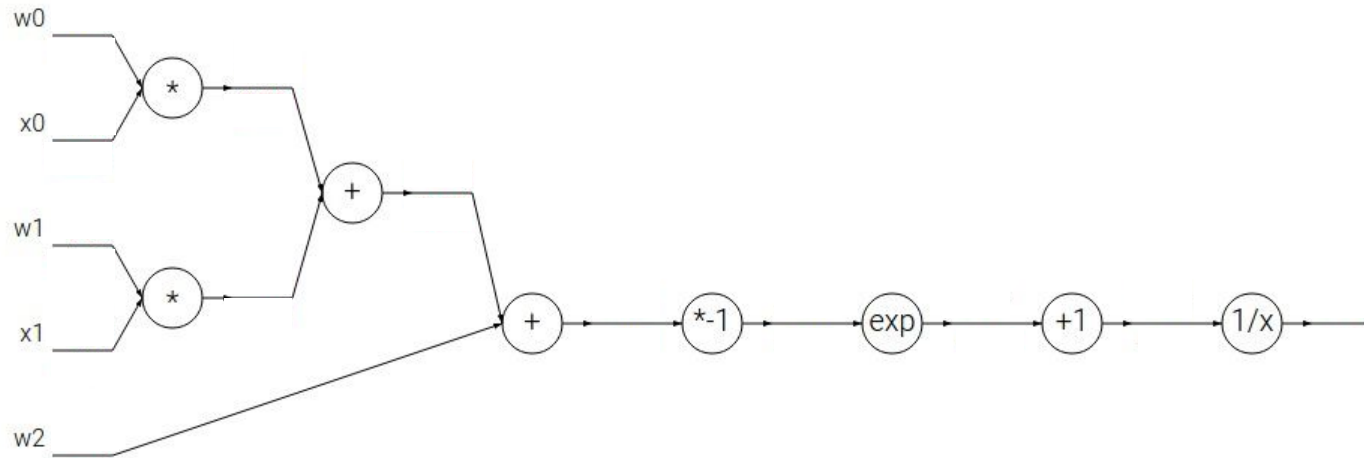




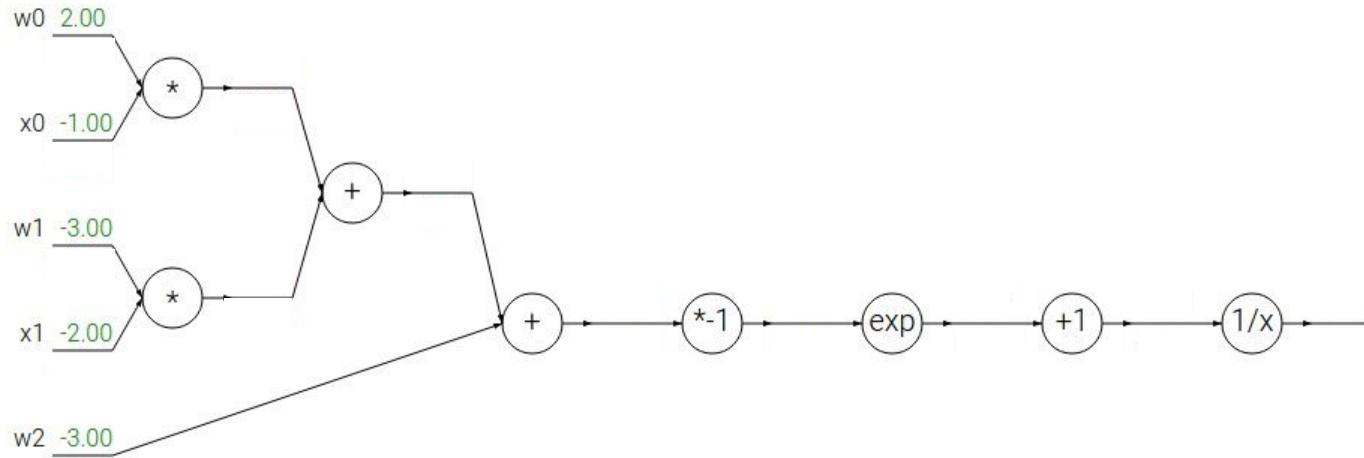




Another example:  $f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$

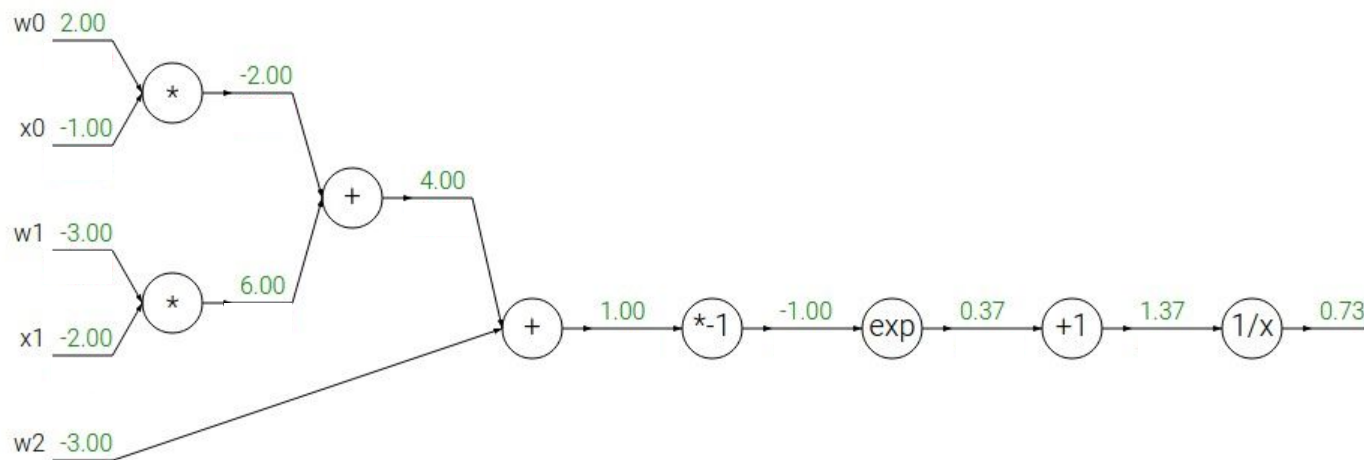


Another example:  $f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$



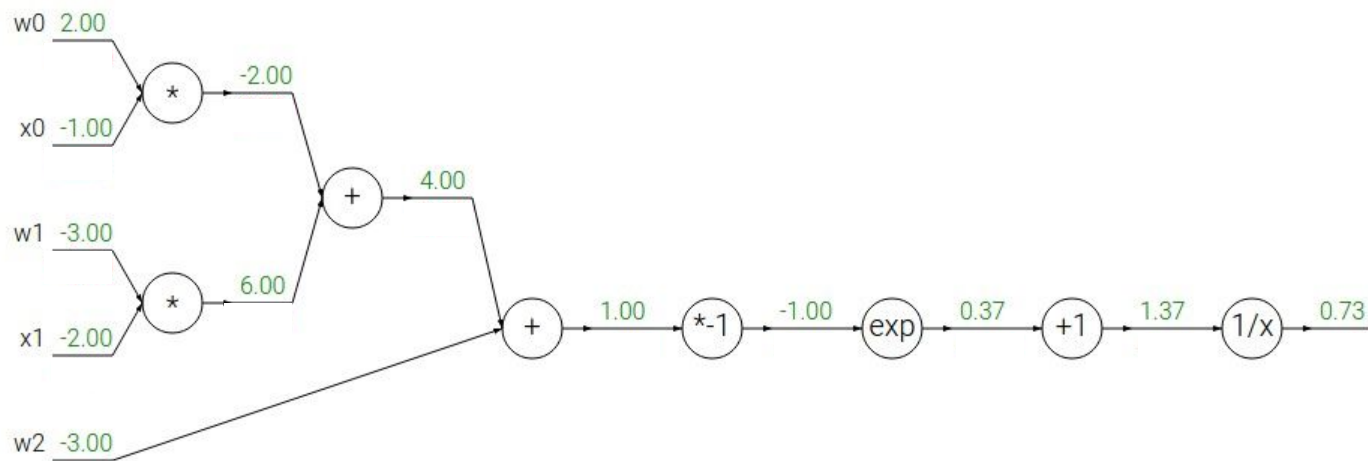
Another example:

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



Another example:

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



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

→

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

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

→

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

$$f_a(x) = ax$$

→

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

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

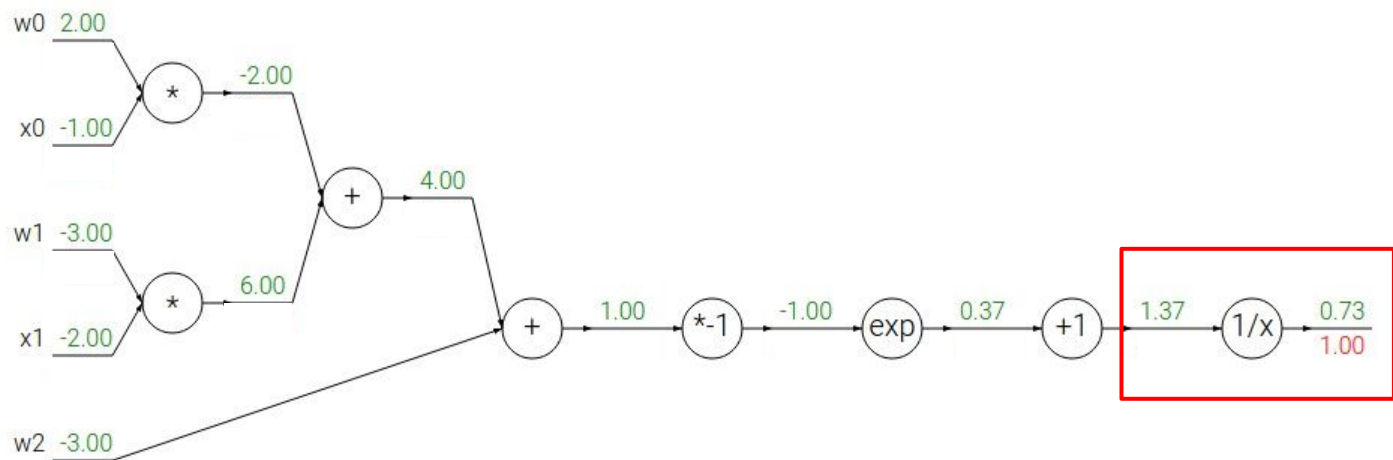
→

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



Another example:

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



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

→

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

$$f_a(x) = ax$$

→

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

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

→

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

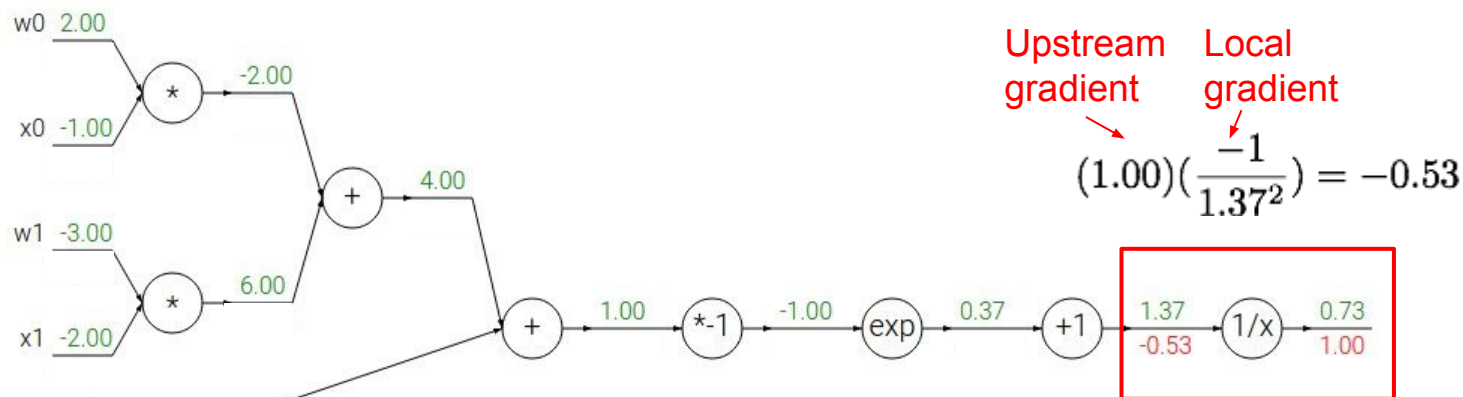
$$f_c(x) = c + x$$

→

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

Another example:

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



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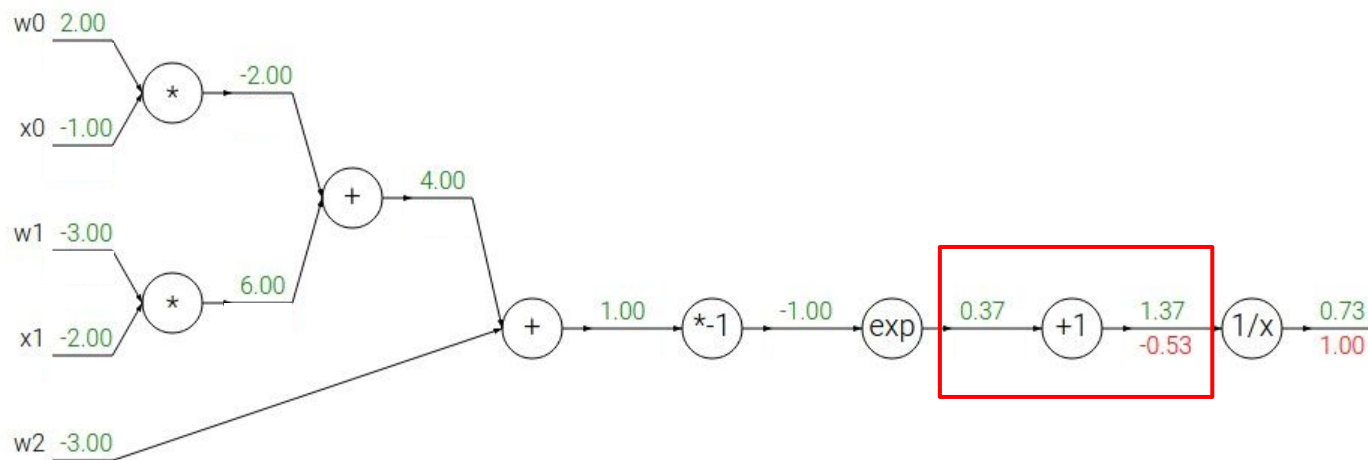
$$f_c(x) = c + x$$

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

Another example:

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



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

$$f_a(x) = ax$$

→

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

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

→

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

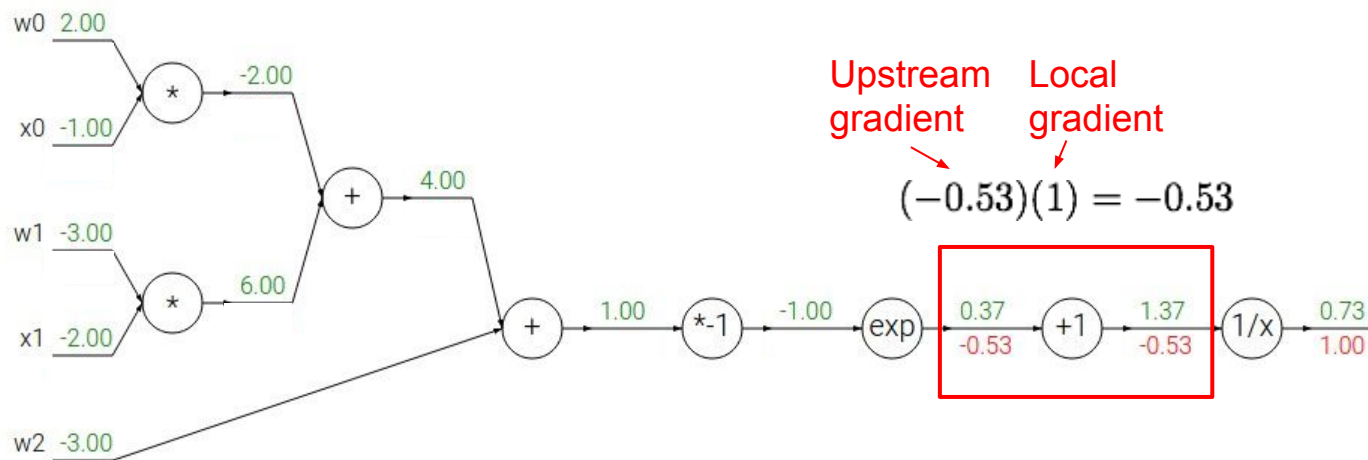
$$f_c(x) = c + x$$

→

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

Another example:

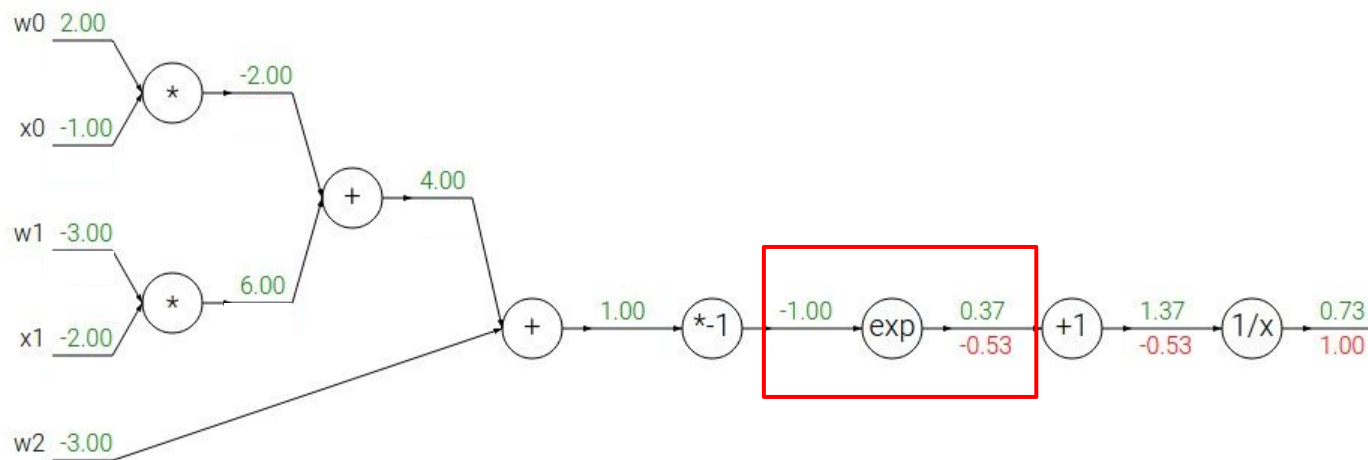
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

Another example:

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



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

→

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

$$f_a(x) = ax$$

→

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

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

→

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

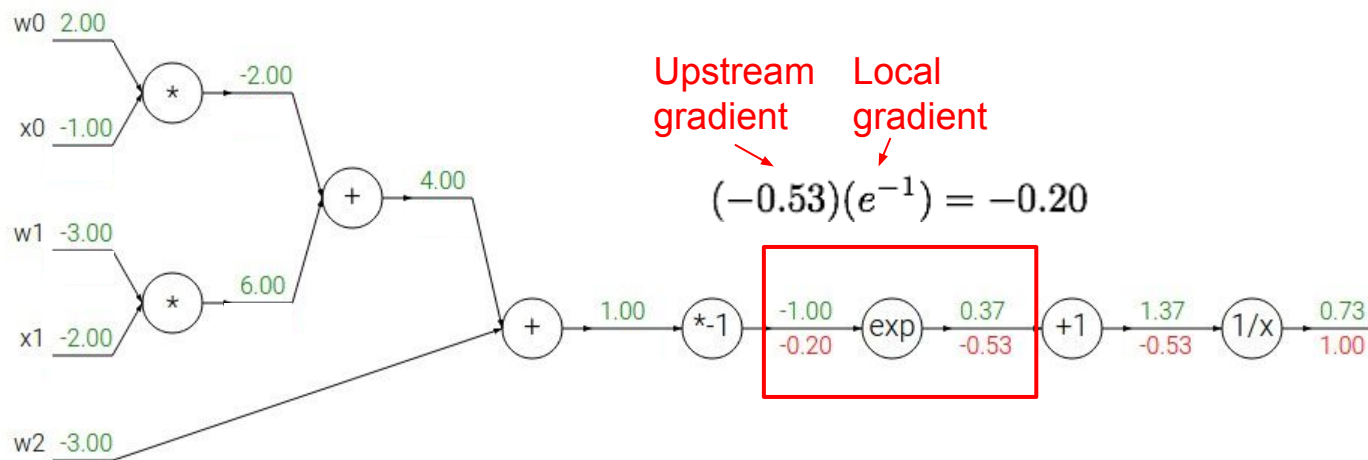
$$f_c(x) = c + x$$

→

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

Another example:

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



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

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

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

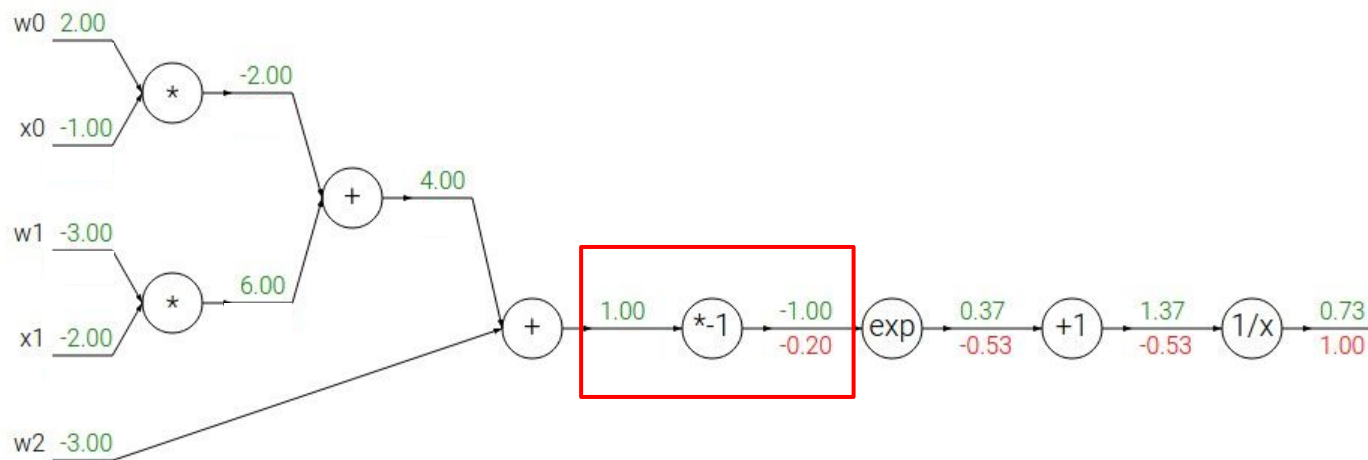
$$f_c(x) = c + x$$

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

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

Another example:

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



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

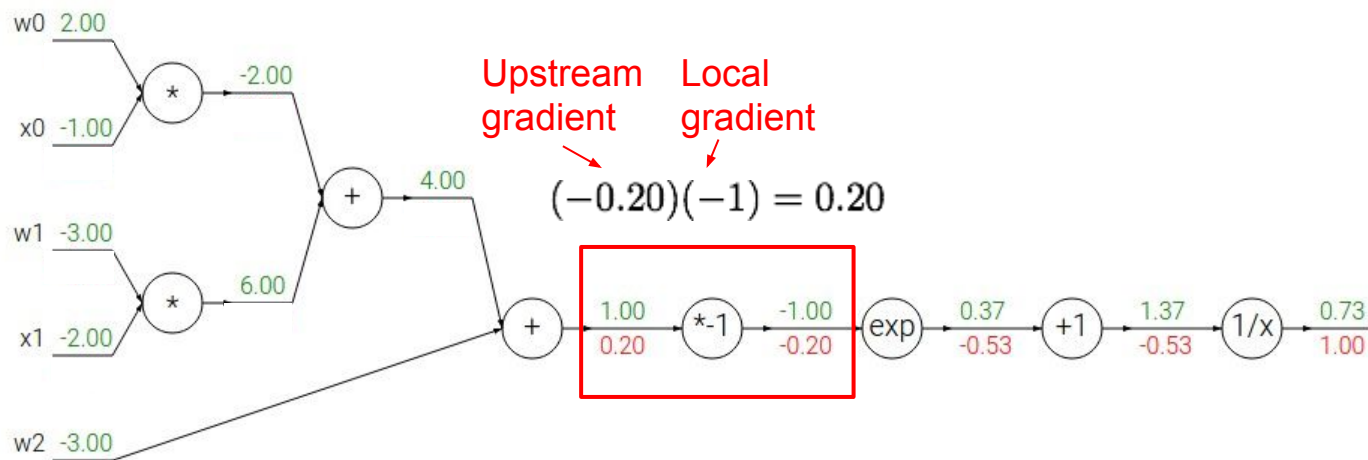
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



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

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

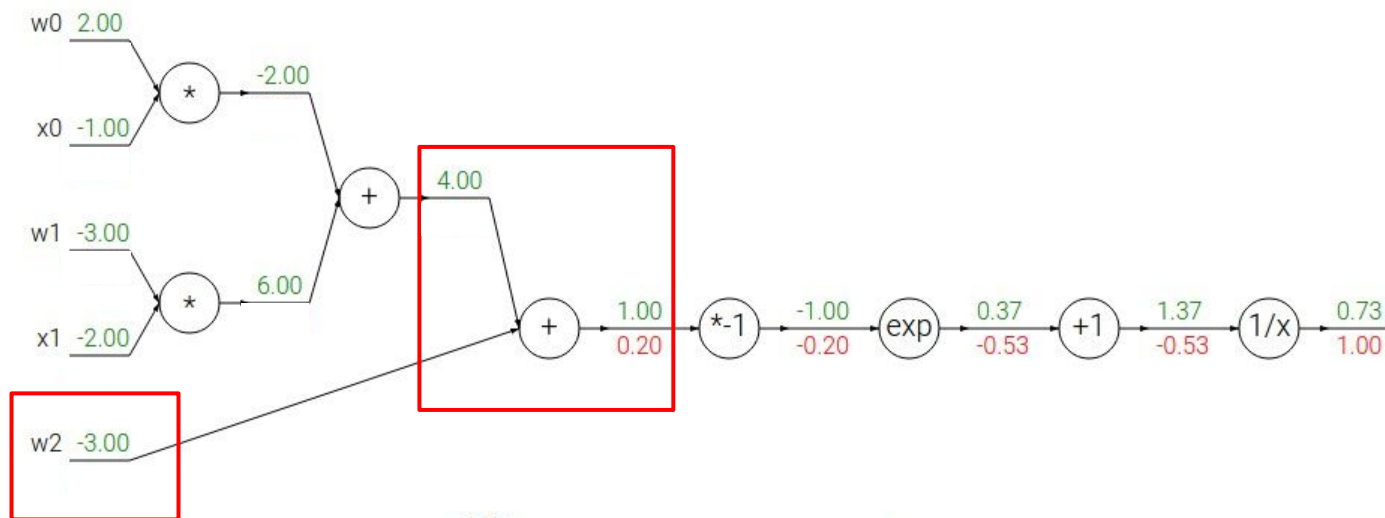
$$f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$$

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



Another example:

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



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

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

$$f_a(x) = ax$$

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

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

→

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

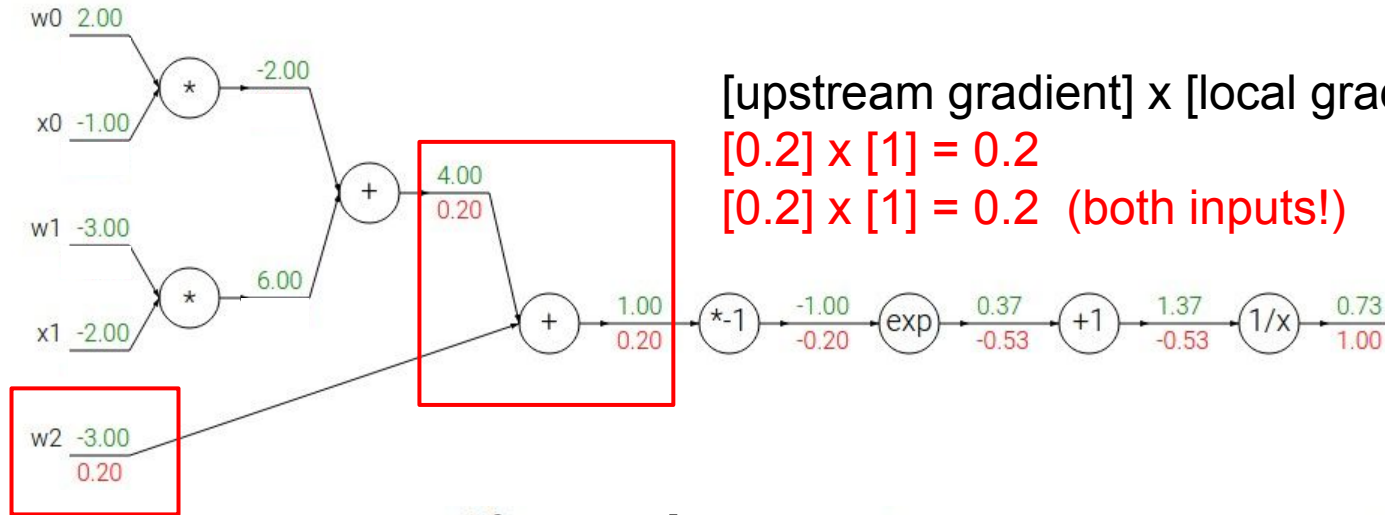
$$f_c(x) = c + x$$

→

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

Another example:

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



[upstream gradient] x [local gradient]

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

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

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

→

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

$$f_a(x) = ax$$

→

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

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

→

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

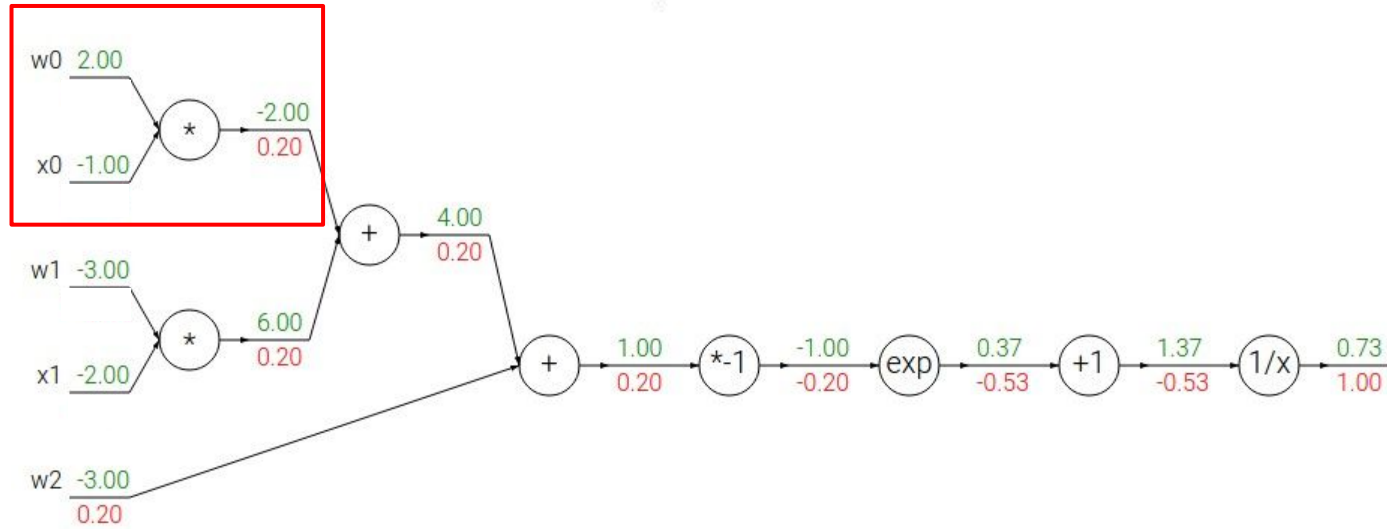
$$f_c(x) = c + x$$

→

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

Another example:

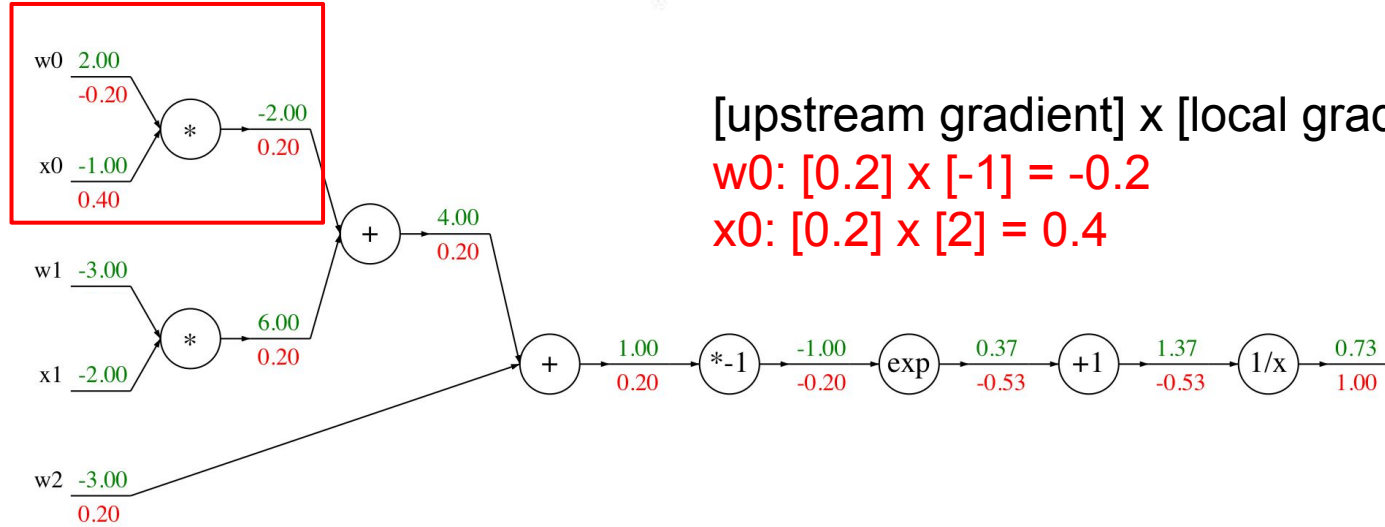
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

Another example:

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



[upstream gradient] x [local gradient]

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

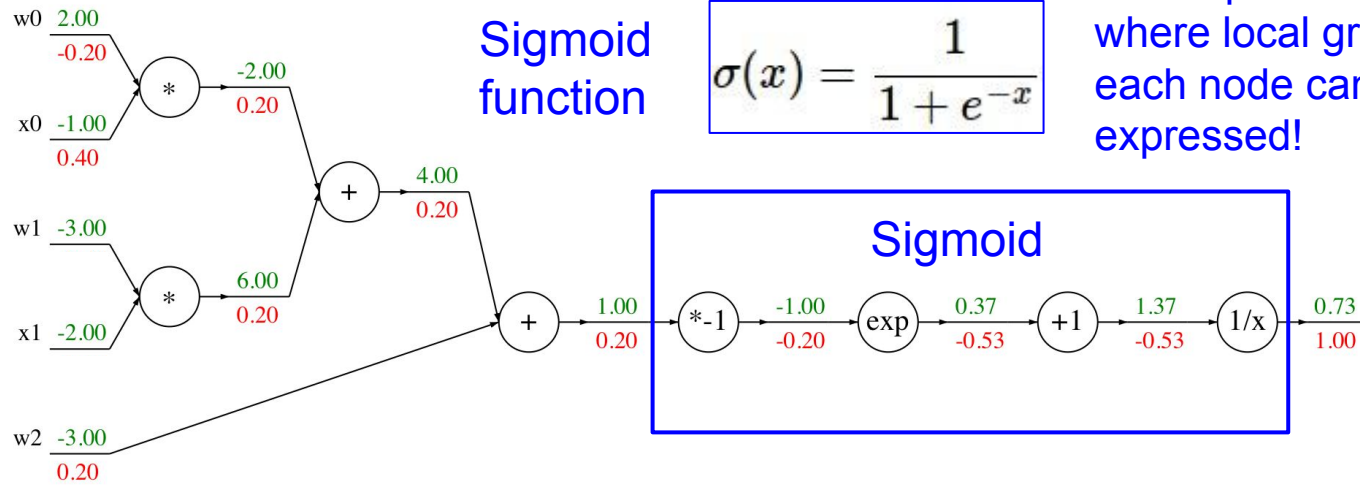
$$x_0: [0.2] \times [2] = 0.4$$

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

Another example:

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

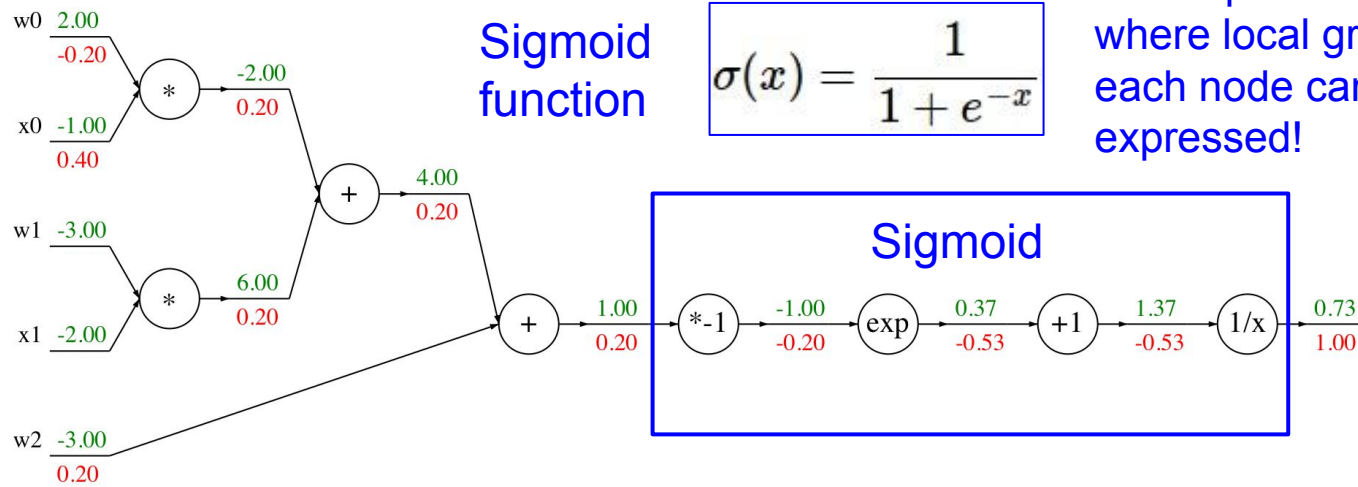
Computational graph representation may not be unique. Choose one where local gradients at each node can be easily expressed!



Another example:

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

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



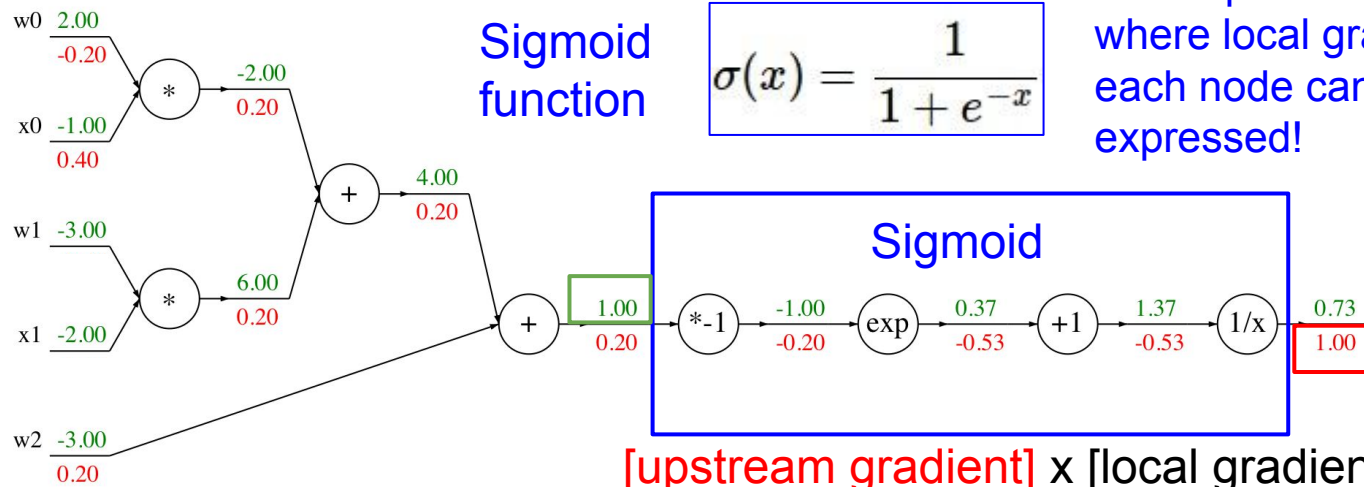
Sigmoid local gradient:

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

Another example:

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

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



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

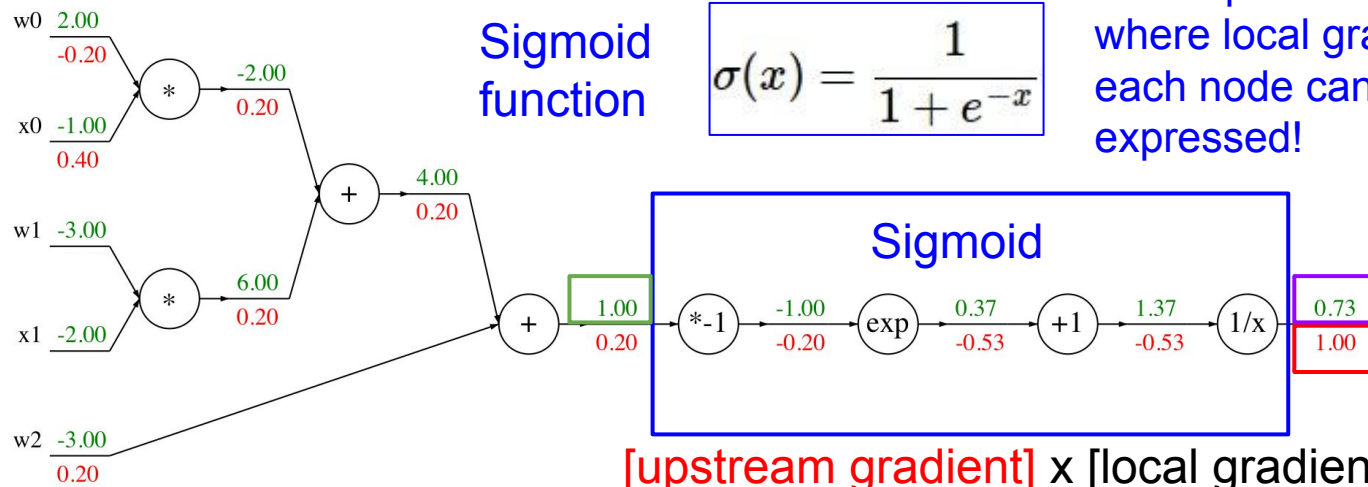
Sigmoid local gradient:

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

Another example:

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

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



Sigmoid function

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

Sigmoid

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

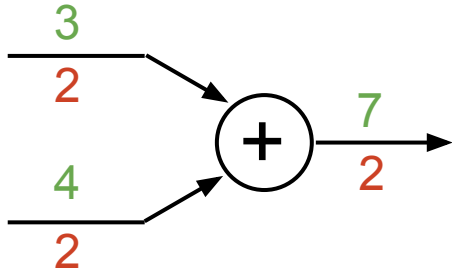
Sigmoid local gradient:

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



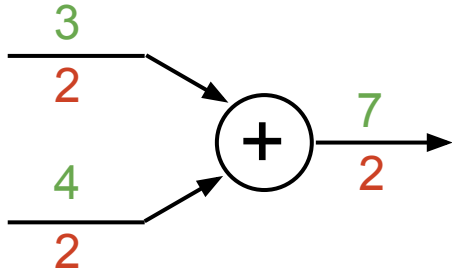
# Patterns in gradient flow

**add** gate: gradient distributor

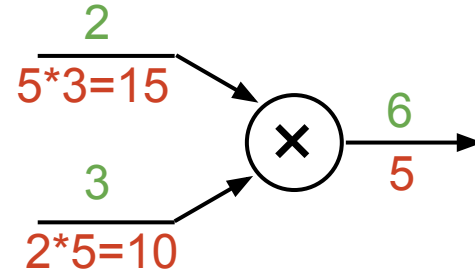


# Patterns in gradient flow

**add** gate: gradient distributor

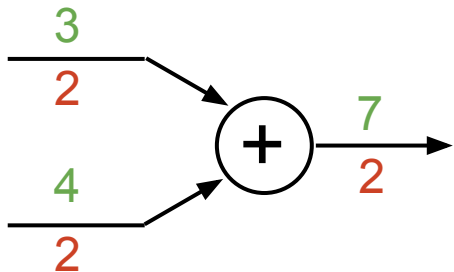


**mul** gate: “swap multiplier”

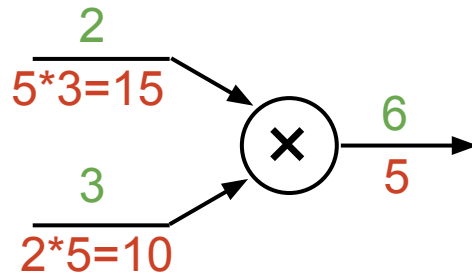


# Patterns in gradient flow

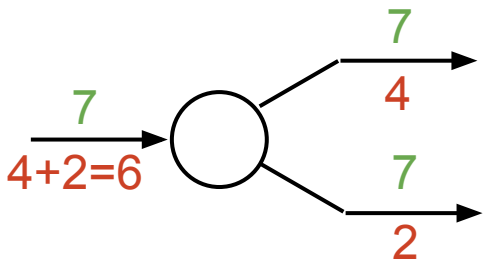
**add** gate: gradient distributor



**mul** gate: “swap multiplier”

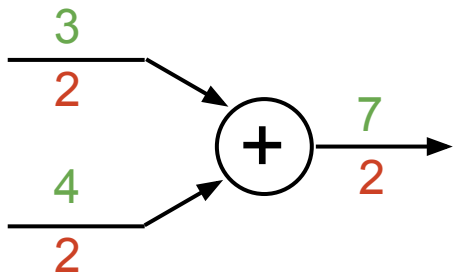


**copy** gate: gradient adder

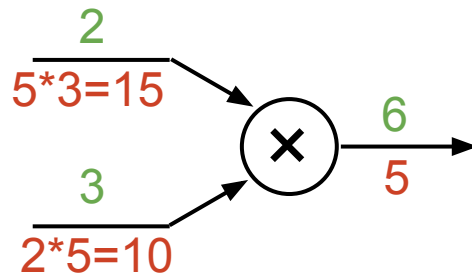


# Patterns in gradient flow

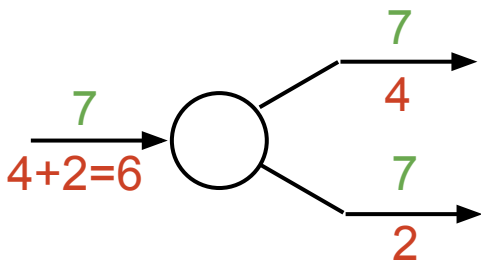
**add** gate: gradient distributor



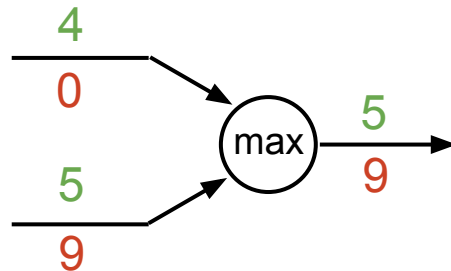
**mul** gate: “swap multiplier”



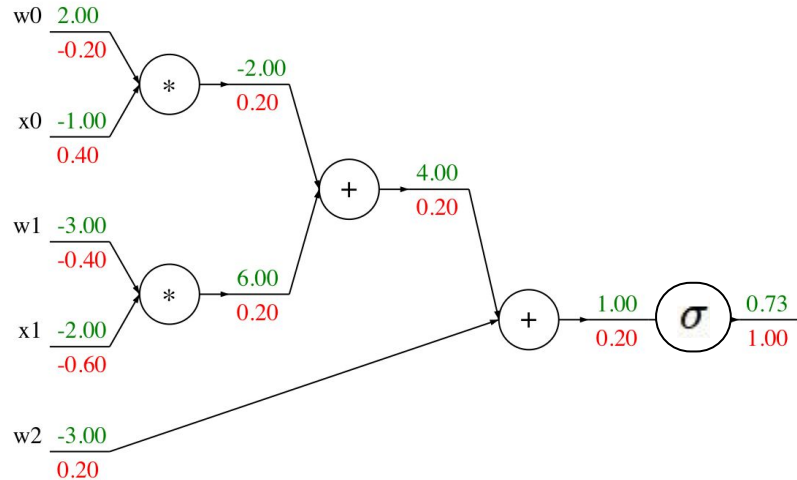
**copy** gate: gradient adder



**max** gate: gradient router



# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

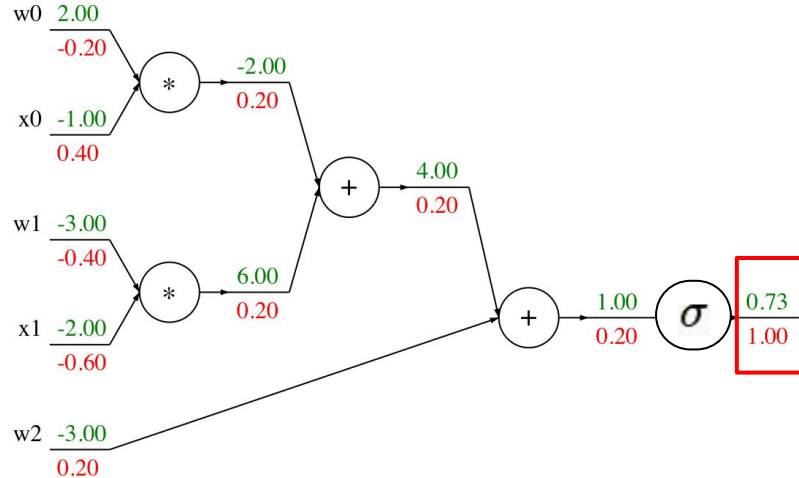
```
def f(w0, x0, w1, x1, w2):
```

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

Backward pass:  
Compute grads

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

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

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

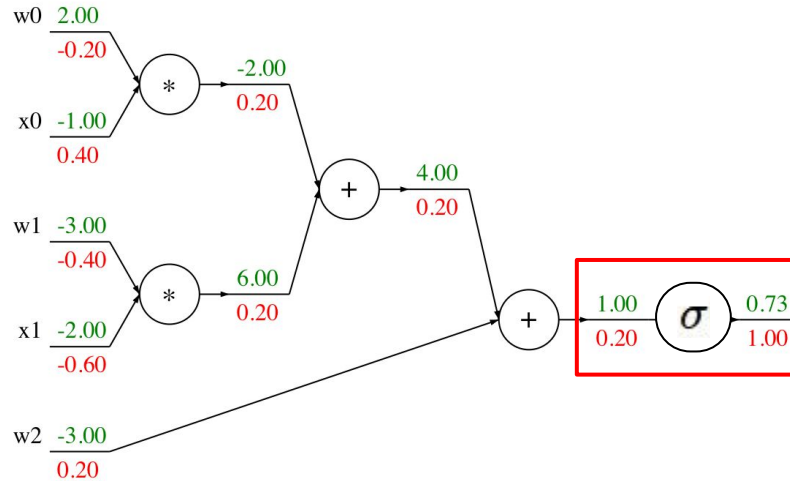
```
    s0 = w0 * x0
    s1 = w1 * x1
    s2 = s0 + s1
    s3 = s2 + w2
    L = sigmoid(s3)
```

Base case

```
    grad_L = 1.0
```

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

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

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

```
    s0 = w0 * x0
```

```
    s1 = w1 * x1
```

```
    s2 = s0 + s1
```

```
    s3 = s2 + w2
```

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

Sigmoid

```
    grad_L = 1.0
```

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

```
    grad_w2 = grad_s3
```

```
    grad_s2 = grad_s3
```

```
    grad_s0 = grad_s2
```

```
    grad_s1 = grad_s2
```

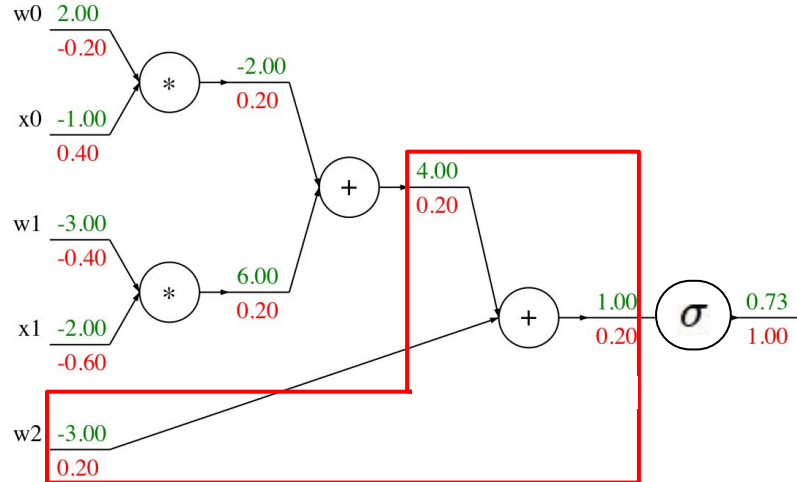
```
    grad_w1 = grad_s1 * x1
```

```
    grad_x1 = grad_s1 * w1
```

```
    grad_w0 = grad_s0 * x0
```

```
    grad_x0 = grad_s0 * w0
```

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

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

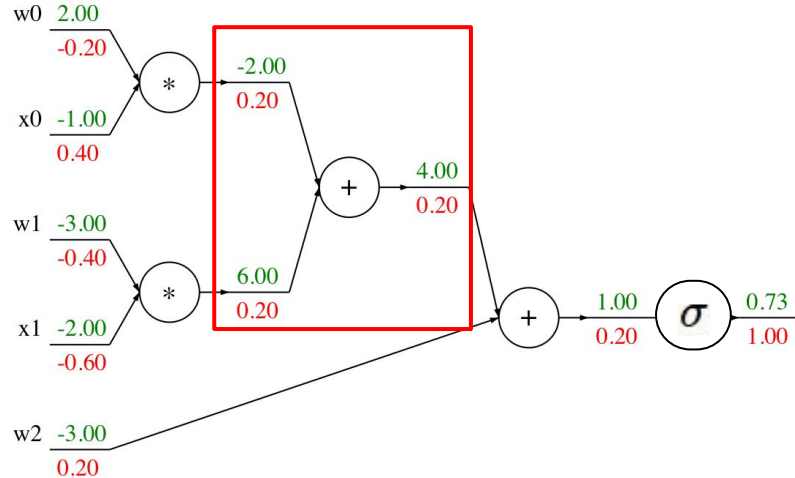
```
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

Add gate

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



# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

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

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

```
    grad_L = 1.0
```

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

```
    grad_w2 = grad_s3
```

```
    grad_s2 = grad_s3
```

```
    grad_s0 = grad_s2
```

```
    grad_s1 = grad_s2
```

```
    grad_w1 = grad_s1 * x1
```

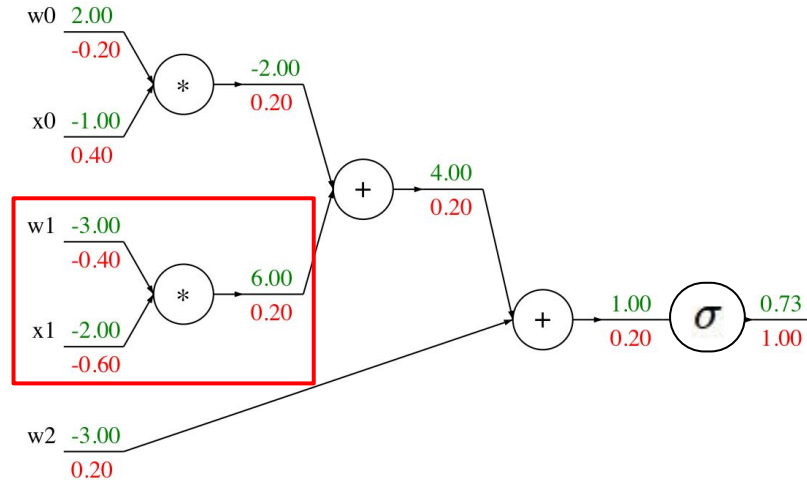
```
    grad_x1 = grad_s1 * w1
```

```
    grad_w0 = grad_s0 * x0
```

```
    grad_x0 = grad_s0 * w0
```

Add gate

# Backprop Implementation: “Flat” code



Forward pass:  
Compute output

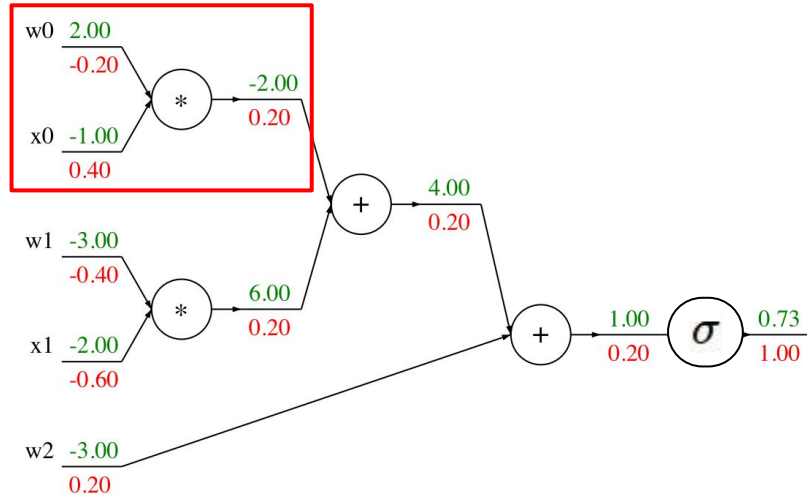
```
def f(w0, x0, w1, x1, w2):
```

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

```
    grad_L = 1.0  
    grad_s3 = grad_L * (1 - L) * L  
    grad_w2 = grad_s3  
    grad_s2 = grad_s3  
    grad_s0 = grad_s2  
    grad_s1 = grad_s2  
    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
```

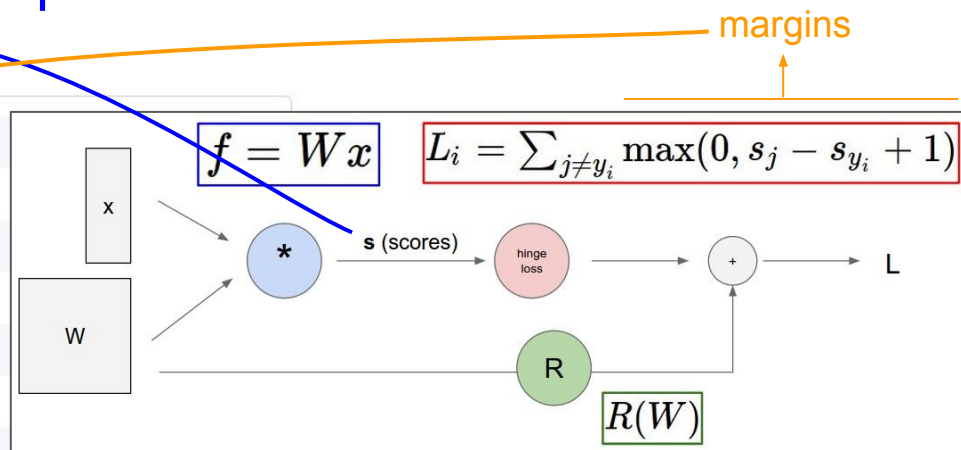
Multiply gate

# “Flat” Backprop: Do this for assignment 2!

Stage your forward/backward computation!

E.g. for the SVM:

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



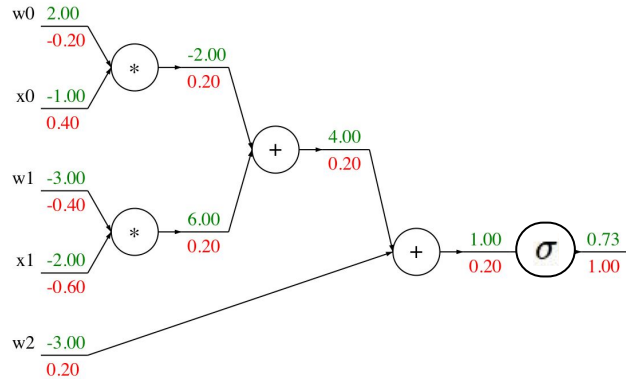
# “Flat” Backprop: Do this for assignment 1!

E.g. for two-layer neural net:

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

# Backprop Implementation: Modularized API

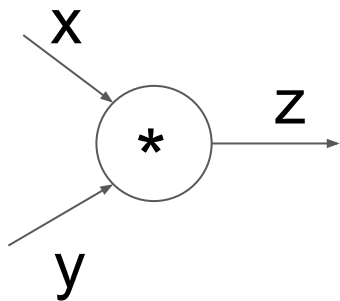
Graph (or Net) object (*rough pseudo code*)



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

# Modularized implementation: forward / backward API

Gate / Node / Function object: Actual PyTorch code



(x,y,z are scalars)

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

Need to stash  
some values for  
use in backward

Upstream  
gradient

Multiply upstream  
and local gradients

# Example: PyTorch operators

pytorch / pytorch

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Projects 4

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

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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)

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Col2Im.c

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ELU.c

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FeatureLPPooling.c

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GatedLinearUnit.c

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MSECriterion.c

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MultiLabelMarginCriterion.c

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MultiMarginCriterion.c

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Sigmoid.c

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SmoothL1Criterion.c

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SoftMarginCriterion.c

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SoftPlus.c

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SoftShrink.c

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SpatialAdaptiveAveragePooling.c

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SpatialAdaptiveMaxPooling.c

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SpatialAveragePooling.c

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



# PyTorch sigmoid layer

Forward

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



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

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

[Source](#)

# PyTorch sigmoid layer

Forward

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



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

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

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

Forward actually  
defined elsewhere...

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

[Source](#)

# PyTorch sigmoid layer

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

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

Forward

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

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

Backward

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

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

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

[Source](#)

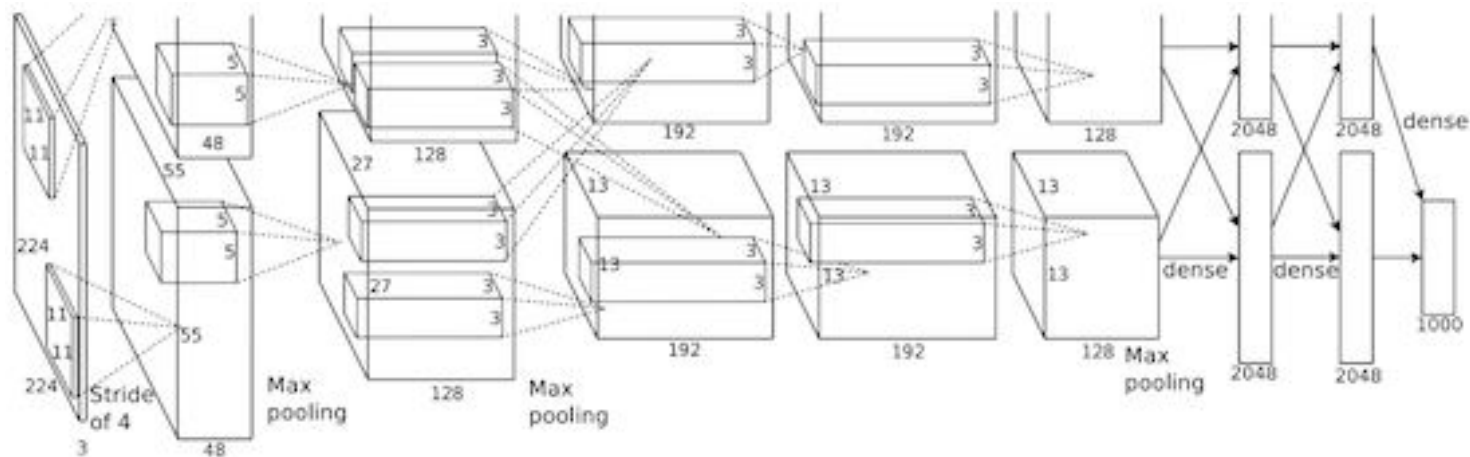
# Summary for today:

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

So far: backprop with scalars

Next time: vector-valued functions!

# Next Time: Convolutional neural networks



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

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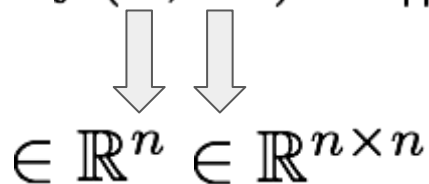
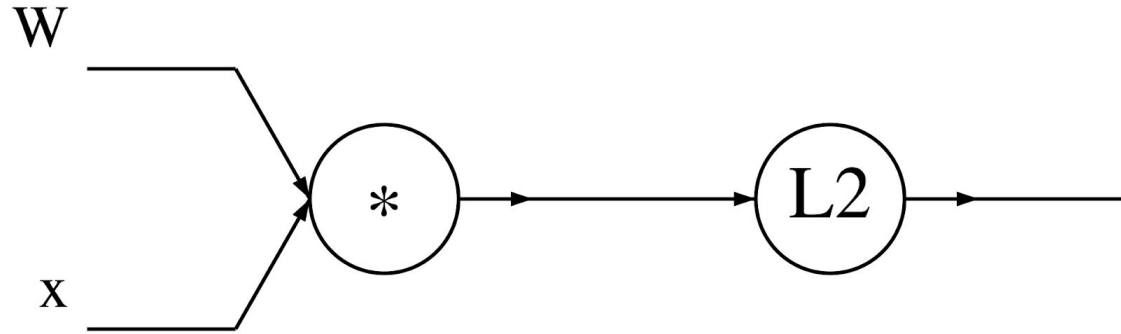


Diagram illustrating the domains of the variables  $x$  and  $W$  in the vectorized example:

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



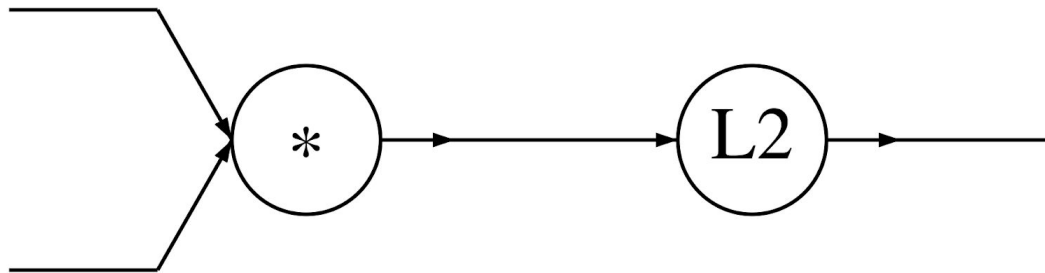
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$$\begin{bmatrix} 0.1 & 0.5 \\ -0.3 & 0.8 \end{bmatrix} \mathbf{W}$$

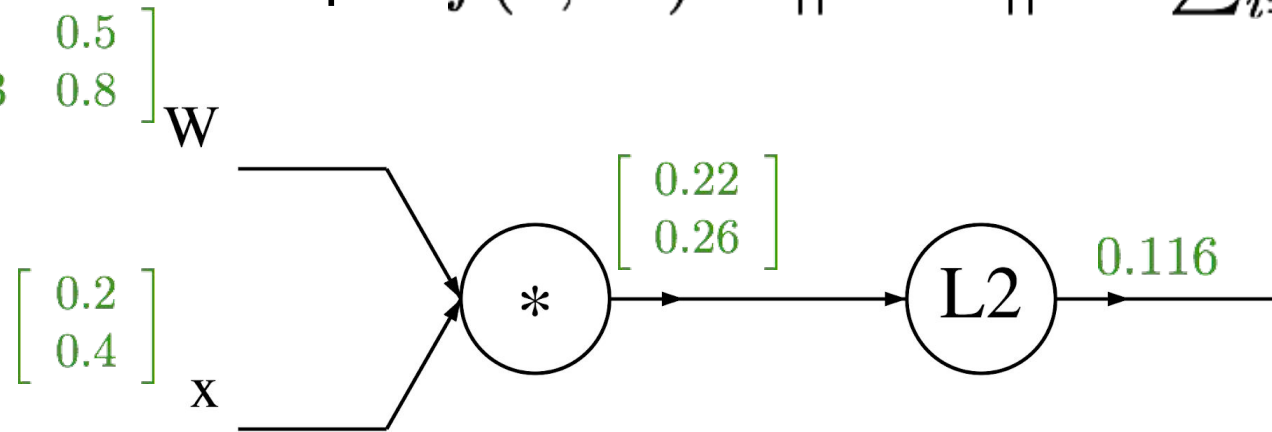
$$\begin{bmatrix} 0.2 \\ 0.4 \end{bmatrix} \mathbf{x}$$



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

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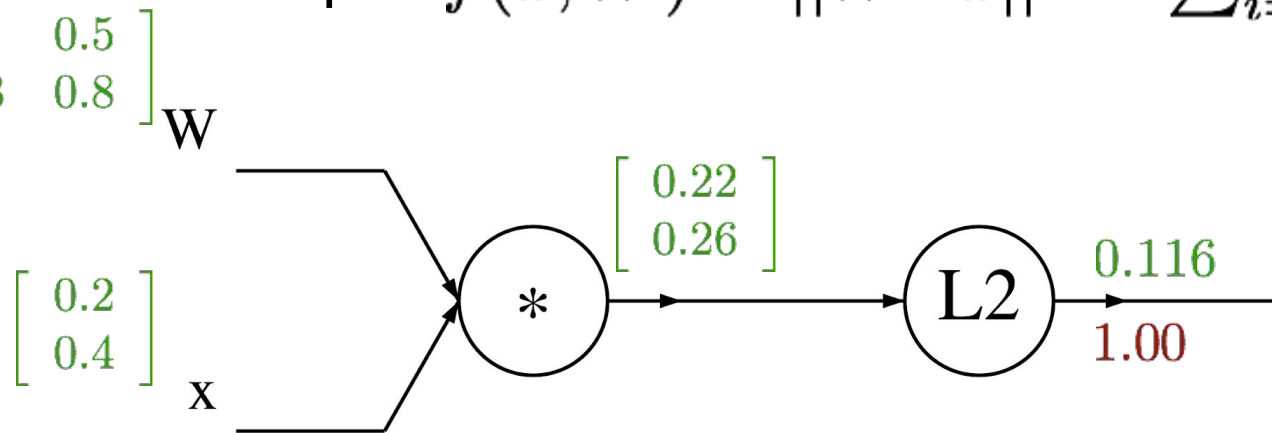
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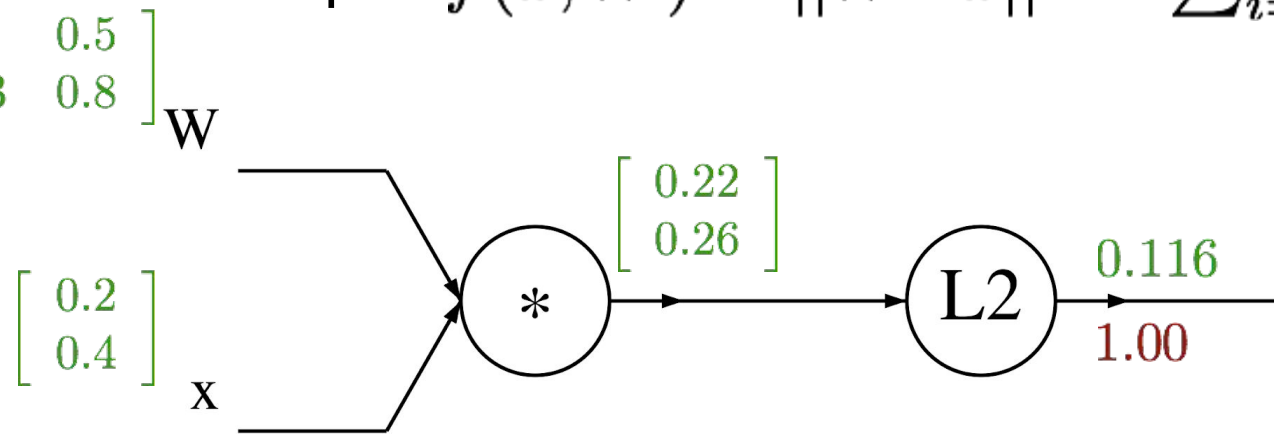
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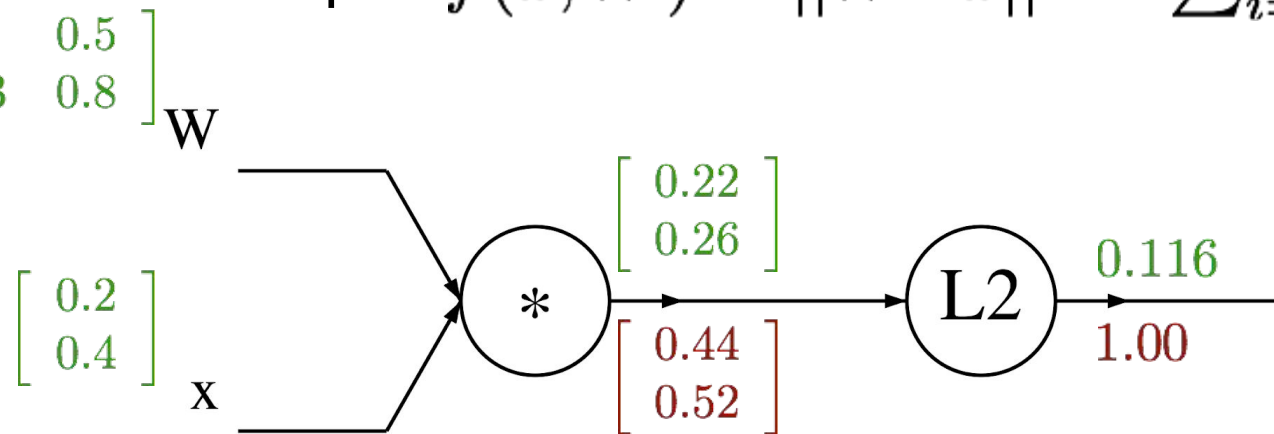
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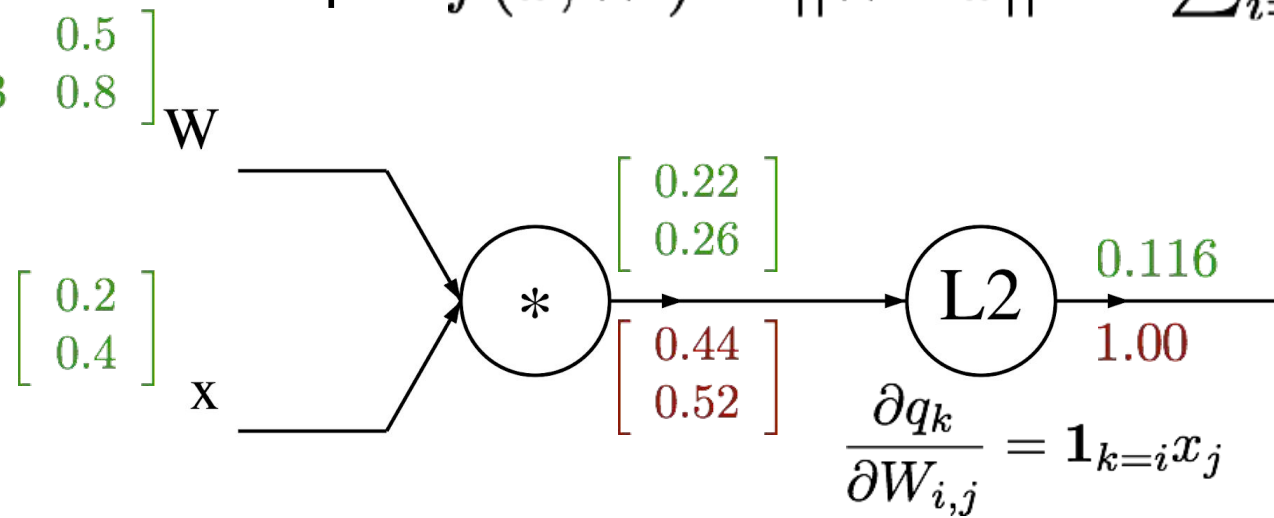
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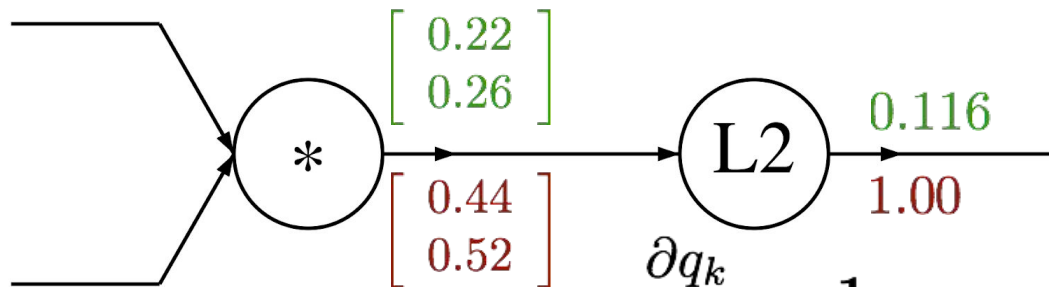
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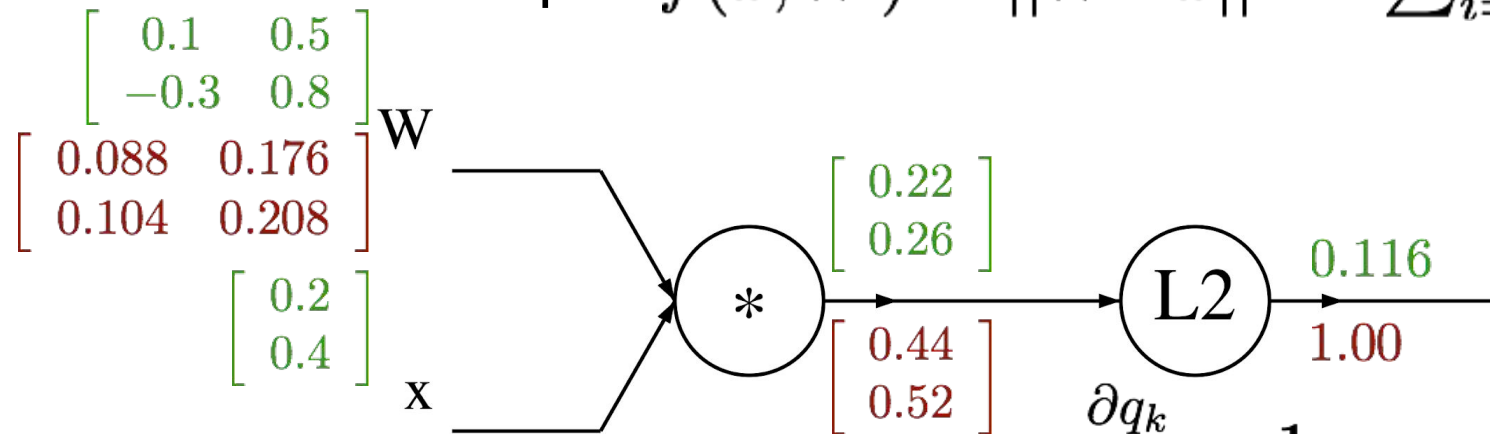
$$\begin{aligned} \frac{\partial f}{\partial W_{i,j}} &= \sum_k \frac{\partial f}{\partial q_k} \frac{\partial q_k}{\partial W_{i,j}} \\ &= \sum_k (2q_k) (\mathbf{1}_{k=i} x_j) \\ &= 2q_i x_j \end{aligned}$$

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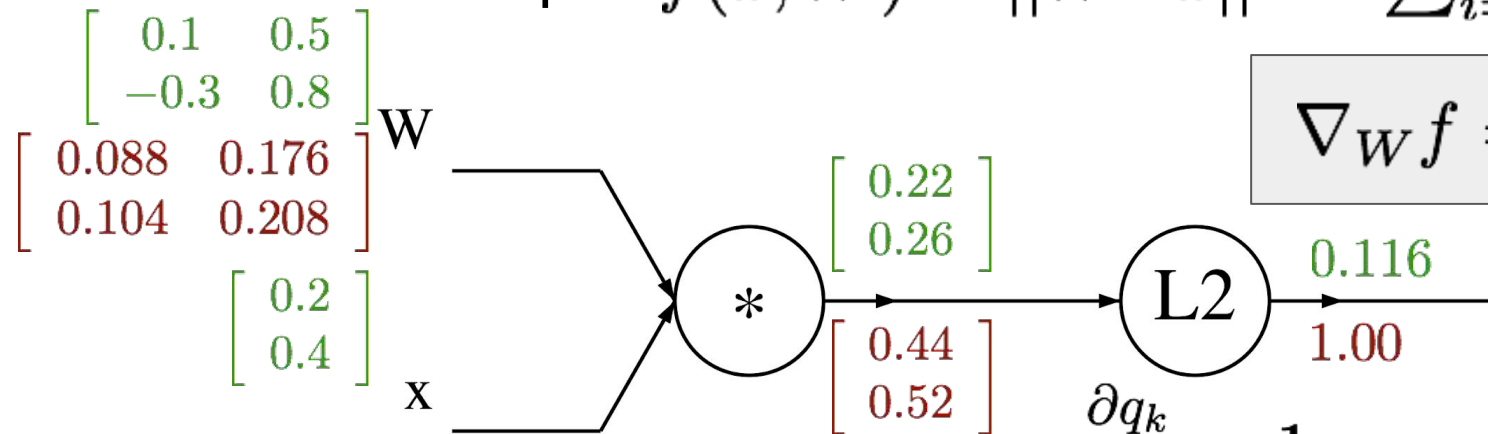


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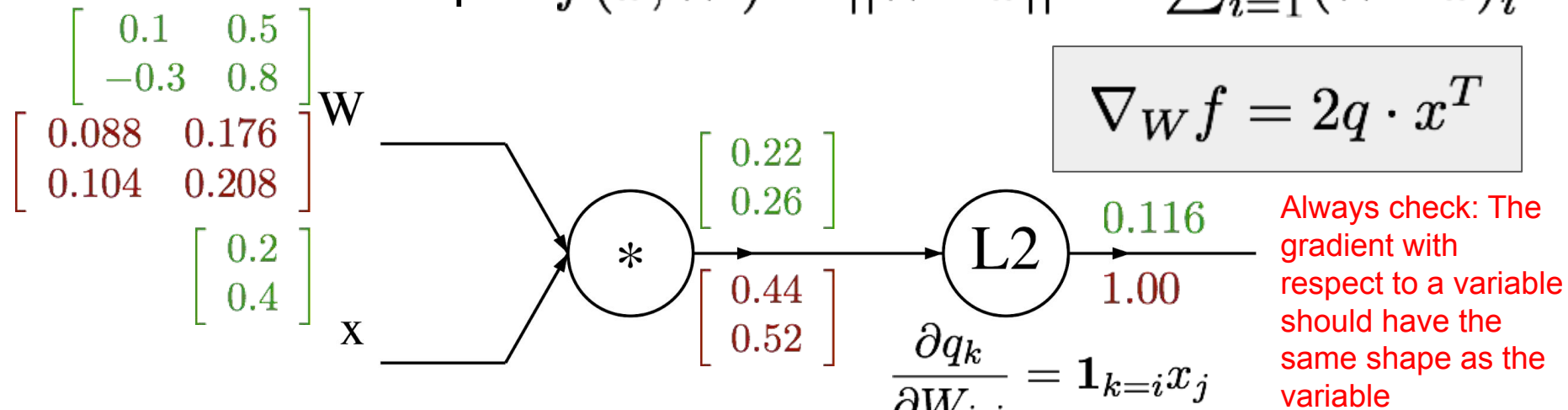
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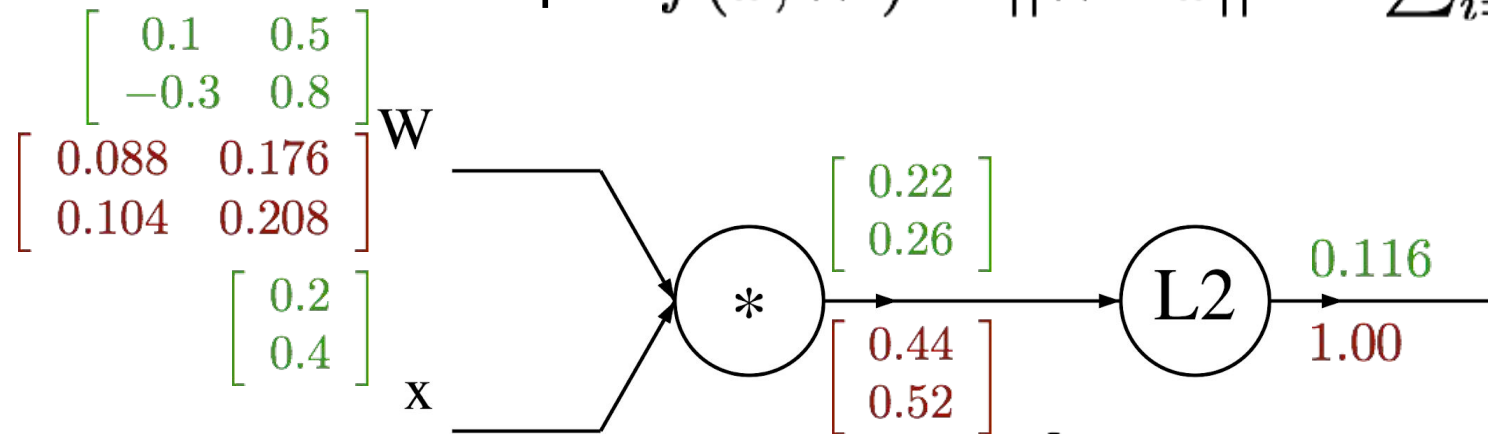
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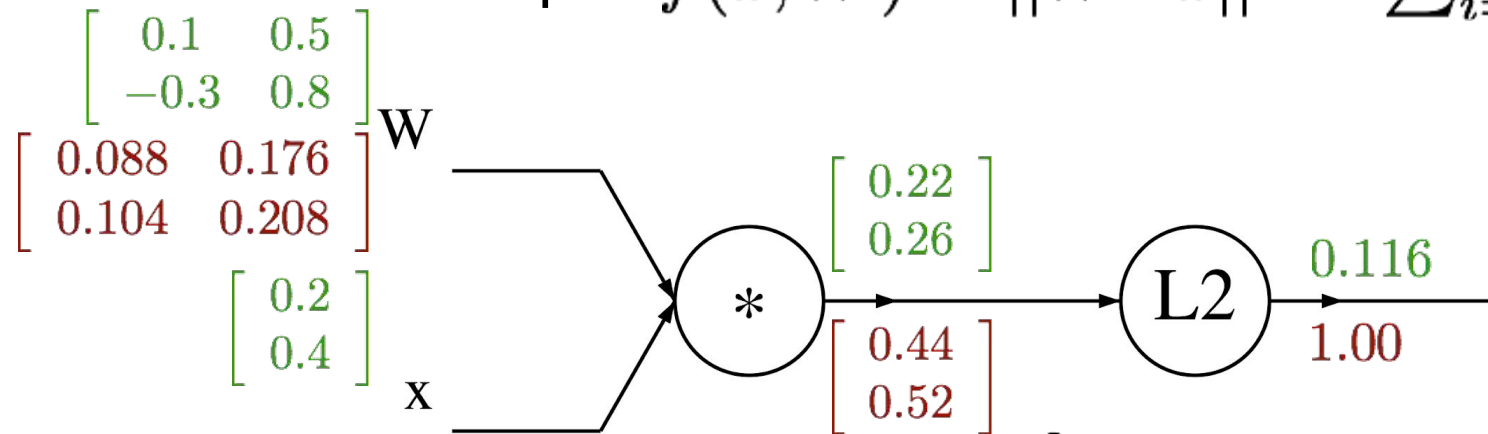


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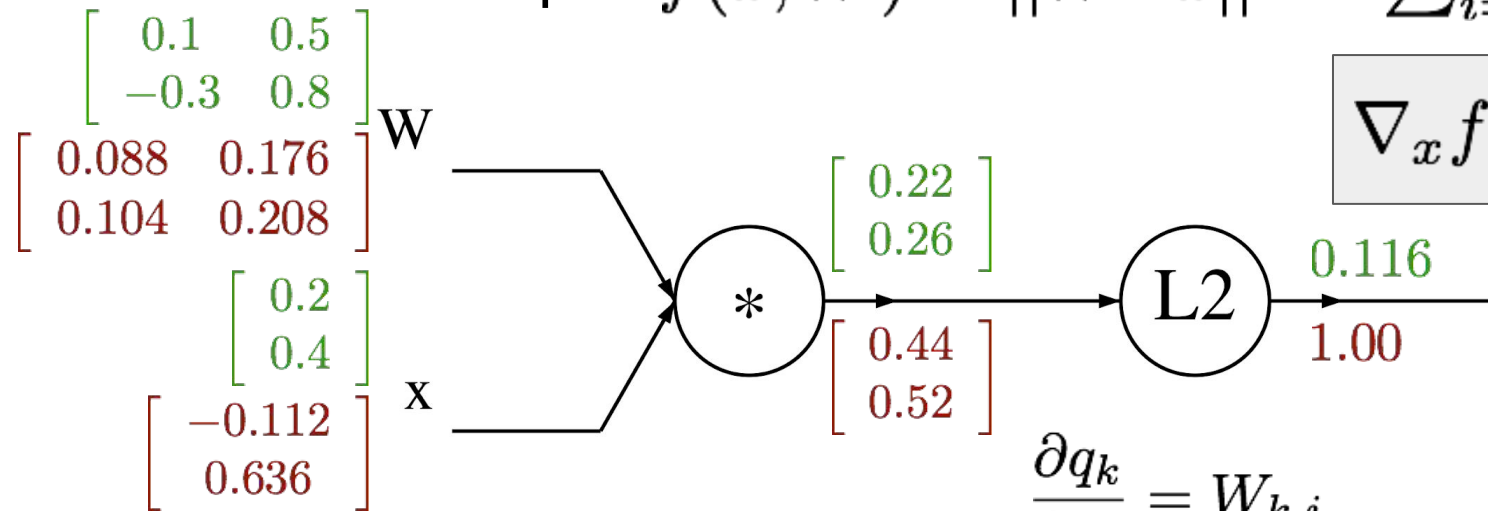


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$$\nabla_x f = 2W^T \cdot q$$

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In discussion section: A matrix example...

$$z_1 = XW_1$$

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

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

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

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

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

