Lecture 4: Backpropagation and Neural Networks part 1

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Recall From Last Time…

Where we are…

$$s = f(x, \boldsymbol{W}) = \boldsymbol{W}x$$

Score function

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

SVM loss

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

Softmax loss

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

Data loss + Regularization loss

Want $\nabla_{\mathrm{W}} L$ = …

gradient of Loss respect to W

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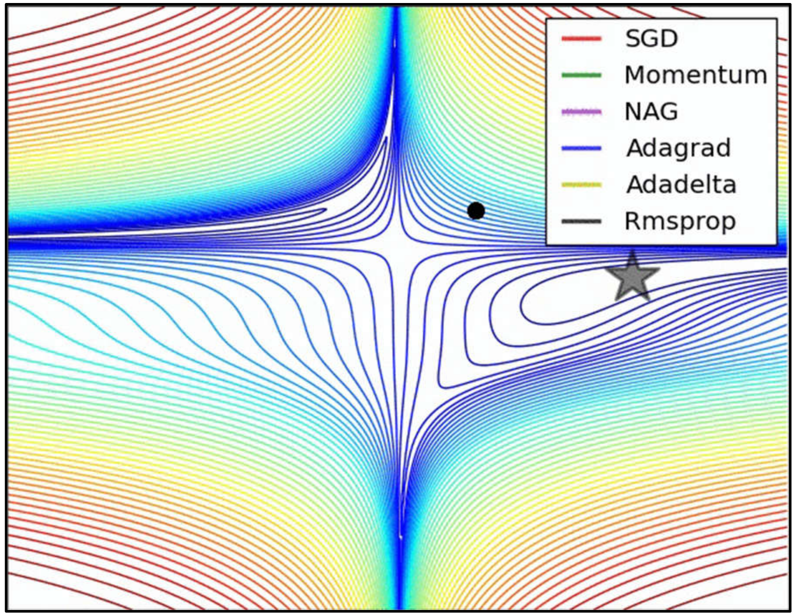
Recall From Last Time…

Optimization




```
# 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
```

(image credits to Alec Radford)

Recall From Last Time…

Gradient Descent

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

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

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

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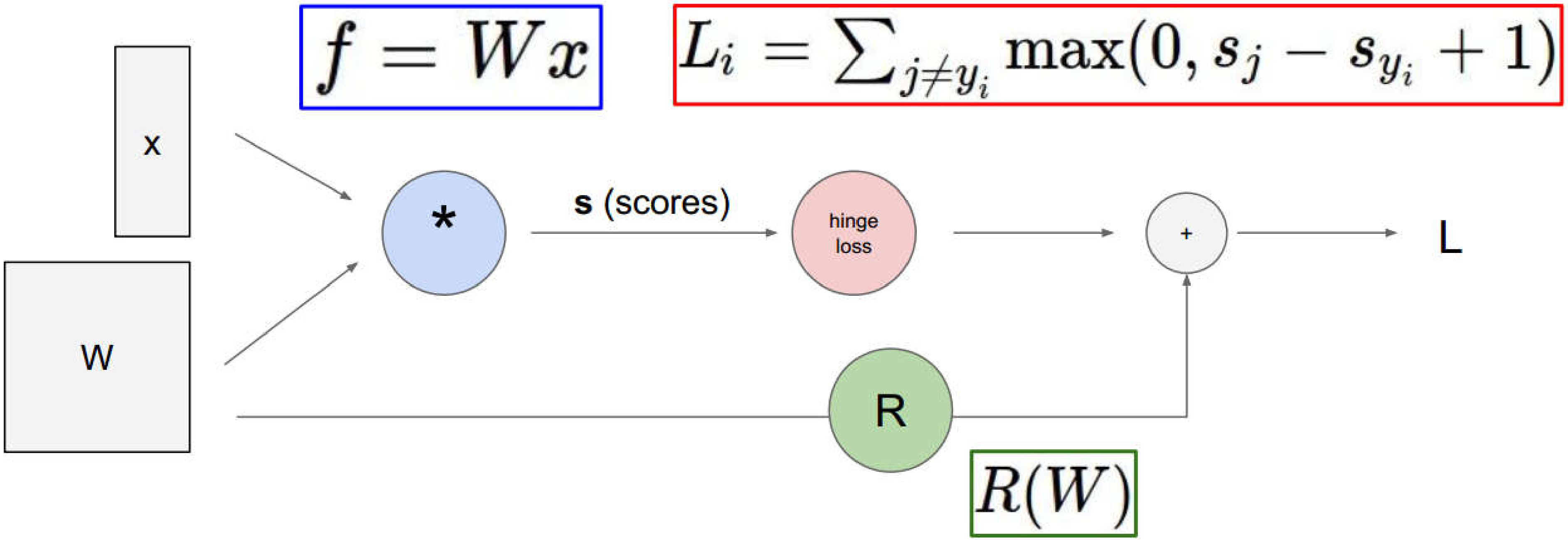
Backpropagation

Computational Graph



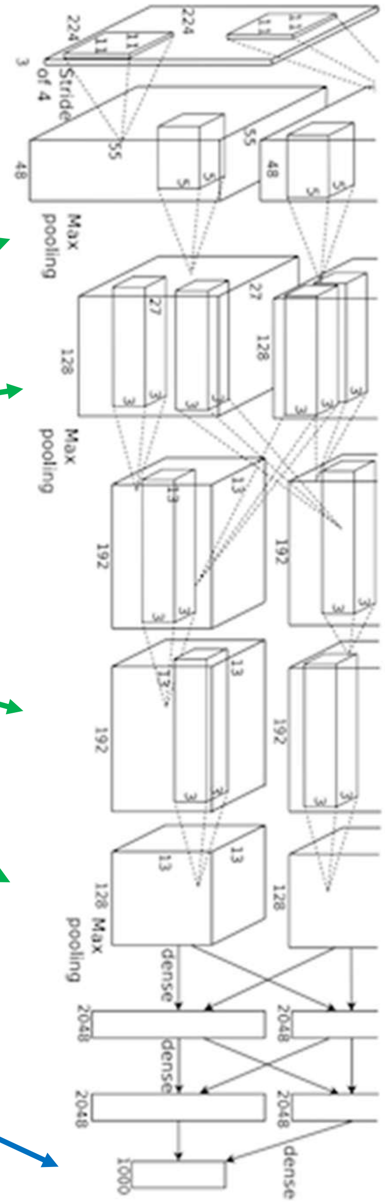
Computation graph of the SVM loss

Convolutional Network (AlexNet)

Input image

weights

loss



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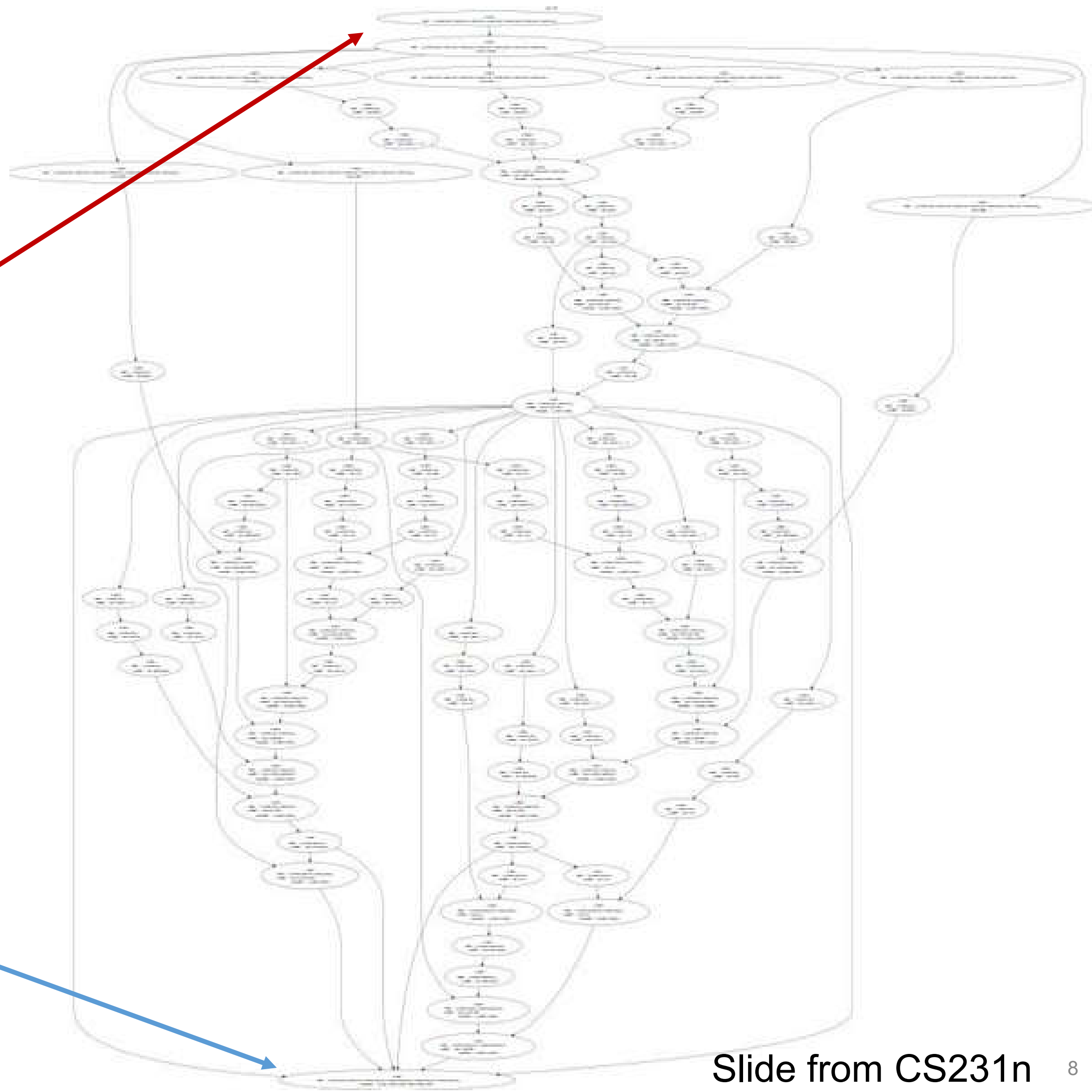
Neural Turing Machine

Input tape



loss

A paper from deepmind

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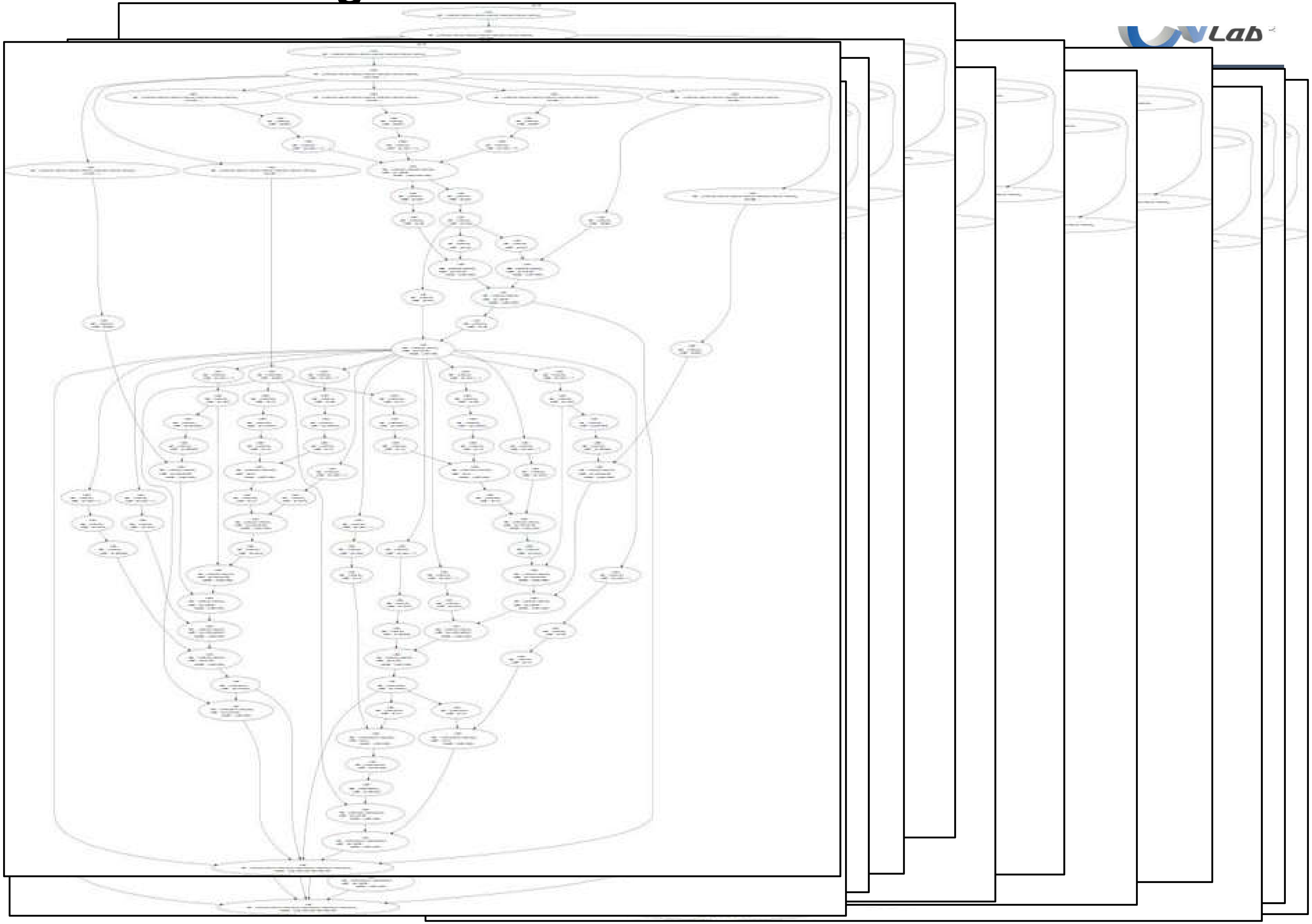
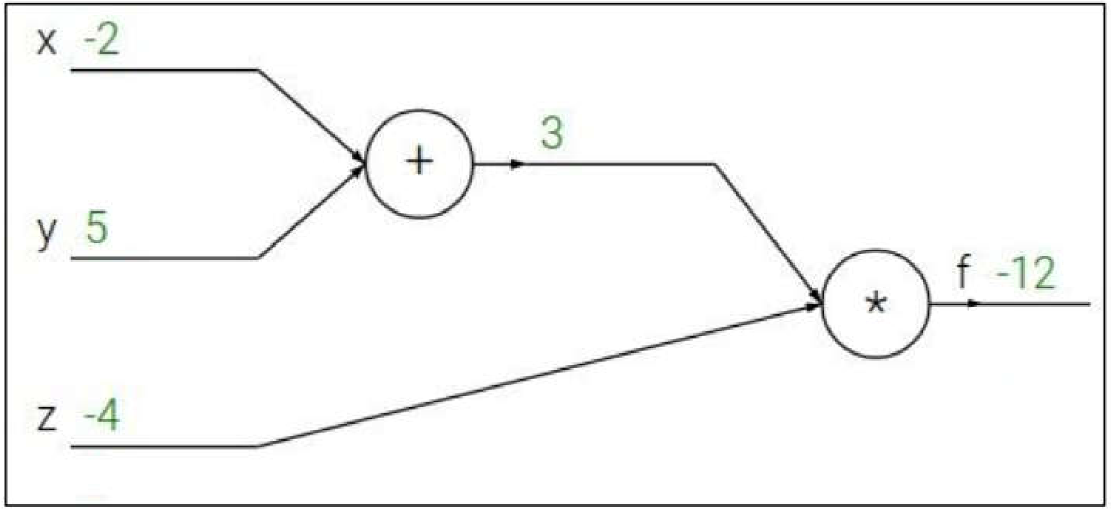
Neural Turing Machine



Start from Simple

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

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



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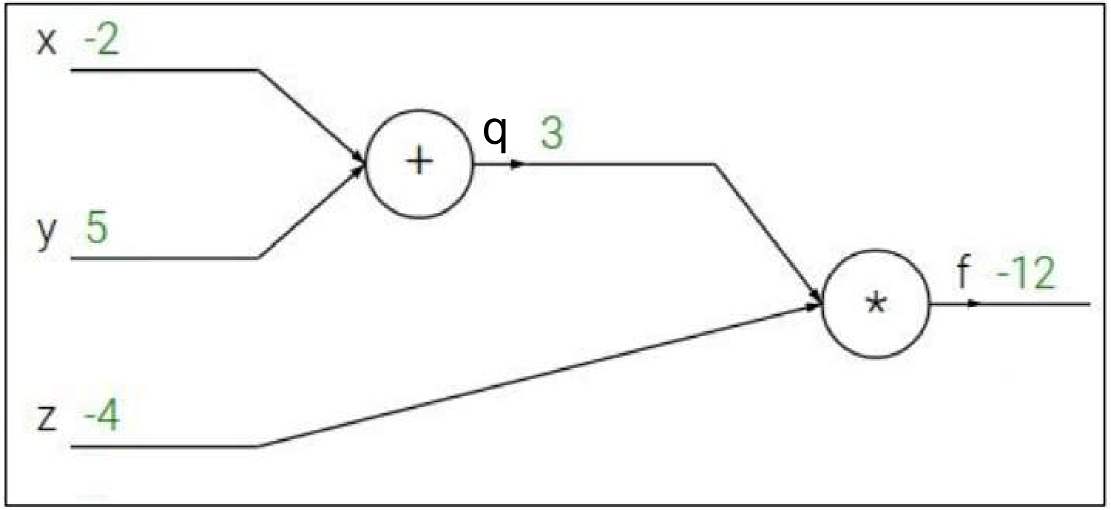

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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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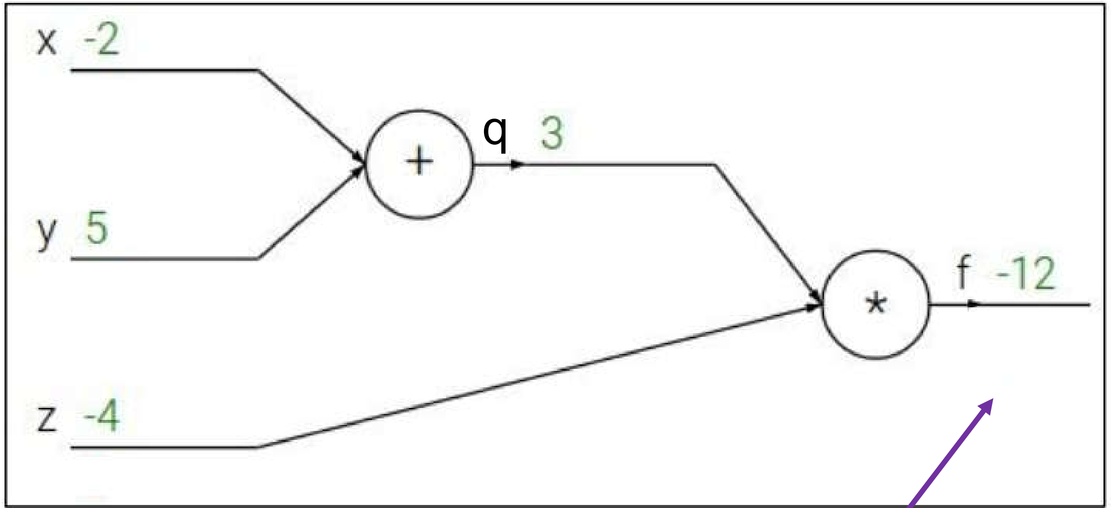

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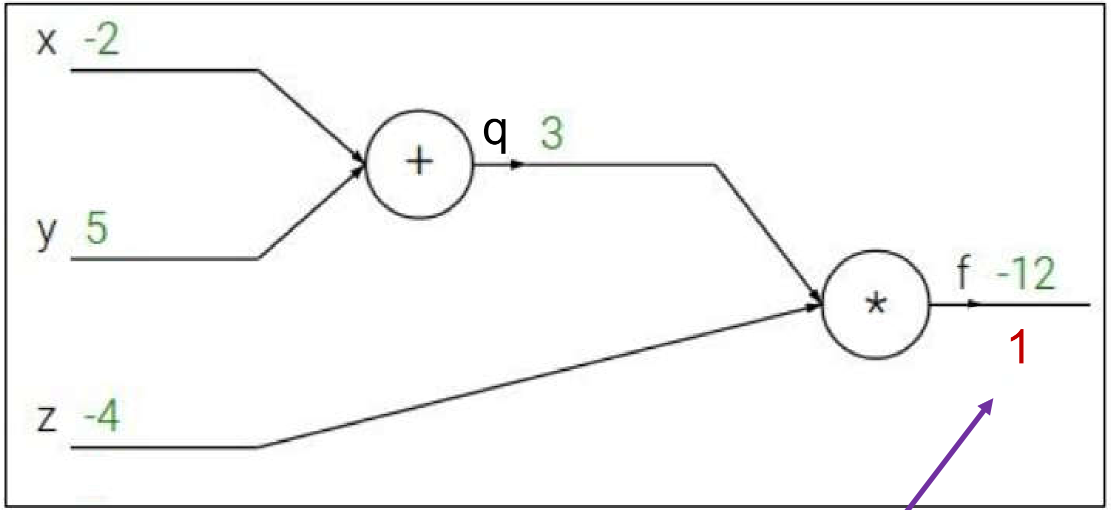

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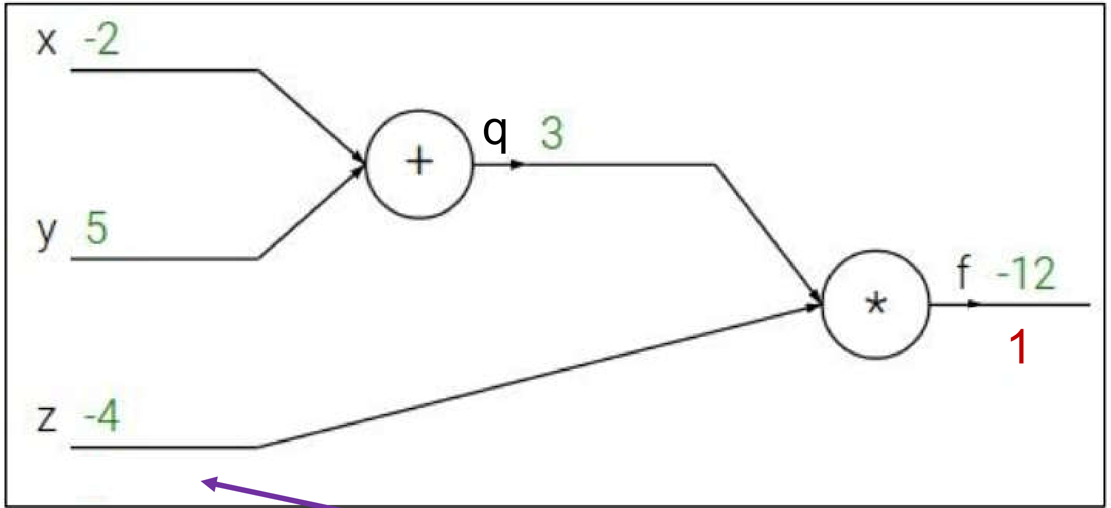

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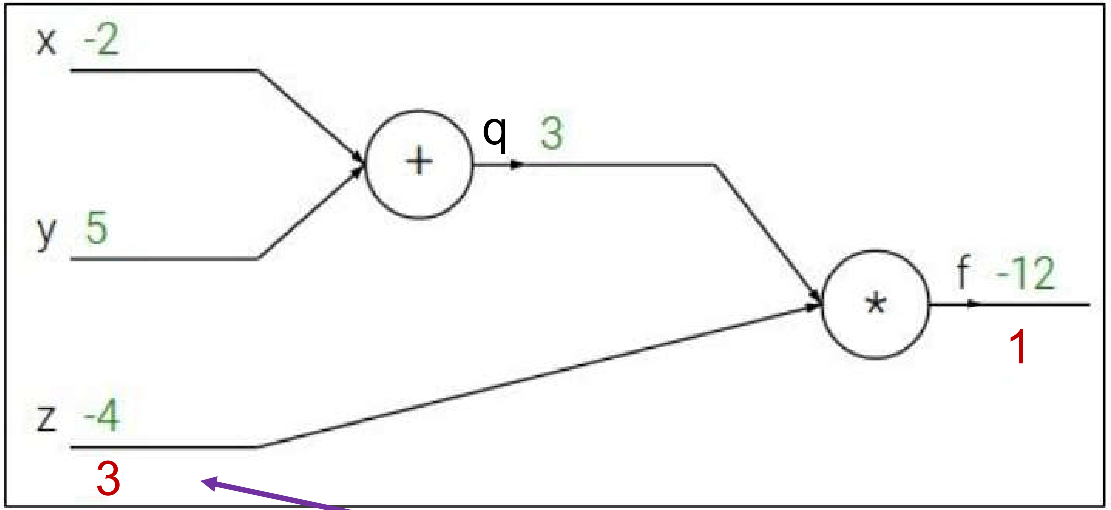

$$\frac{\partial f}{\partial z}$$

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

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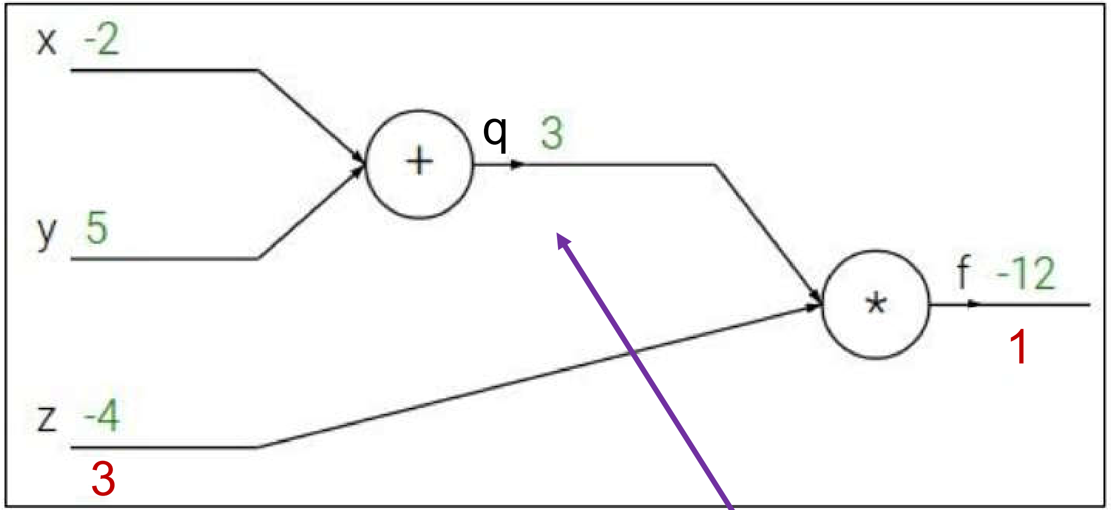

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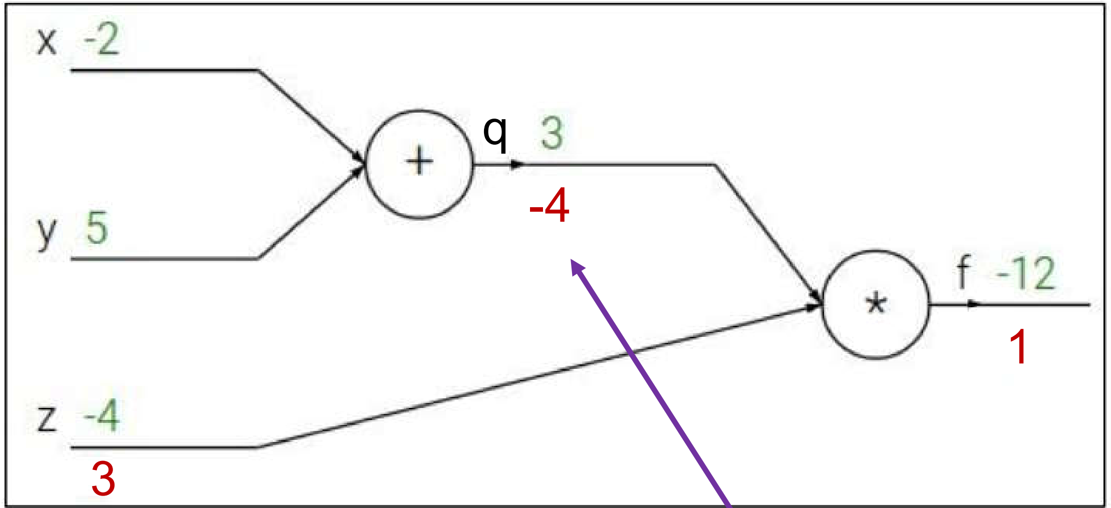

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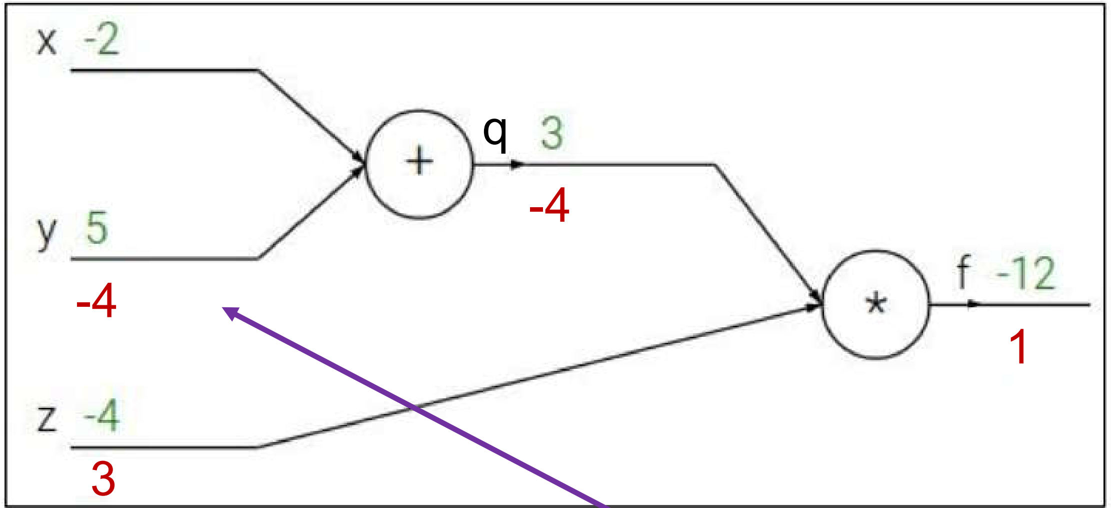

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$$\boxed{\frac{\partial f}{\partial y}}$$

Chain rule:

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

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

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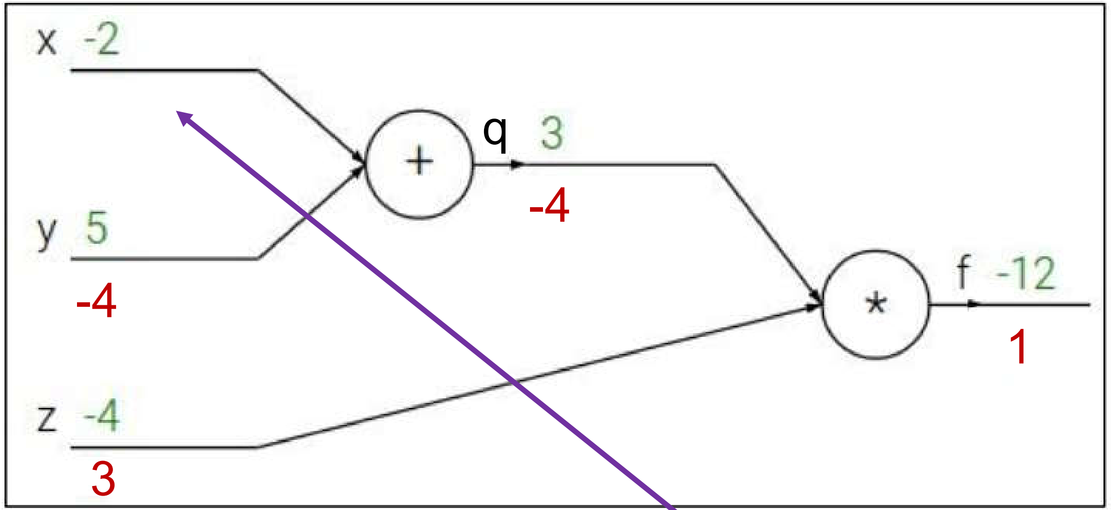

$$\frac{\partial f}{\partial x}$$

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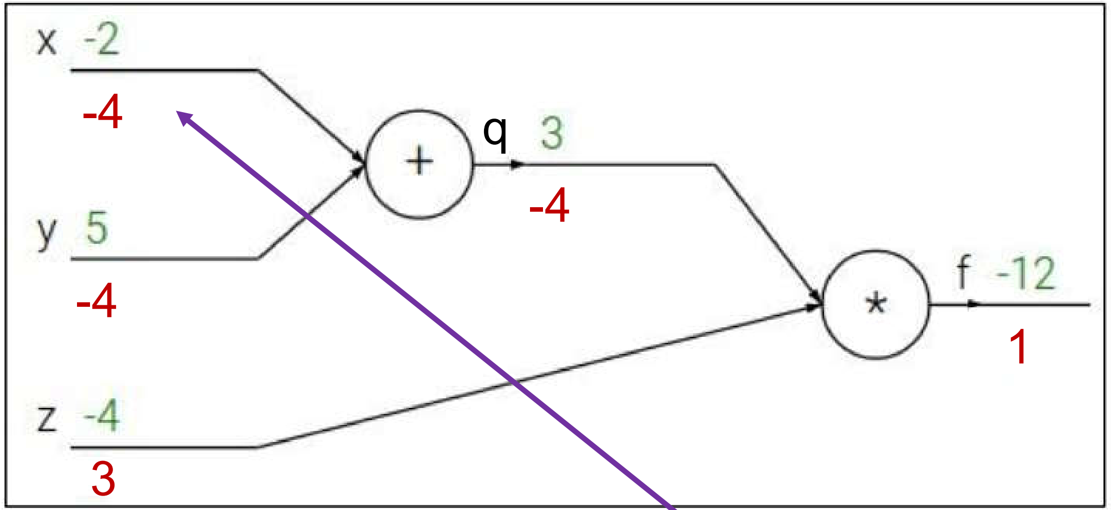

$$\frac{\partial f}{\partial x}$$

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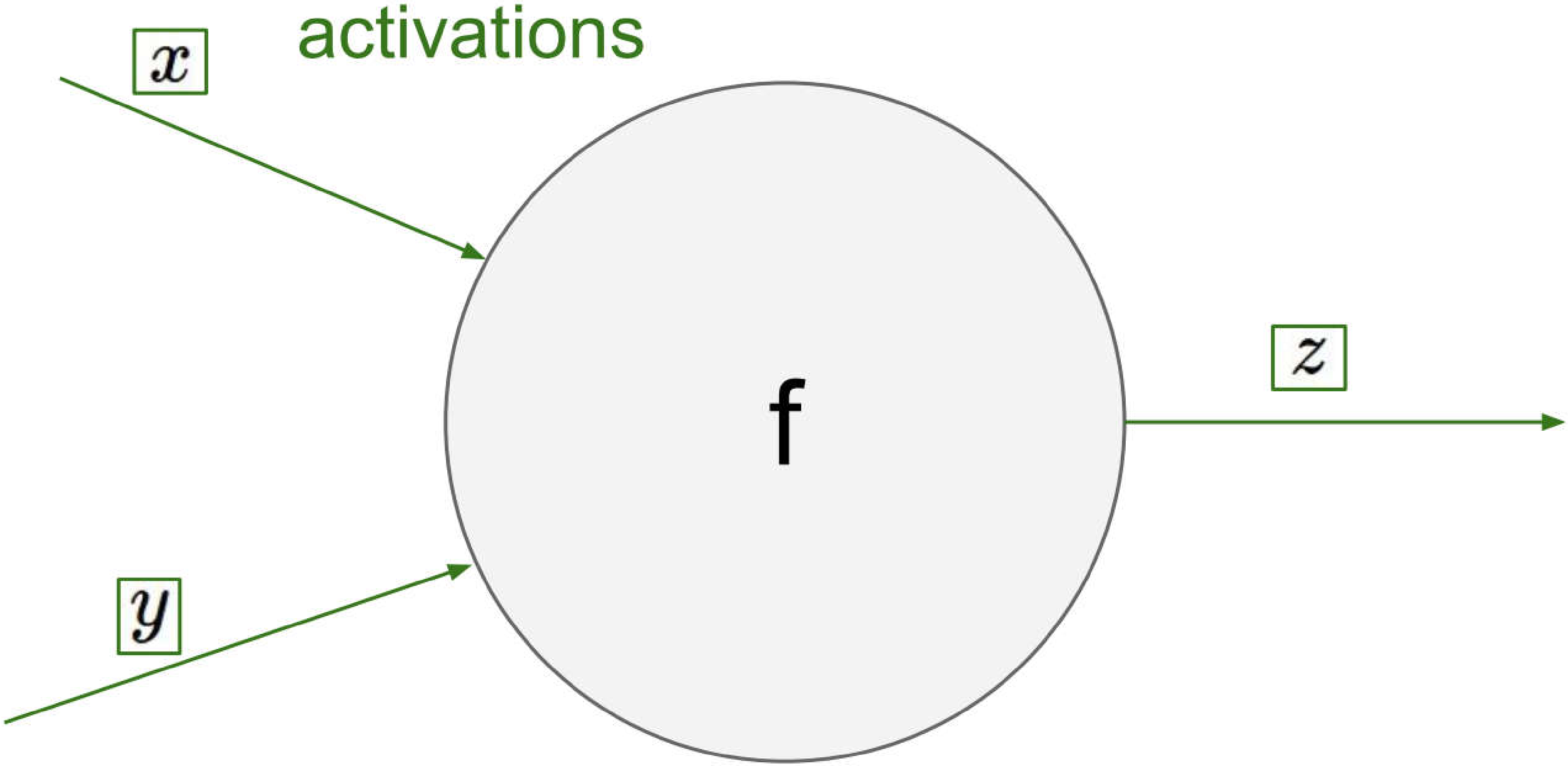
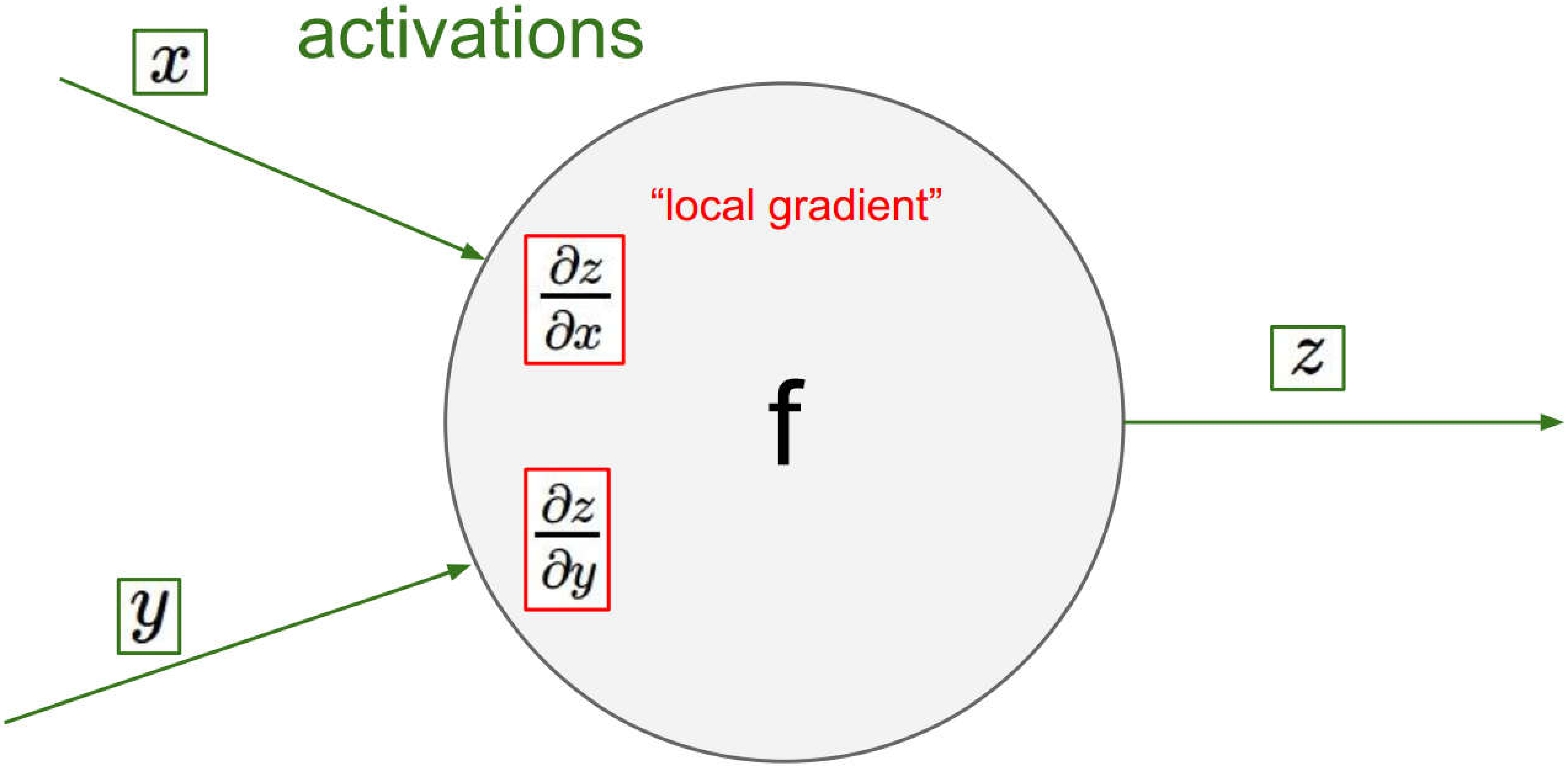
Backpropagation



Backpropagation



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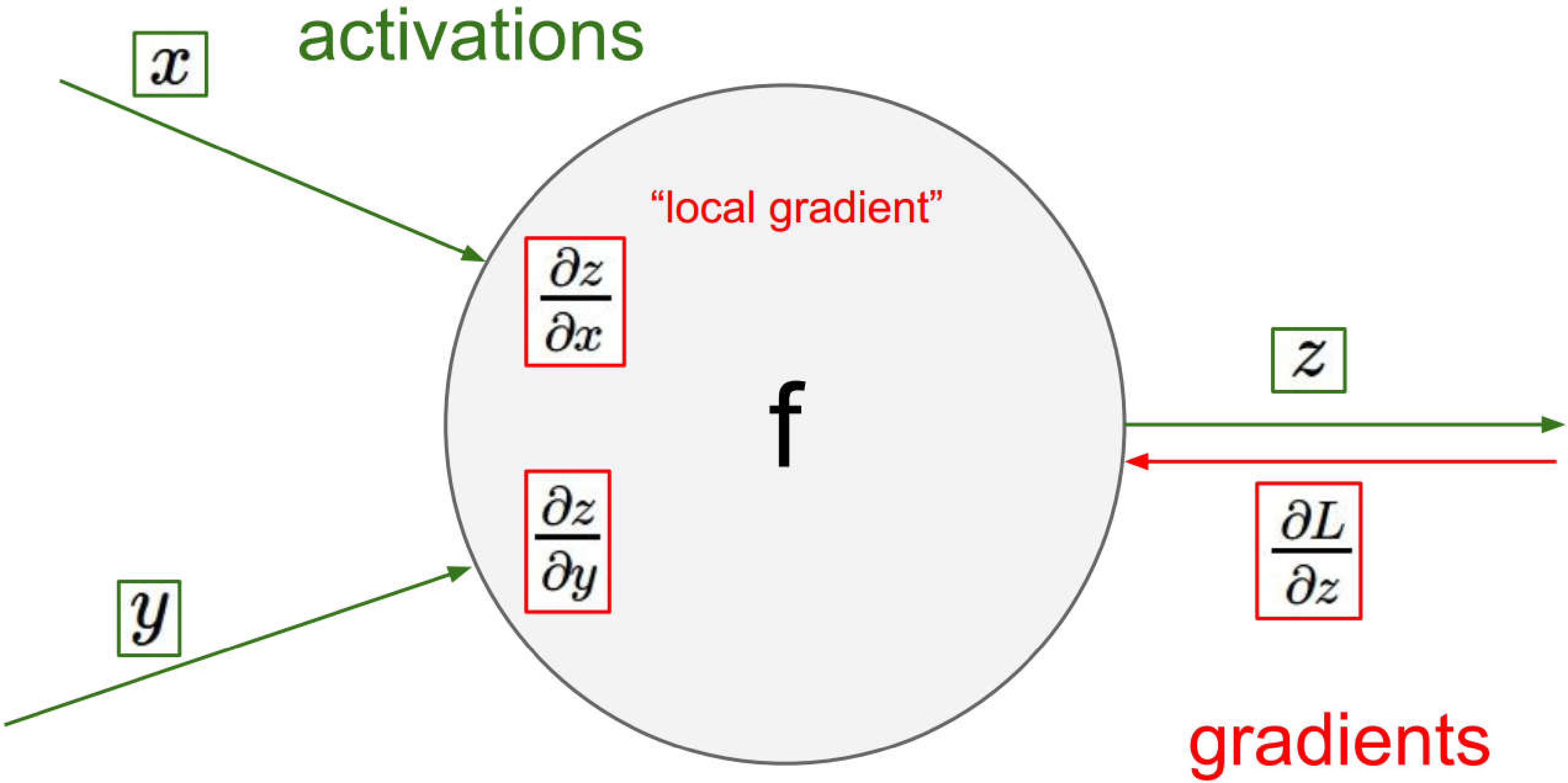

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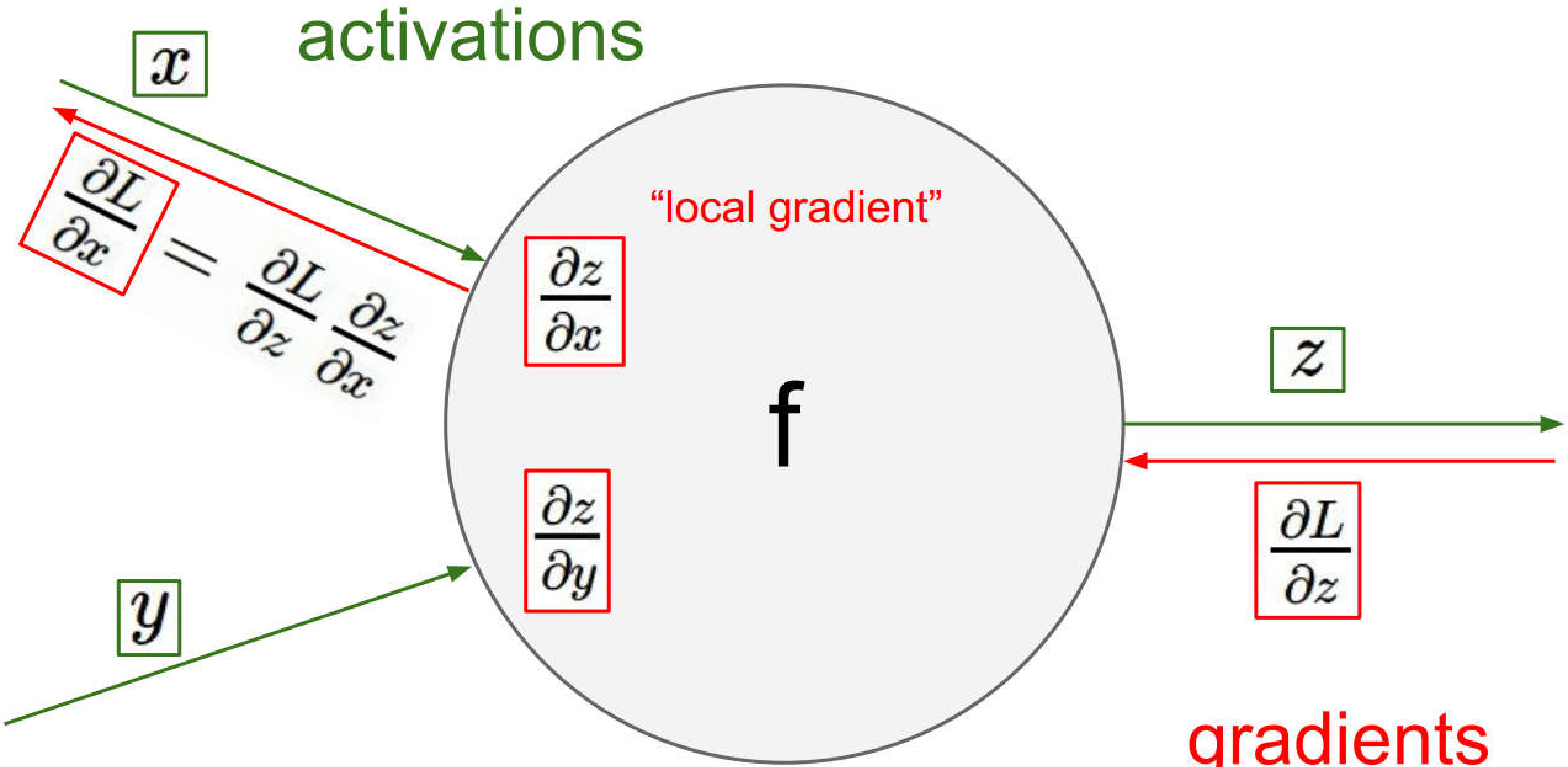
Backpropagation



Chain Rule

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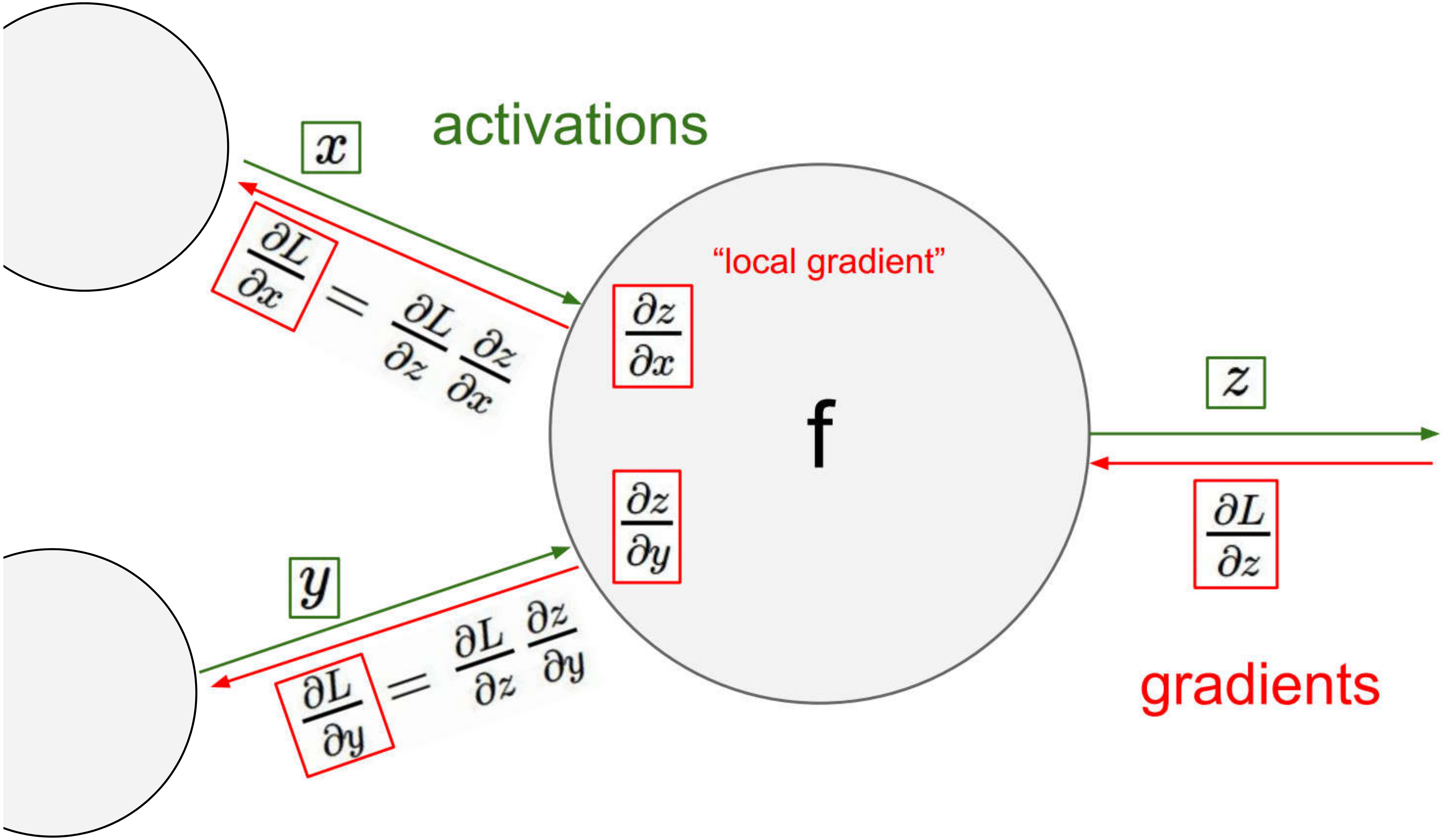
Backpropagation



Chain rule

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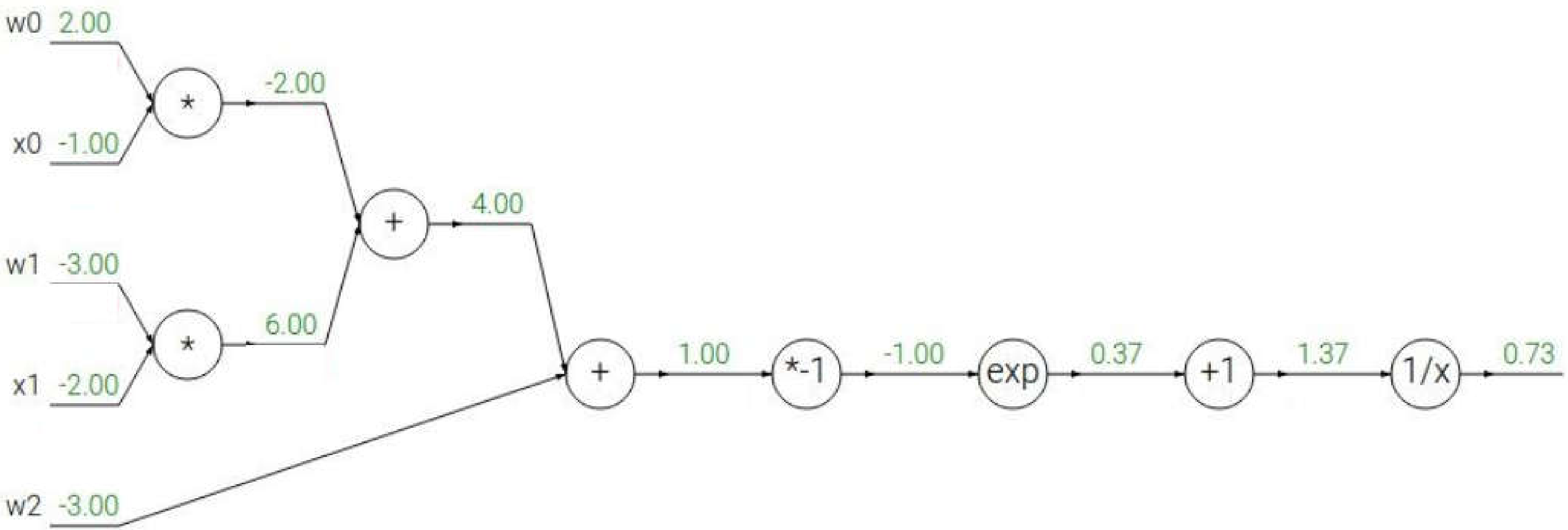
Another Example

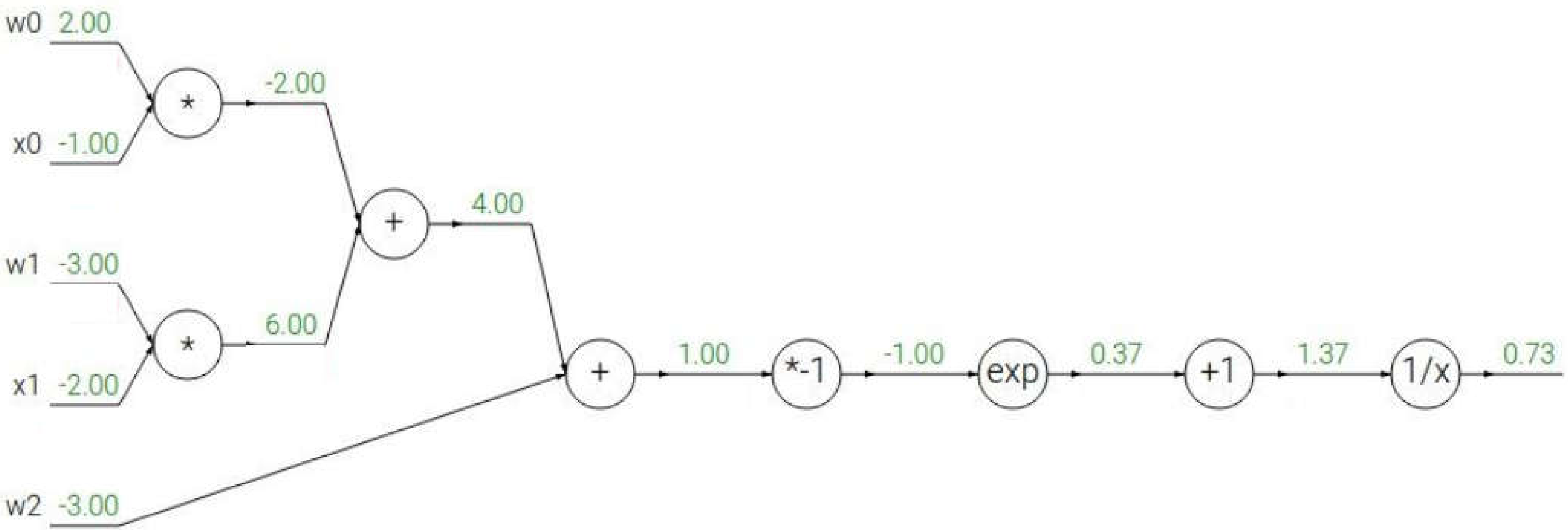
Sigmoid Neuron: $f(\boldsymbol{w}, \boldsymbol{x}) = \dfrac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$



Computation graph of sigmoid neuron

Another Example

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



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

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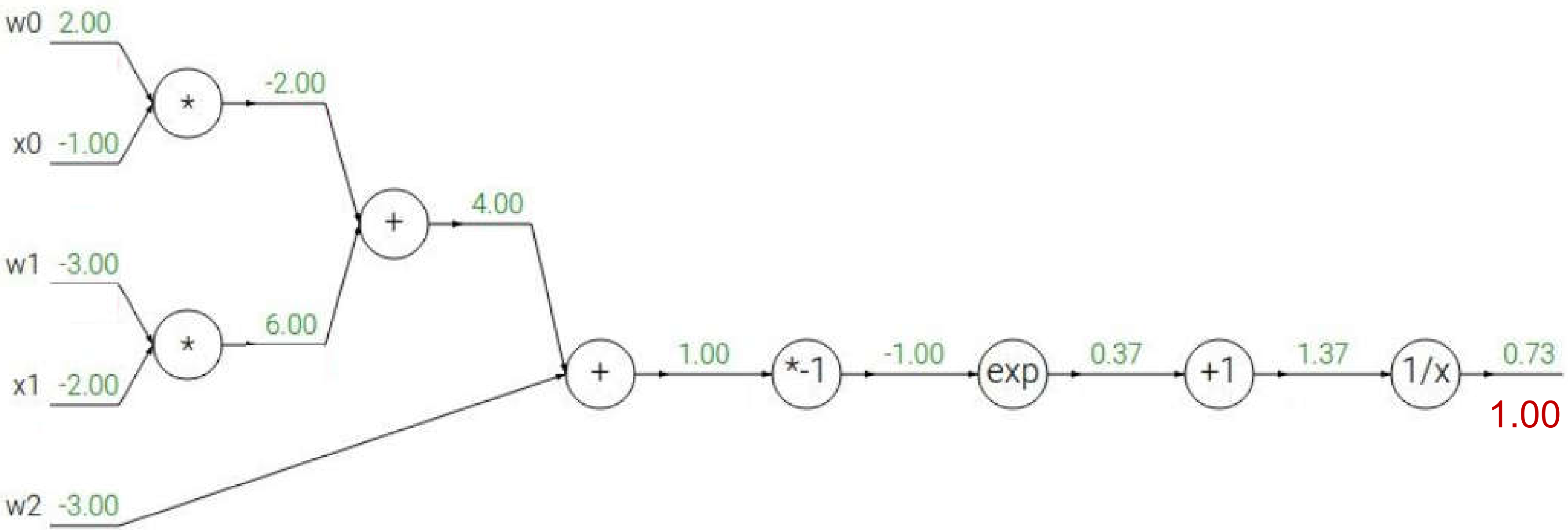

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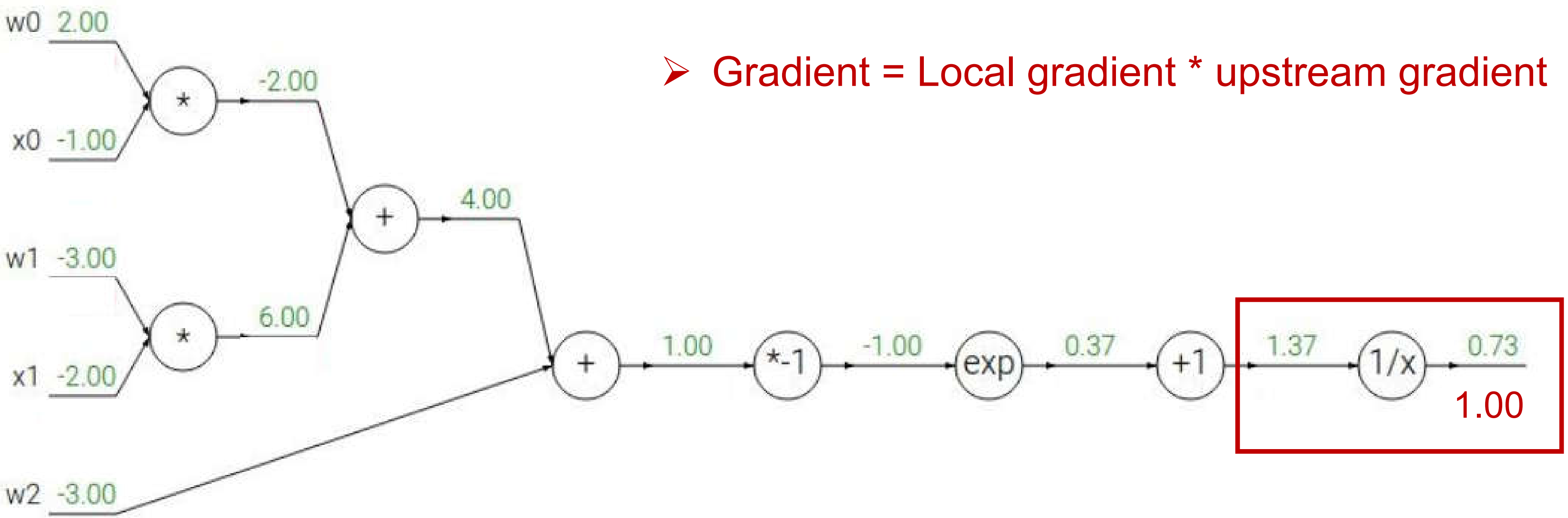
➢ Gradient = Local gradient * upstream gradient



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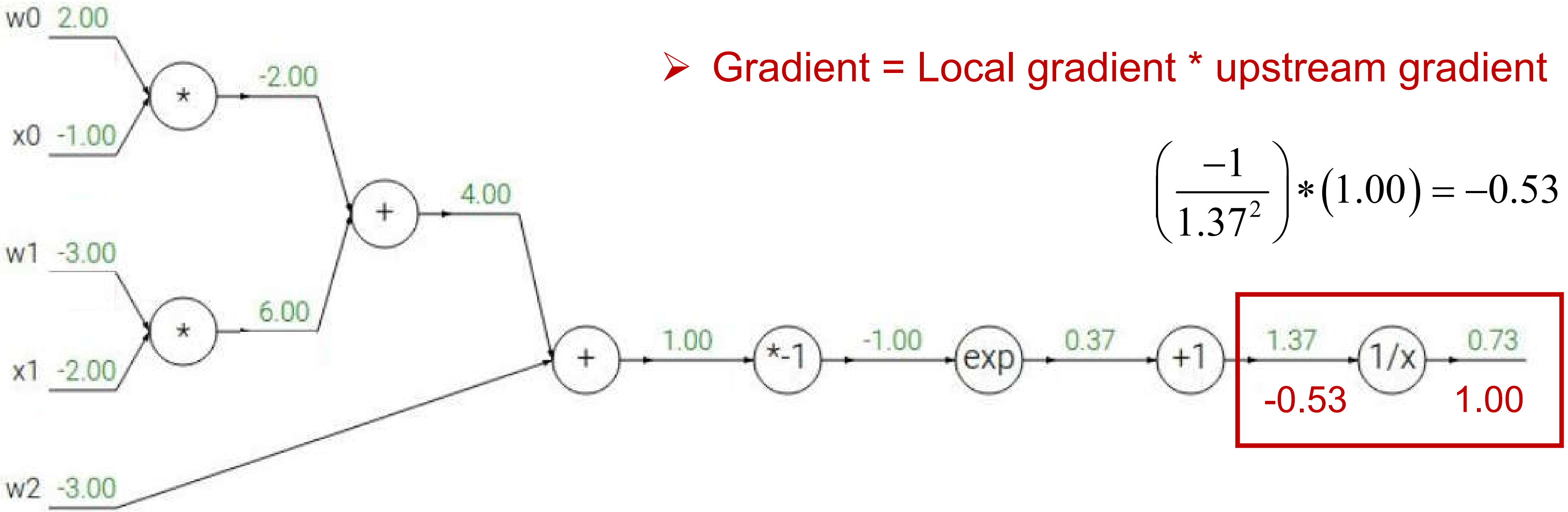

➢ Gradient = Local gradient * upstream gradient

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

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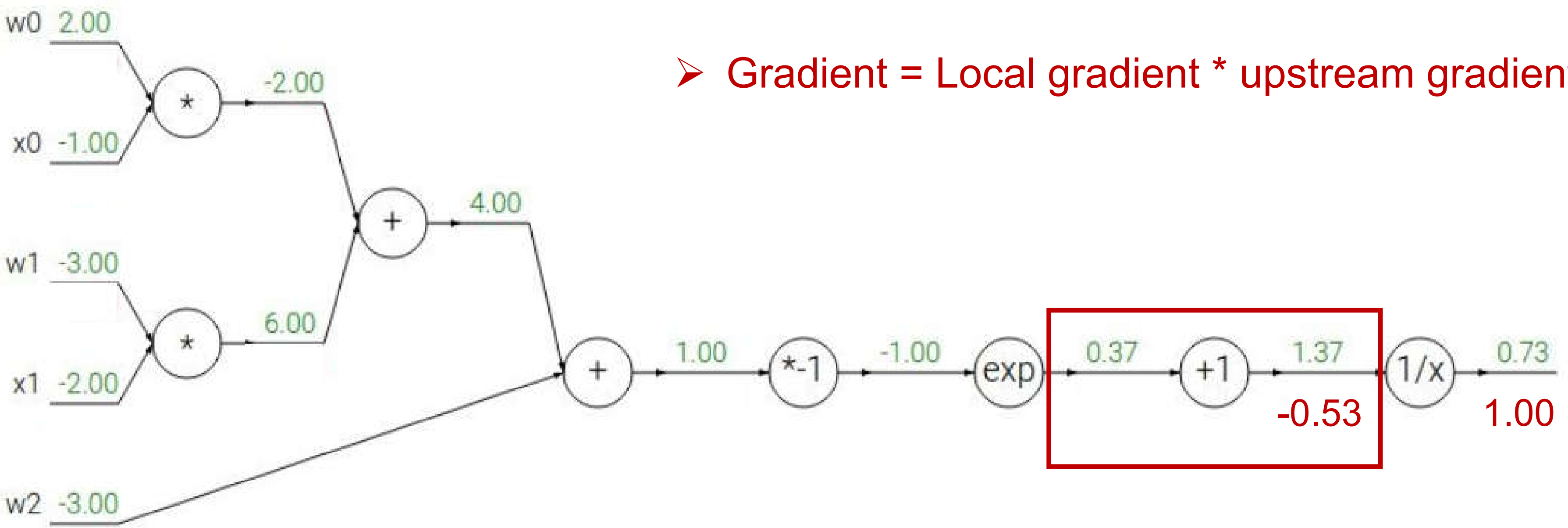

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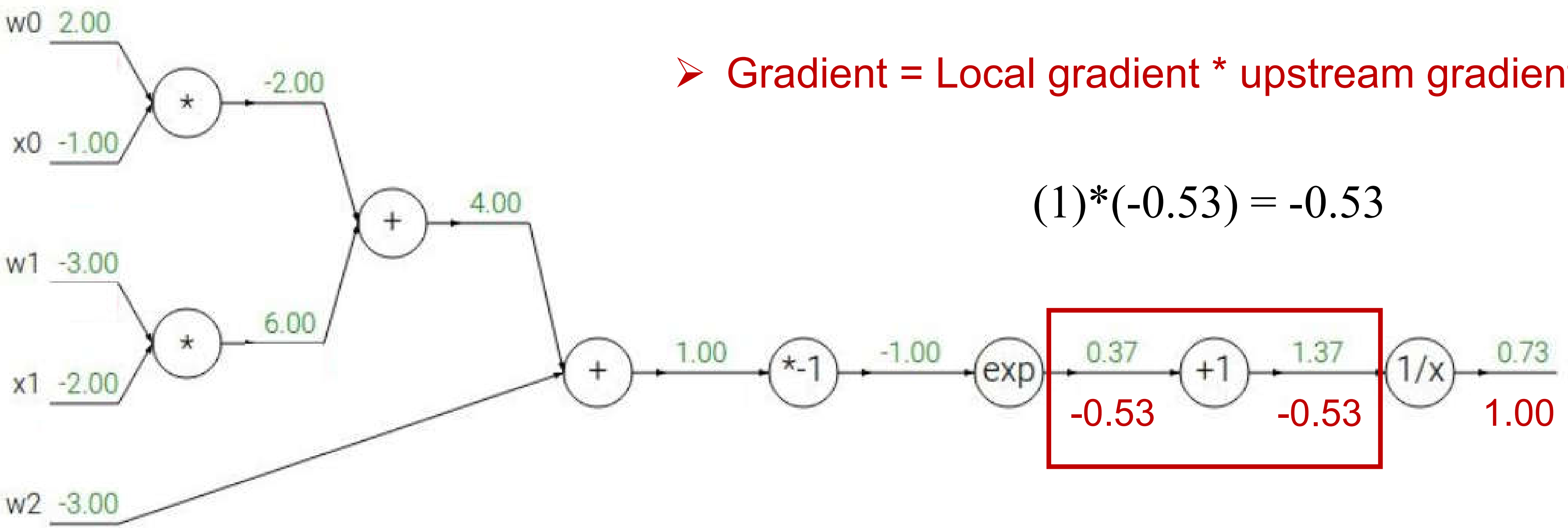

➢ Gradient = Local gradient * upstream gradient

(1)*(-0.53) = -0.53

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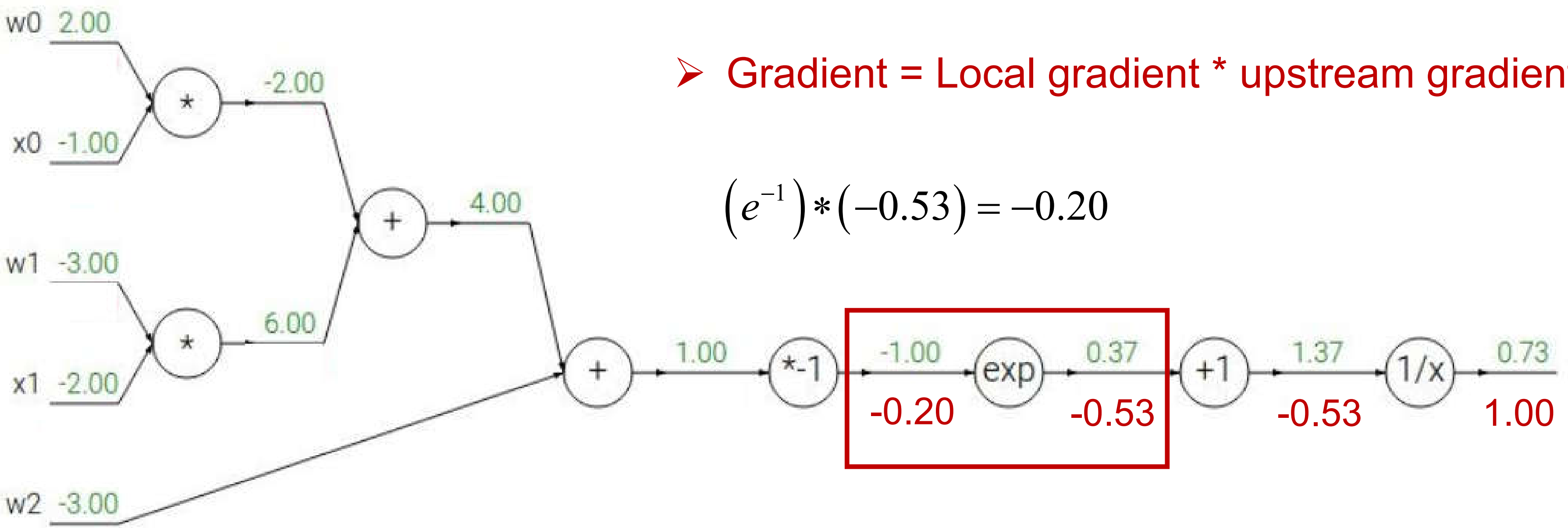
$$\left(e^{-1}\right) * (-0.53) = -0.20$$



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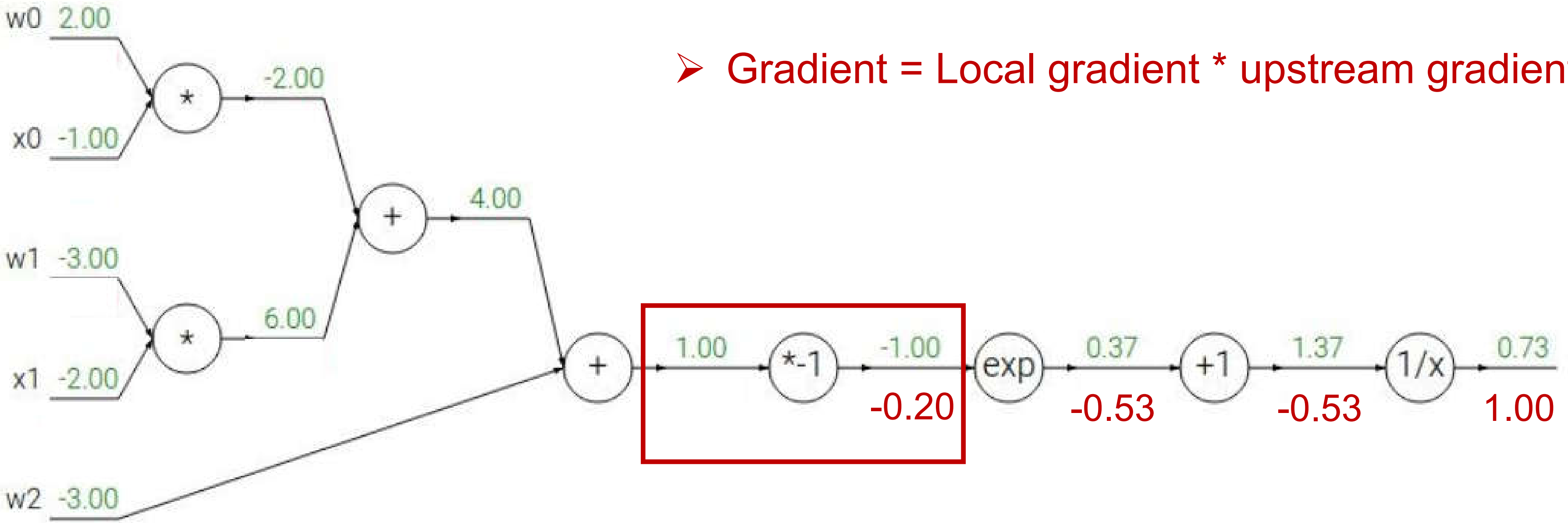

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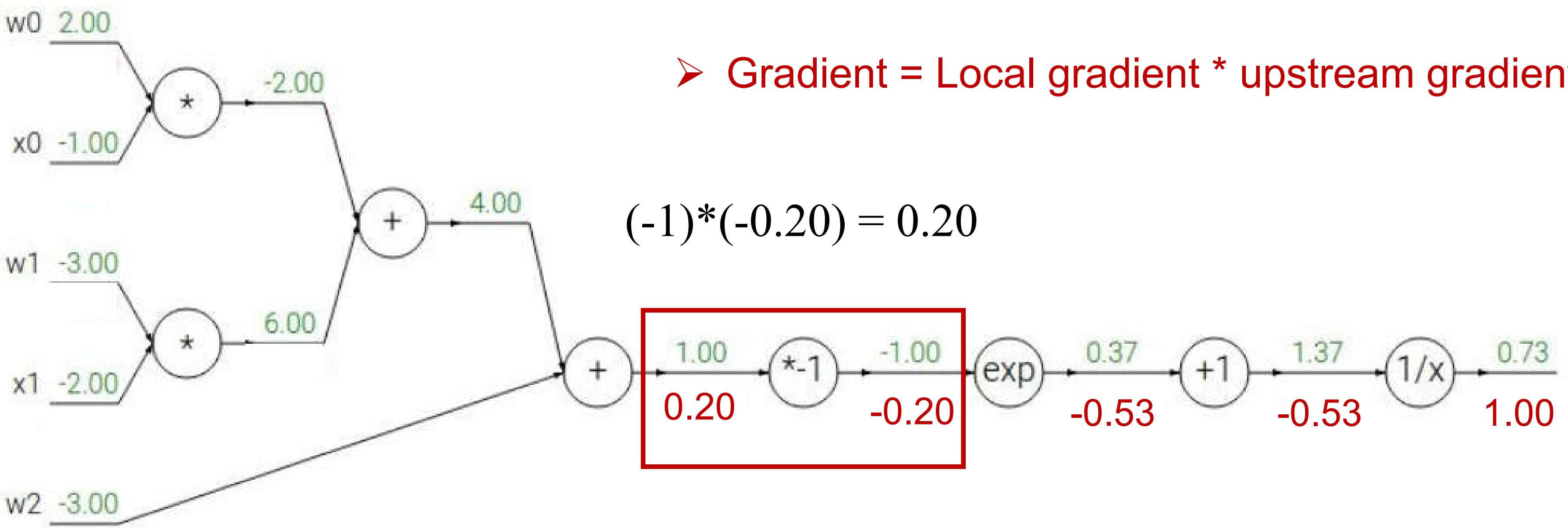

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$$(1)*(0.20) = 0.20$$

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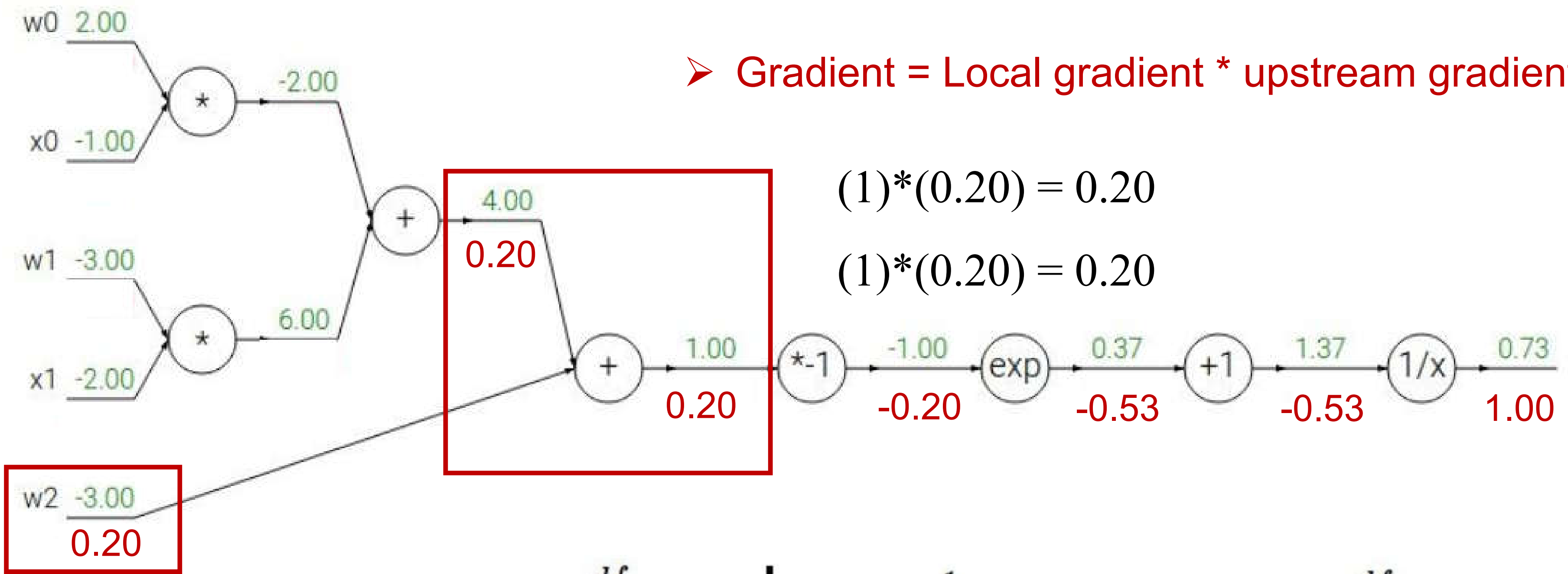

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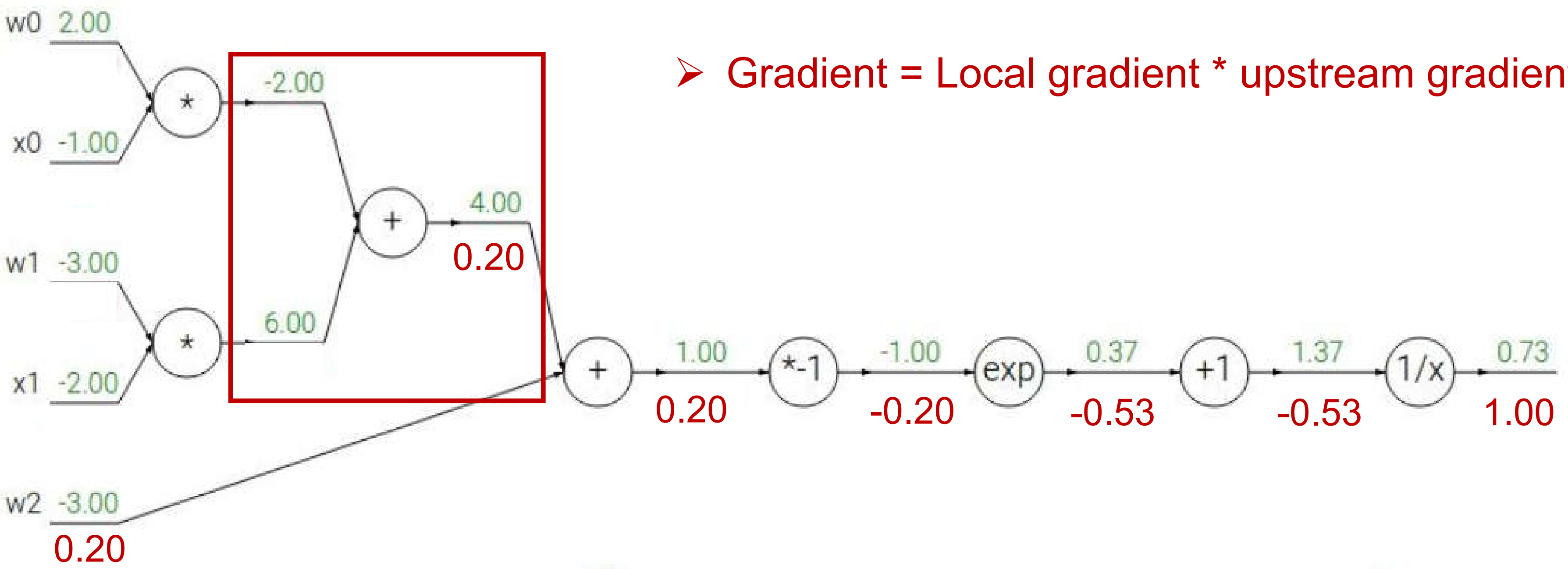

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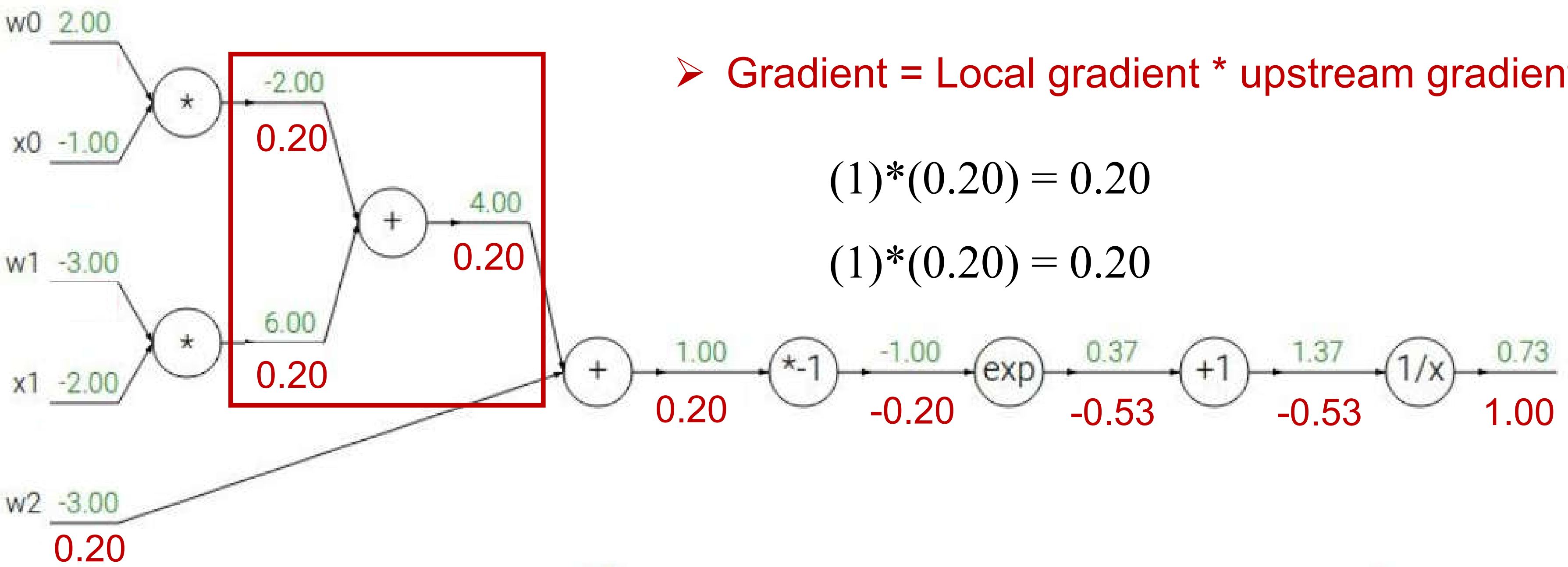

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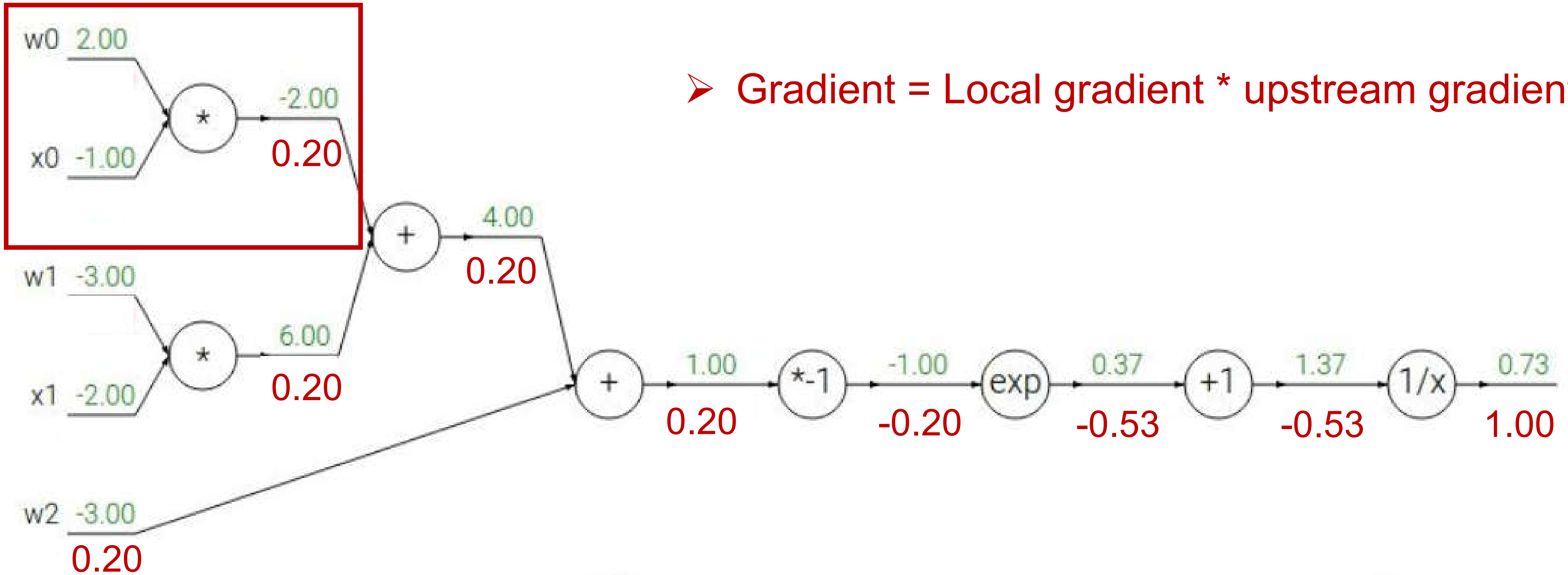
$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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

Another Example

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



- Gradient = Local gradient * upstream gradient

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

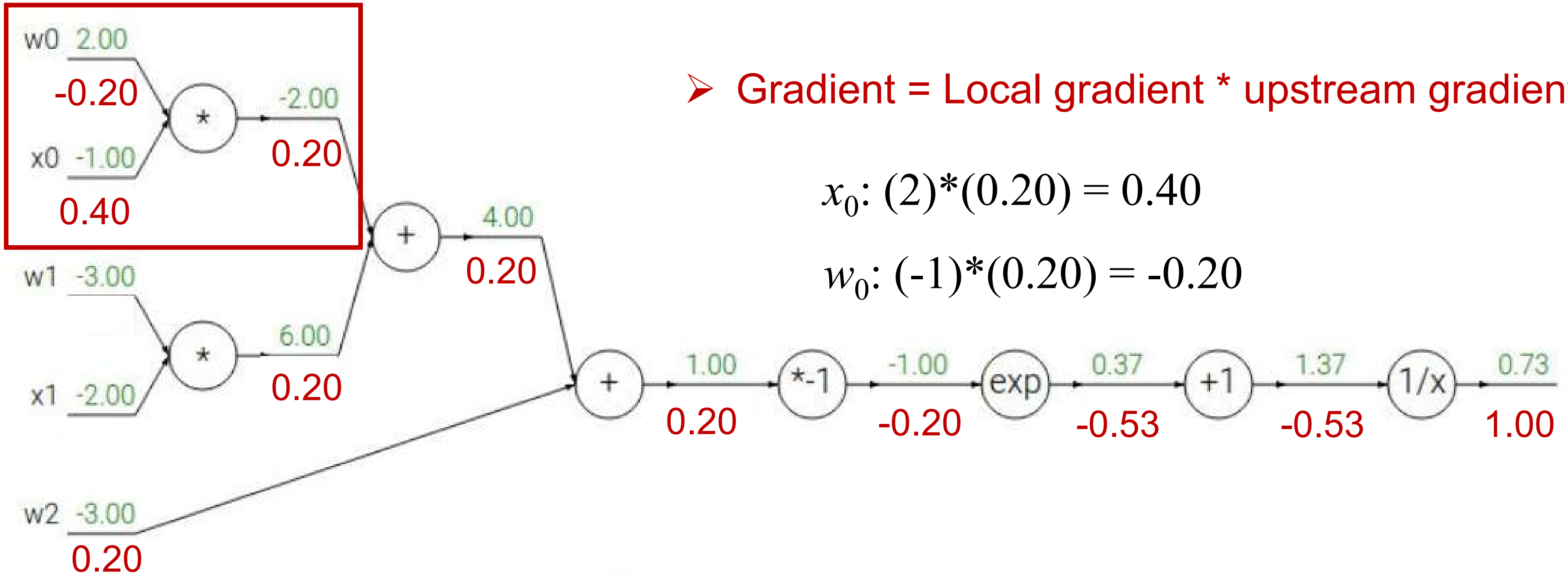
$$\boxed{f_a(x)=ax \quad \rightarrow \quad \frac{df}{dx}=a}$$

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

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

Another Example

Sigmoid Neuron: $f(w,x)=\dfrac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$



- Gradient = Local gradient * upstream gradient

x_0: (2)*(0.20) = 0.40

w_0: (-1)*(0.20) = -0.20

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

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

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

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

Another Example

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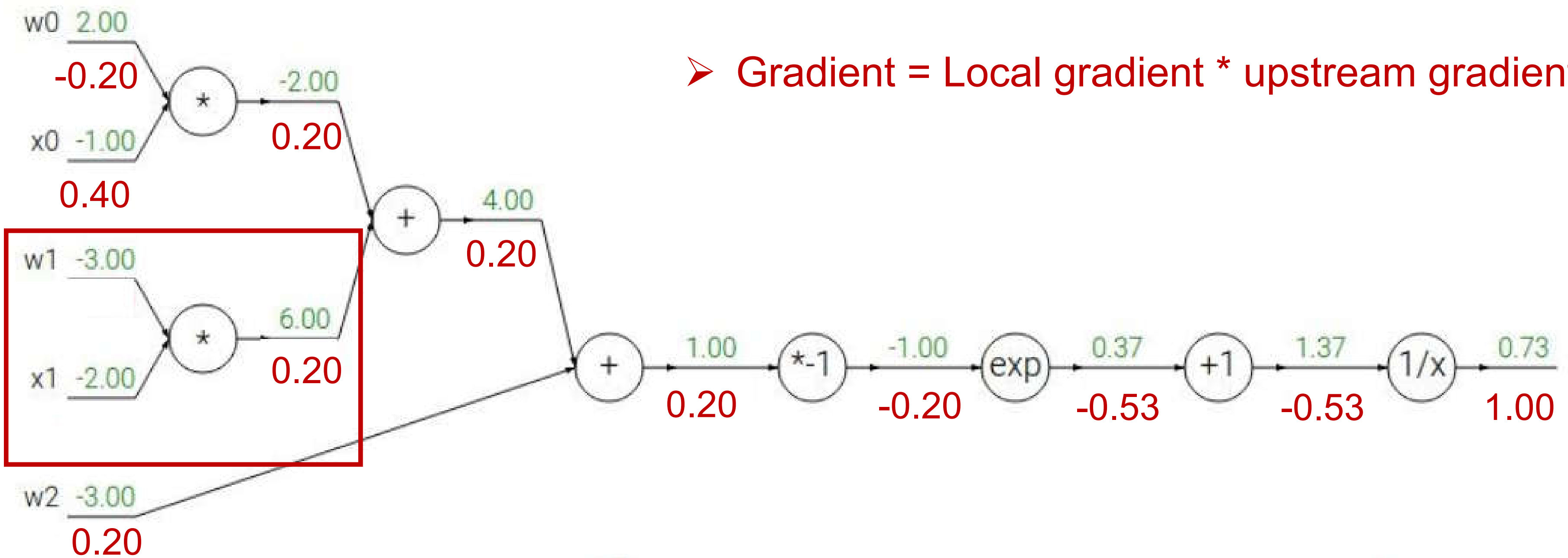


- Gradient = Local gradient * upstream gradient

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

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

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

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

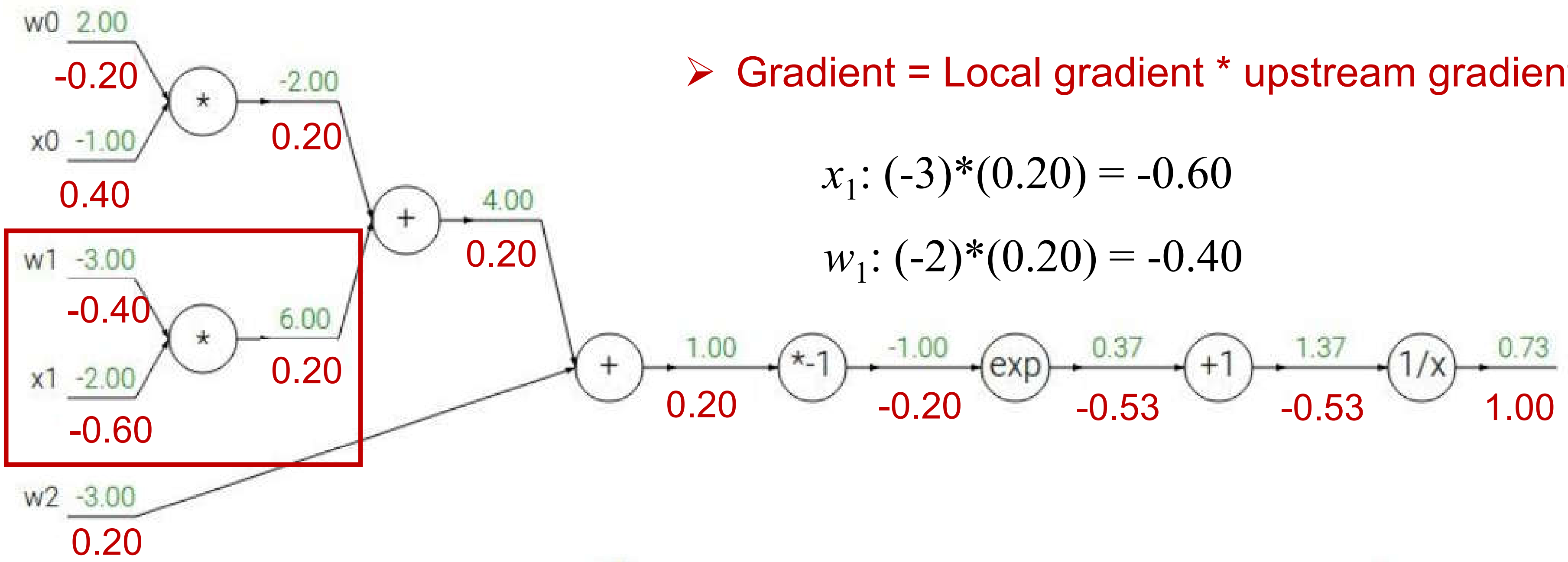
Another Example

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

- Gradient = Local gradient * upstream gradient

x_1: (-3)*(0.20) = -0.60

w_1: (-2)*(0.20) = -0.40



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

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

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

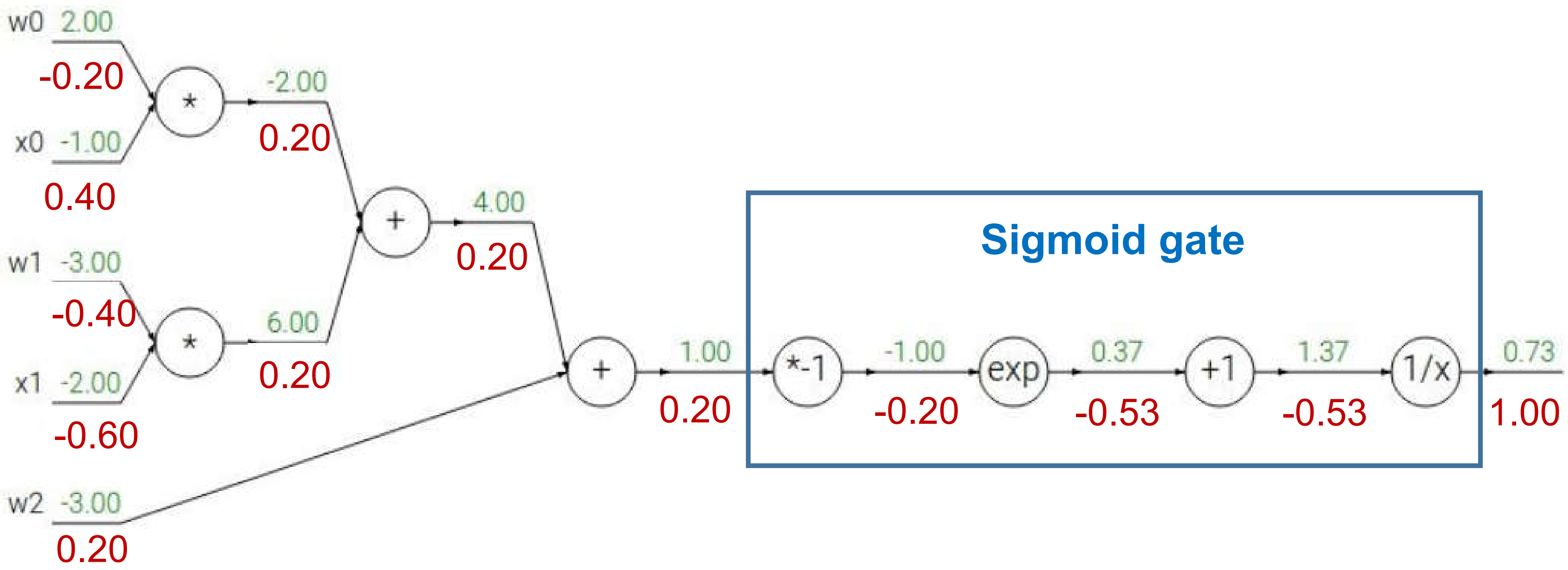
$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

Sigmoid Function

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

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

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



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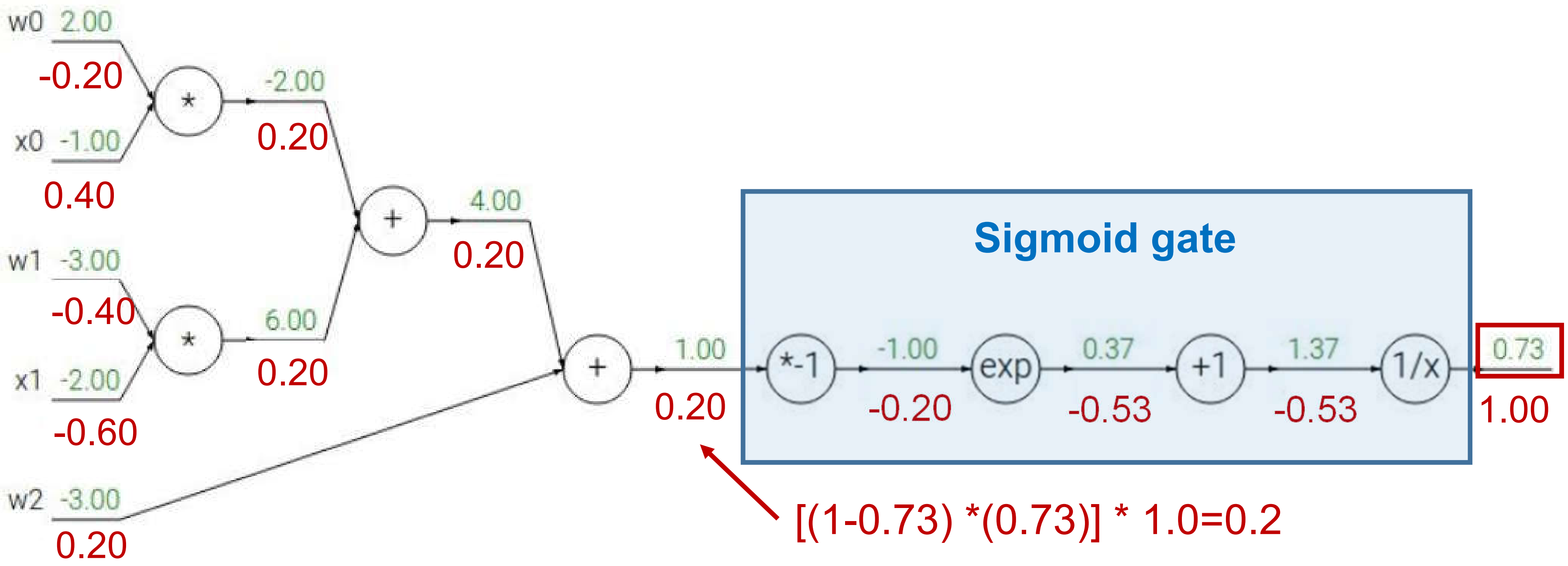
Sigmoid Function

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

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

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



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Patterns in Backward Flow

add gate: gradient distributor

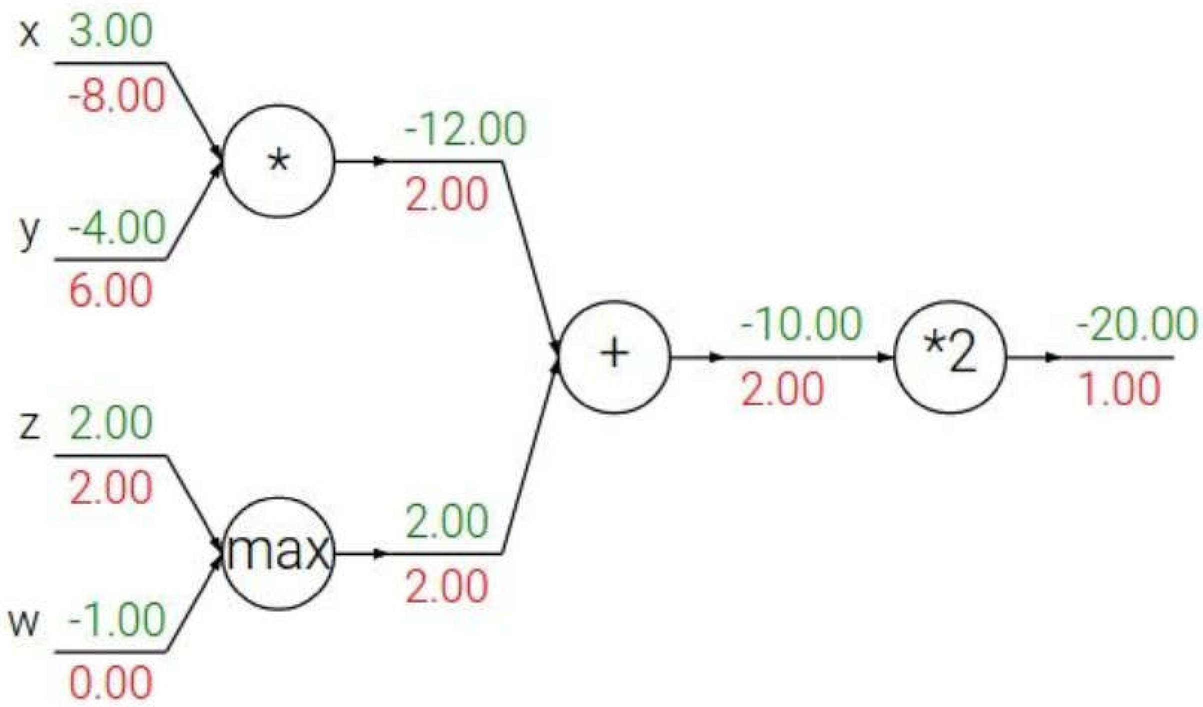
max gate: gradient router

mul gate: gradient “switcher”

max(-1, 2) = 2

max(-1+δ, 2) = 2

max(-1, 2+δ) = 2+δ



Question #1: what will happen in max gate when two inputs are the same?

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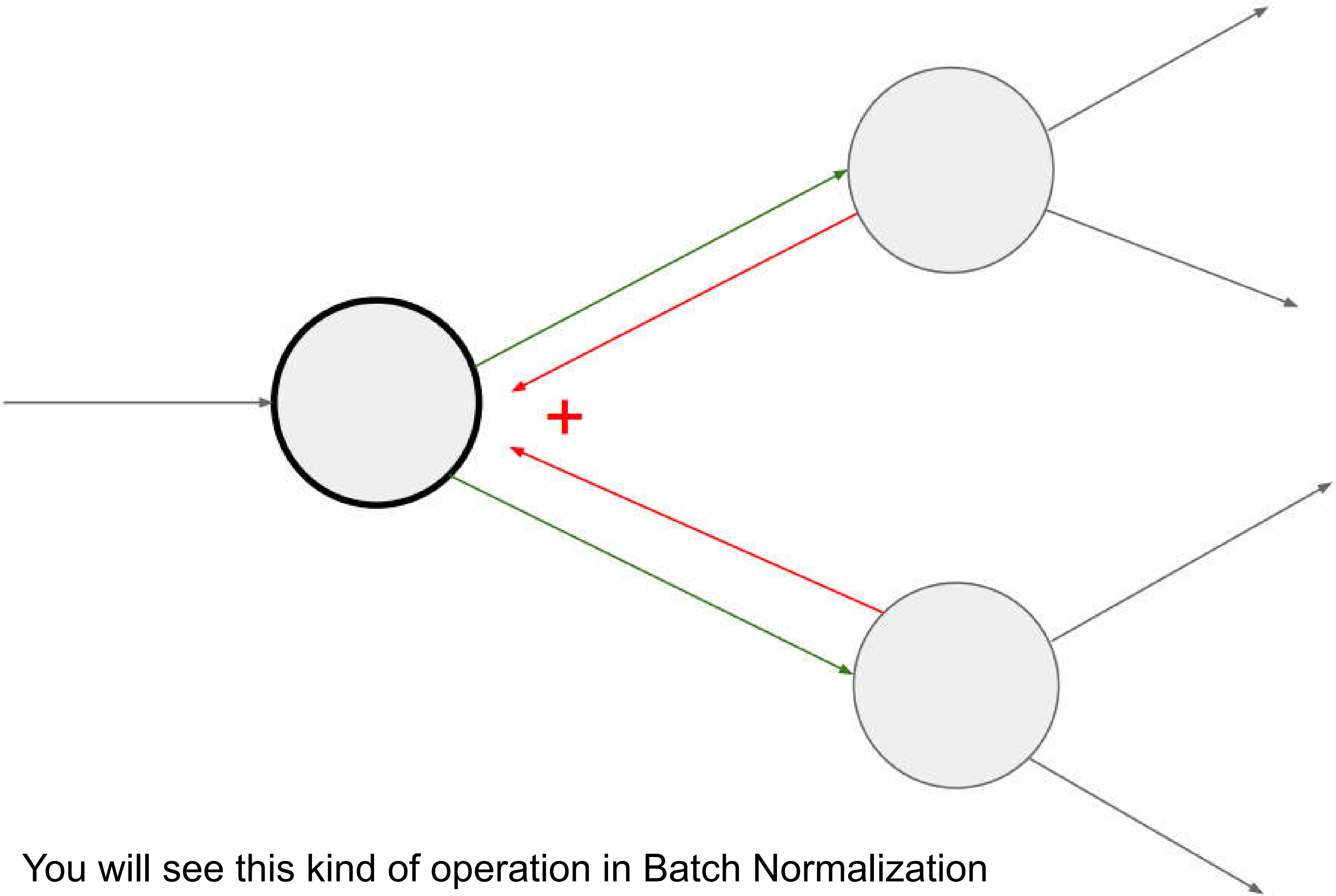
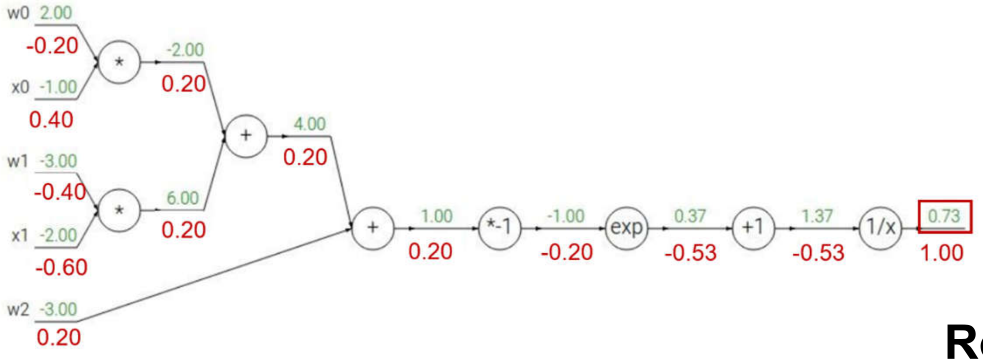
Gradients Add at Branches



- You will see this kind of operation in Batch Normalization

Forward/Backward API

Implementation: Forward/Backward API



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
```

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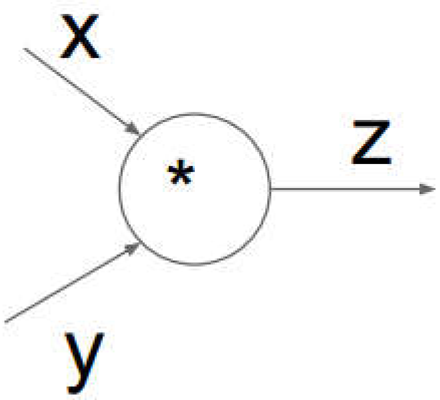
Implementation: Forward/Backward API




```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        return z
    def backward(dz):
        # dx = ... #todo
        # dy = ... #todo
        return [dx, dy]
```

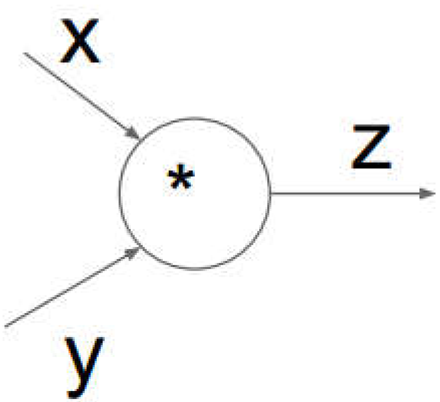
Chain rule

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

$$\frac{\partial L}{\partial x}$$

(x, y, z are scalars)

Implementation: Forward/Backward API




```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
    def backward(dz):
        dx = self.y * dz # [dz/dx * dL/dz]
        dy = self.x * dz # [dz/dy * dL/dz]
        return [dx, dy]
```

cache

(x, y, z are scalars)

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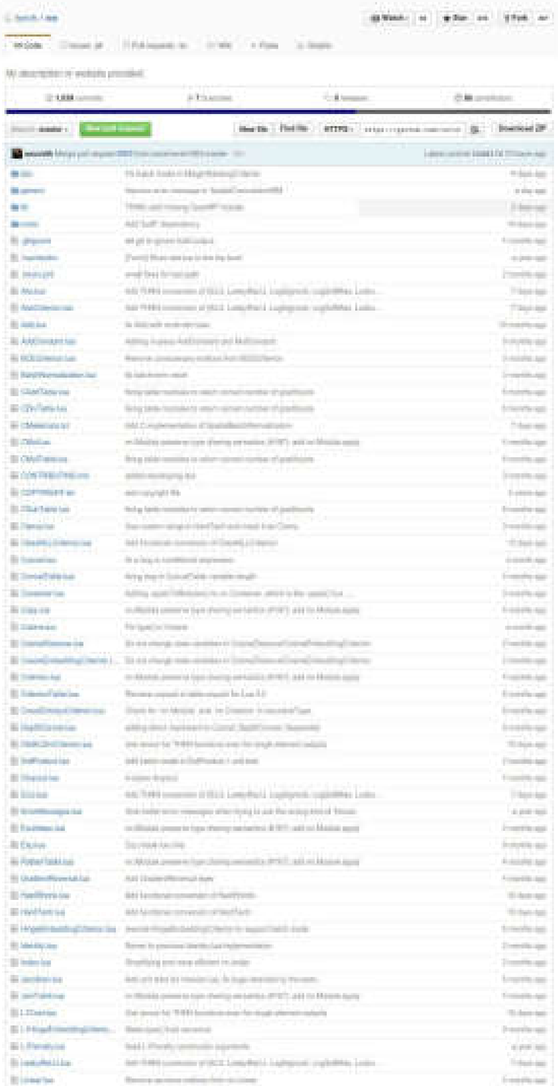
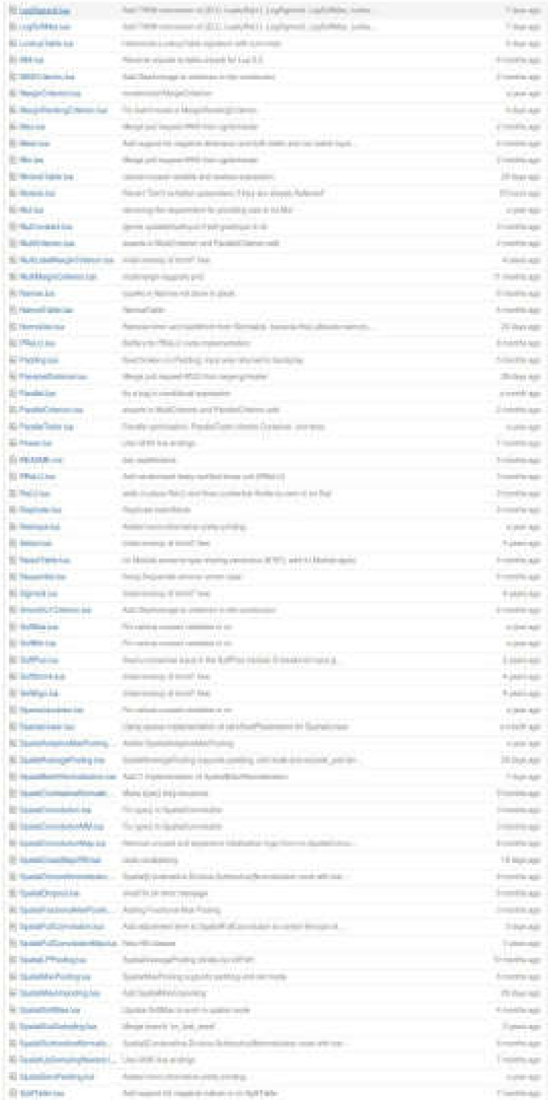
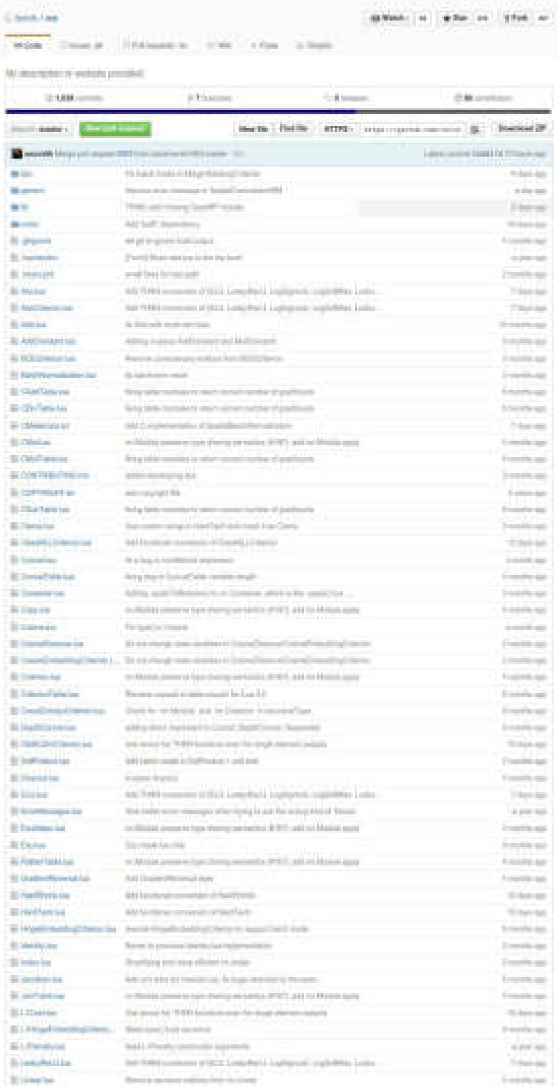
Example: Torch Layers





Example: Torch Layers



=

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Example: Torch MulConstant

```lua
local MulConstant, parent = torch.class('nn.MulConstant', 'nn.Module')

function MulConstant:__init(constant_scalar,ip)
  parent.__init(self)
  assert(type(constant_scalar) == 'number', 'input is not scalar!')
  self.constant_scalar = constant_scalar

  -- default for inplace is false
   self.inplace = ip or false
   if (ip and type(ip) ~= 'boolean') then
      error('in-place flag must be boolean')
   end
end

function MulConstant:updateOutput(input)
  if self.inplace then
    input:mul(self.constant_scalar)
    self.output = input
  else
    self.output:resizeAs(input)
    self.output:copy(input)
    self.output:mul(self.constant_scalar)
  end
  return self.output
end

function MulConstant:updateGradInput(input, gradOutput)
  if self.gradInput then
    if self.inplace then
      gradOutput:mul(self.constant_scalar)
      self.gradInput = gradOutput
      -- restore previous input value
      input:div(self.constant_scalar)
    else
      self.gradInput:resizeAs(gradOutput)
      self.gradInput:copy(gradOutput)
      self.gradInput:mul(self.constant_scalar)
    end
    return self.gradInput
  end
end
```

$$f(X) = aX$$

Initialization()

Forward()

Backward()

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Example: Caffe Layers

Caffe Sigmoid Layer

```cpp
#include <cmath>
#include <vector>

#include "caffe/layers/sigmoid_layer.hpp"

namespace caffe {

template <typename Dtype>
inline Dtype sigmoid(Dtype x) {
  return 1. / (1. + exp(-x));
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Forward_cpu(const vector<Blob<Dtype>*>& bottom,
    const vector<Blob<Dtype>*>& top) {
  const Dtype* bottom_data = bottom[0]->cpu_data();
  Dtype* top_data = top[0]->mutable_cpu_data();
  const int count = bottom[0]->count();
  for (int i = 0; i < count; ++i) {
    top_data[i] = sigmoid(bottom_data[i]);
  }
}

template <typename Dtype>
void SigmoidLayer<Dtype>::Backward_cpu(const vector<Blob<Dtype>*>& top,
    const vector<bool>& propagate_down,
    const vector<Blob<Dtype>*>& bottom) {
  if (propagate_down[0]) {
    const Dtype* top_data = top[0]->cpu_data();
    const Dtype* top_diff = top[0]->cpu_diff();
    Dtype* bottom_diff = bottom[0]->mutable_cpu_diff();
    const int count = bottom[0]->count();
    for (int i = 0; i < count; ++i) {
      const Dtype sigmoid_x = top_data[i];
      bottom_diff[i] = top_diff[i] * sigmoid_x * (1. - sigmoid_x);
    }
  }
}

#ifdef CPU_ONLY
STUB_GPU(SigmoidLayer);
#endif

INSTANTIATE_CLASS(SigmoidLayer);


}  // namespace caffe
```

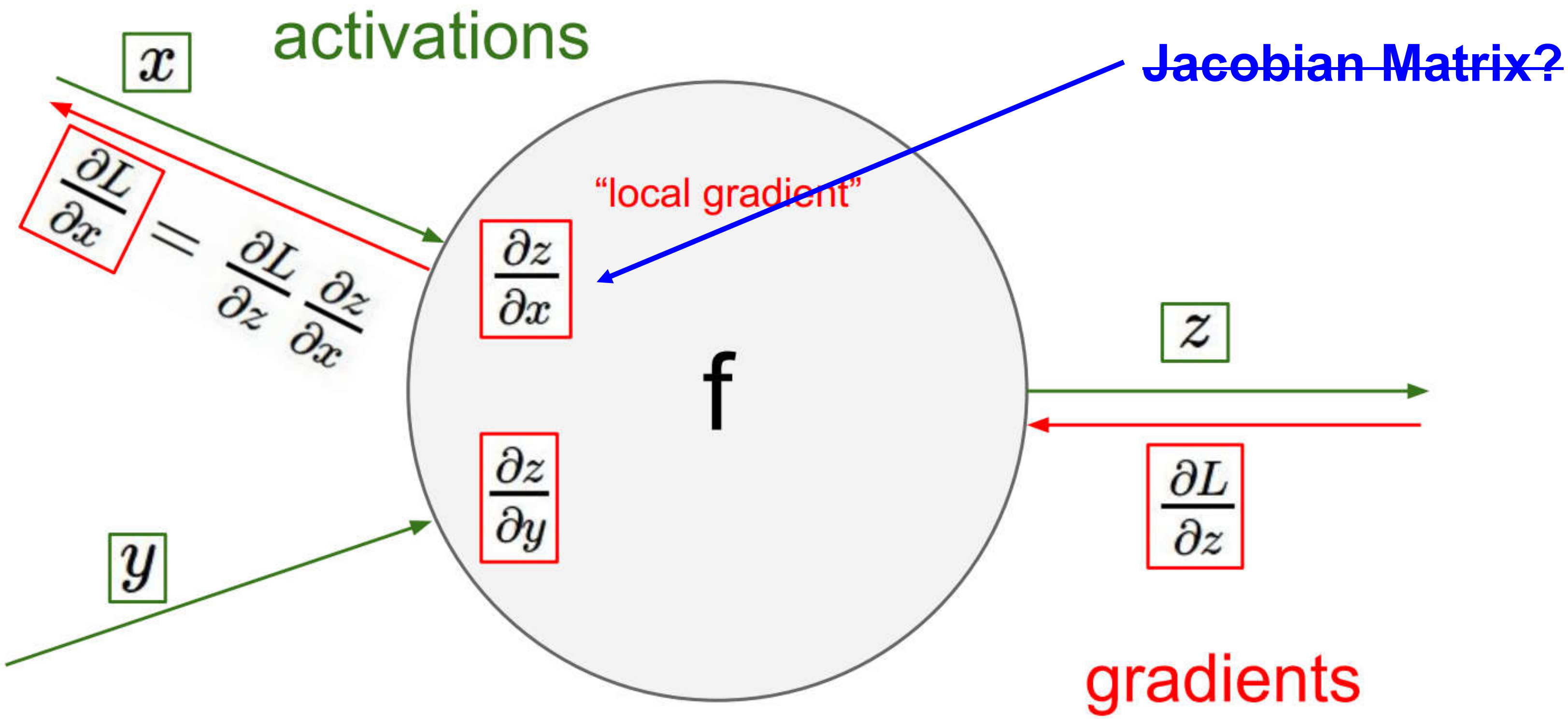
Forward_cpu

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

Backward_cpu

$$\boxed{(1-\sigma(x))\sigma(x)}$$ *top_diff (chain rule)

Gradients for Vectorized Code



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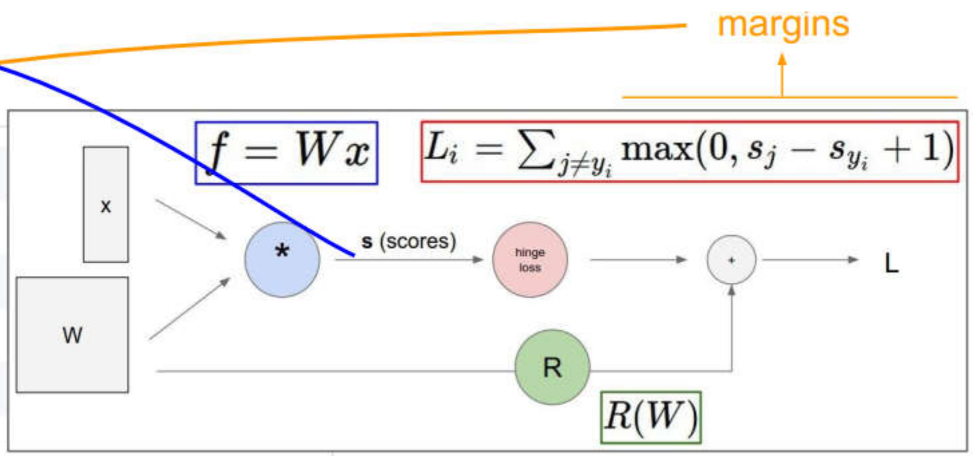
Assignment #1(Q2,Q3): Writing SVM/Softmax

- 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 = #...
```



Computation graph of the SVM loss

Summary so Far

- **Neural nets will be very large:** no hope of writing down gradient formula by hand for all parameters
- **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.

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Neural Network

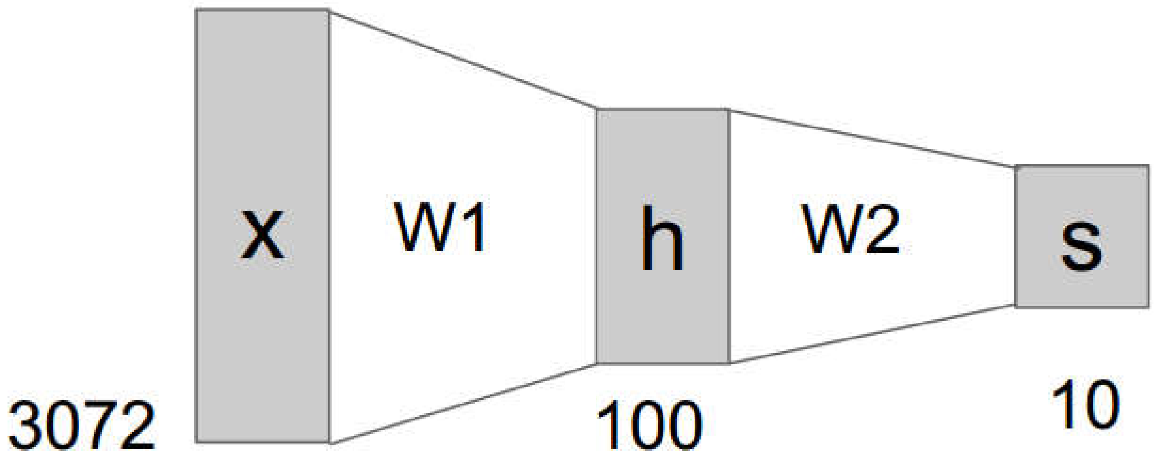
Neural Network: without the Brain Stuff

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

Neural Network: without the Brain Stuff

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

(Now) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$ more complex mathematic expression of X

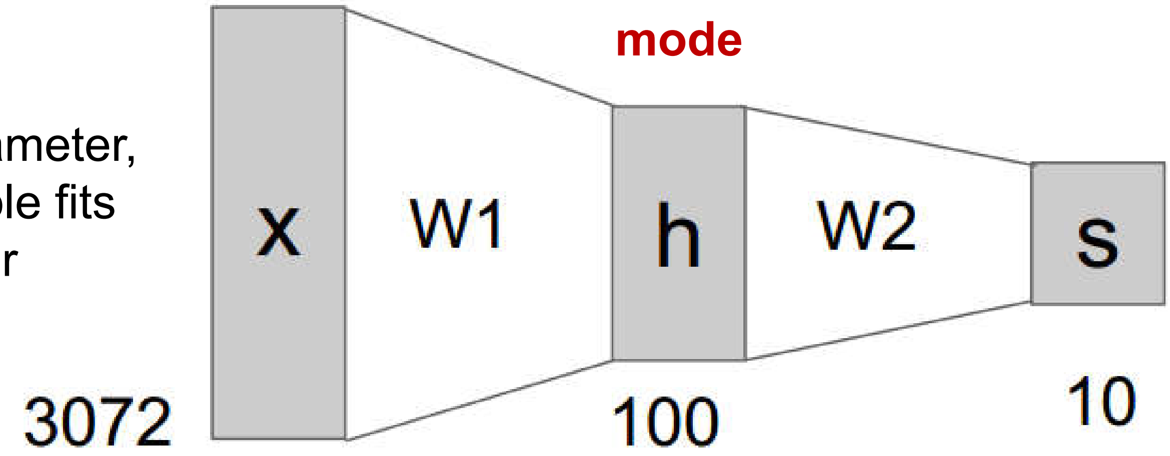


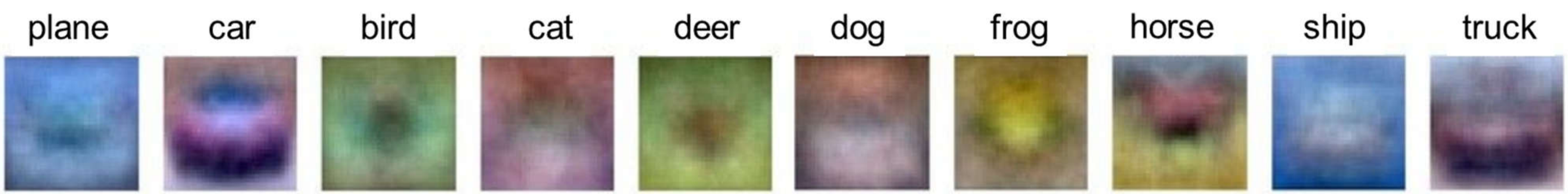
Neural Network: without the Brain Stuff

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

(Now) **2-layer Neural Network** $\boxed{f = W_2 \max(0, W_1 x)}$ more complex mathematic expression of X

- h is a hyperparameter, as big as possible fits in your computer





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Neural Network: Without the Brain Stuff

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

(Now) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$ more complex mathematic expression of X

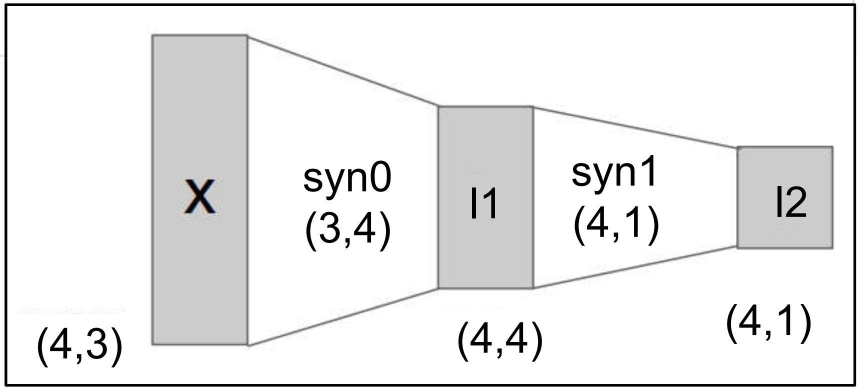
or **3-layer Neural Network** $\boxed{f = W_3 \max(0, W_2 \max(0, W_1 x))}$

Python Code for 2-layer Neural Network

- Full implementation of training a 2-layer Neural Network needs ~11 lines:

```
X = np.array([ [0,0,1],[0,1,1],[1,0,1],[1,1,1] ])
y = np.array([[0,1,1,0]]).T
syn0 = 2*np.random.random((3,4)) - 1
syn1 = 2*np.random.random((4,1)) - 1
for j in xrange(60000):
    l1 = 1/(1+np.exp(-(np.dot(X,syn0))))
    l2 = 1/(1+np.exp(-(np.dot(l1,syn1))))
    l2_delta = (y - l2)*(l2*(1-l2))
    l1_delta = l2_delta.dot(syn1.T) * (l1 * (1-l1))
    syn1 += l1.T.dot(l2_delta)
    syn0 += X.T.dot(l1_delta)
```

Loss = (y – y_predict)



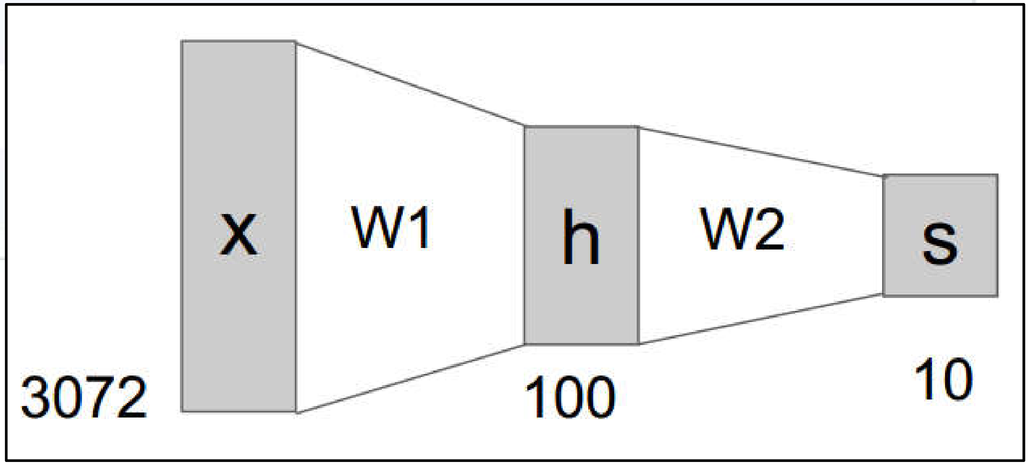
- Sigmoid activation function
- Logistic regression loss

from @iamtrask, http://iamtrask.github.io/2015/07/12/basic-python-network/

Assignment: Writing 2-Layer Net

- Stage your forward/backward computation!

```
# 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 = #...
```



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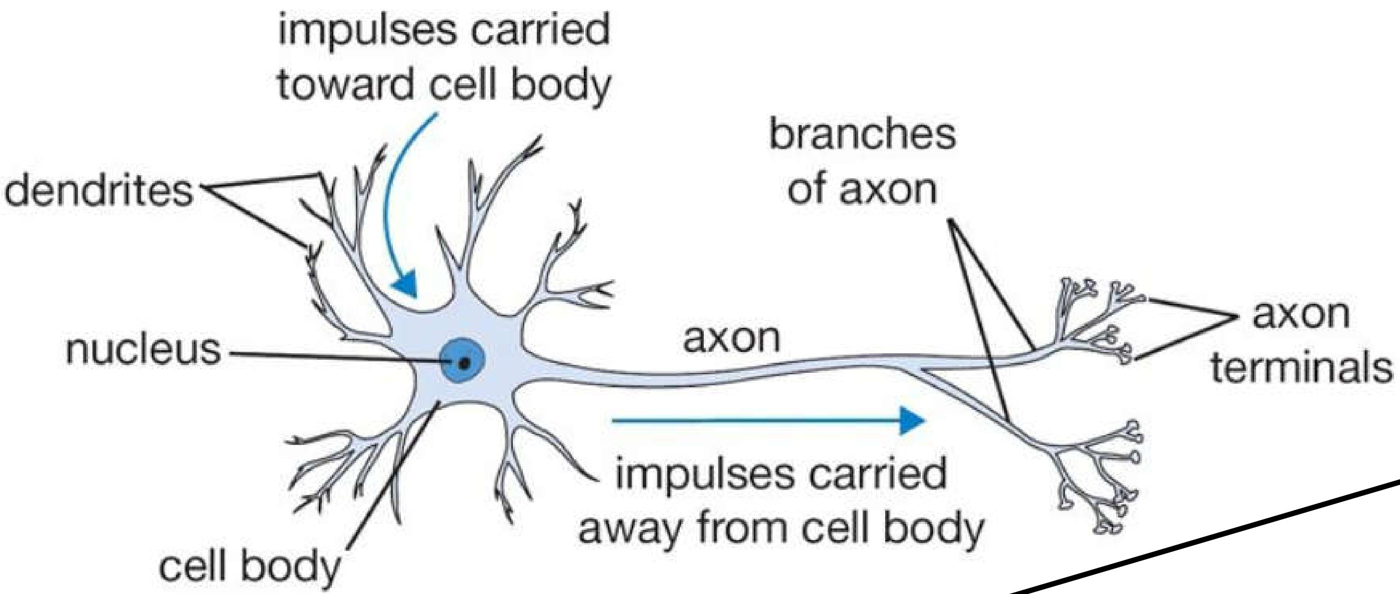
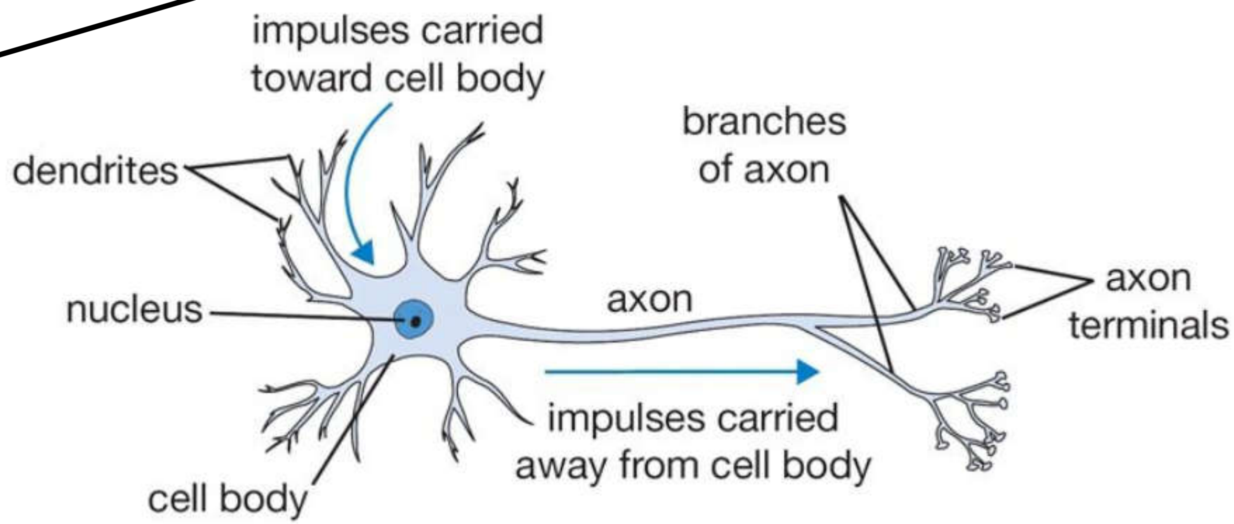
Neural Network Without Brain Stuff

Biological Neuron Without Brain Stuff





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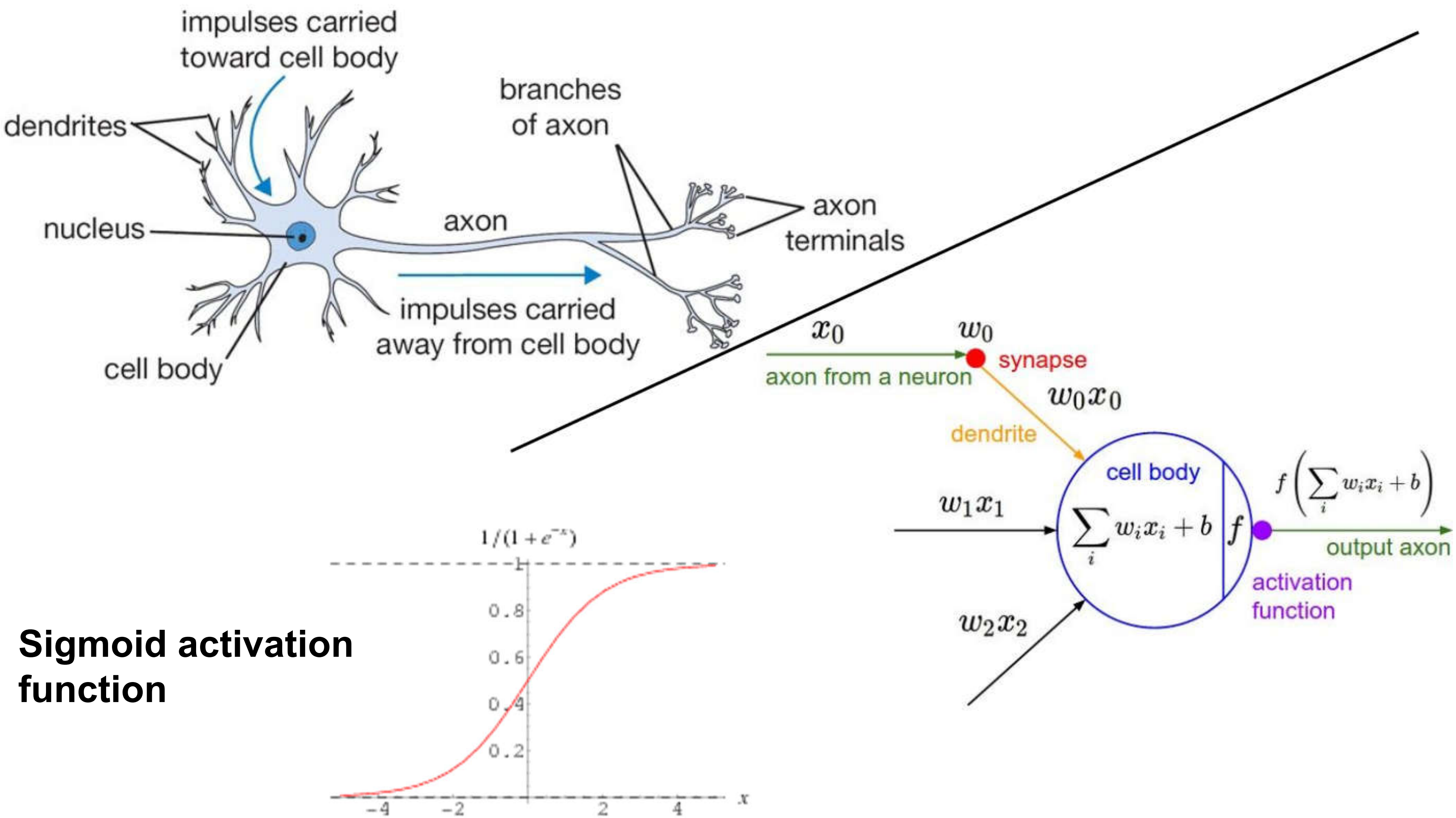
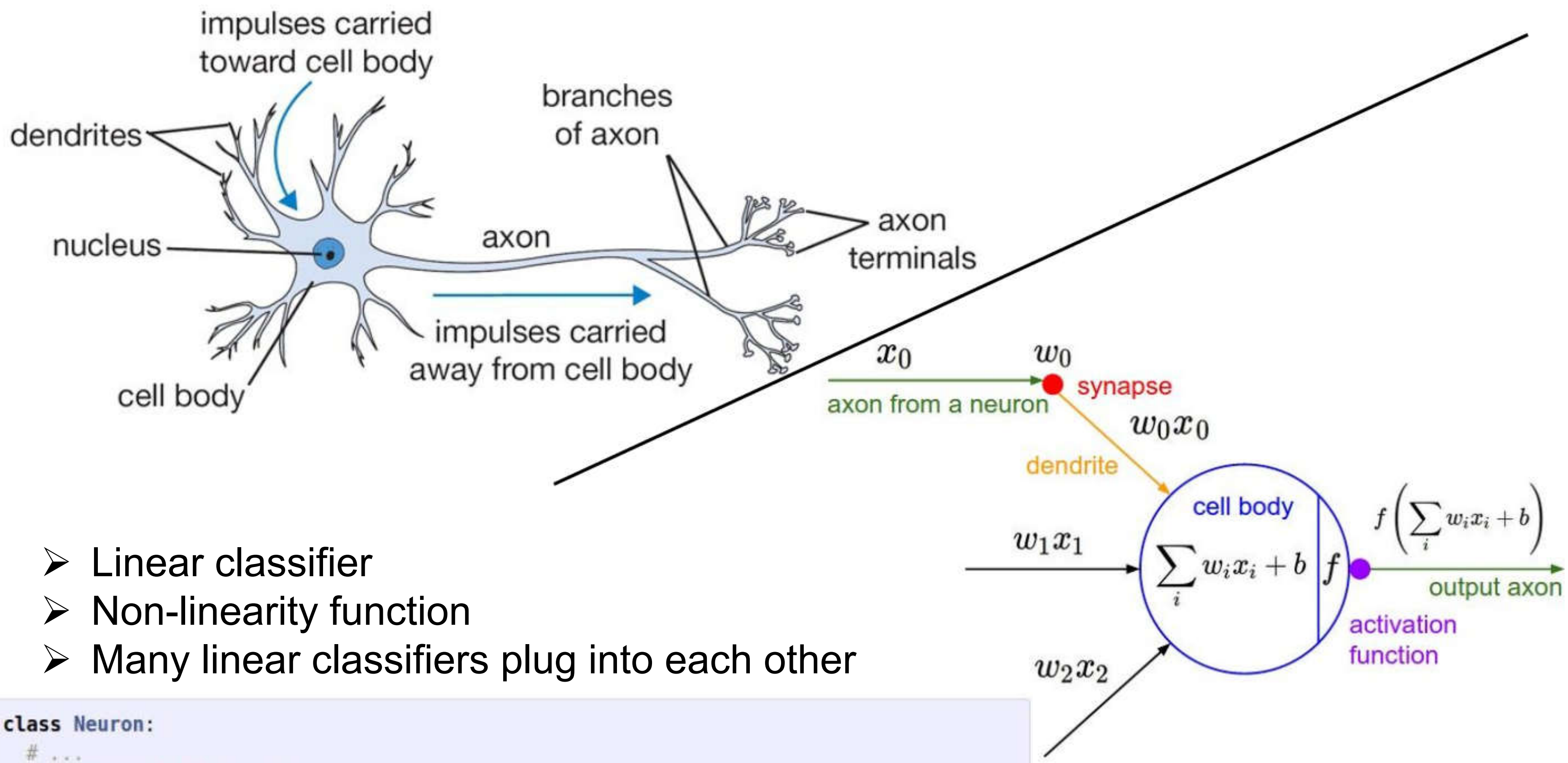
Biological Neuron Without Brain Stuff



Sigmoid activation function

Biological Neuron Without Brain Stuff



- Linear classifier
- Non-linearity function
- Many linear classifiers plug into each other

```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 function
    return firing_rate
```

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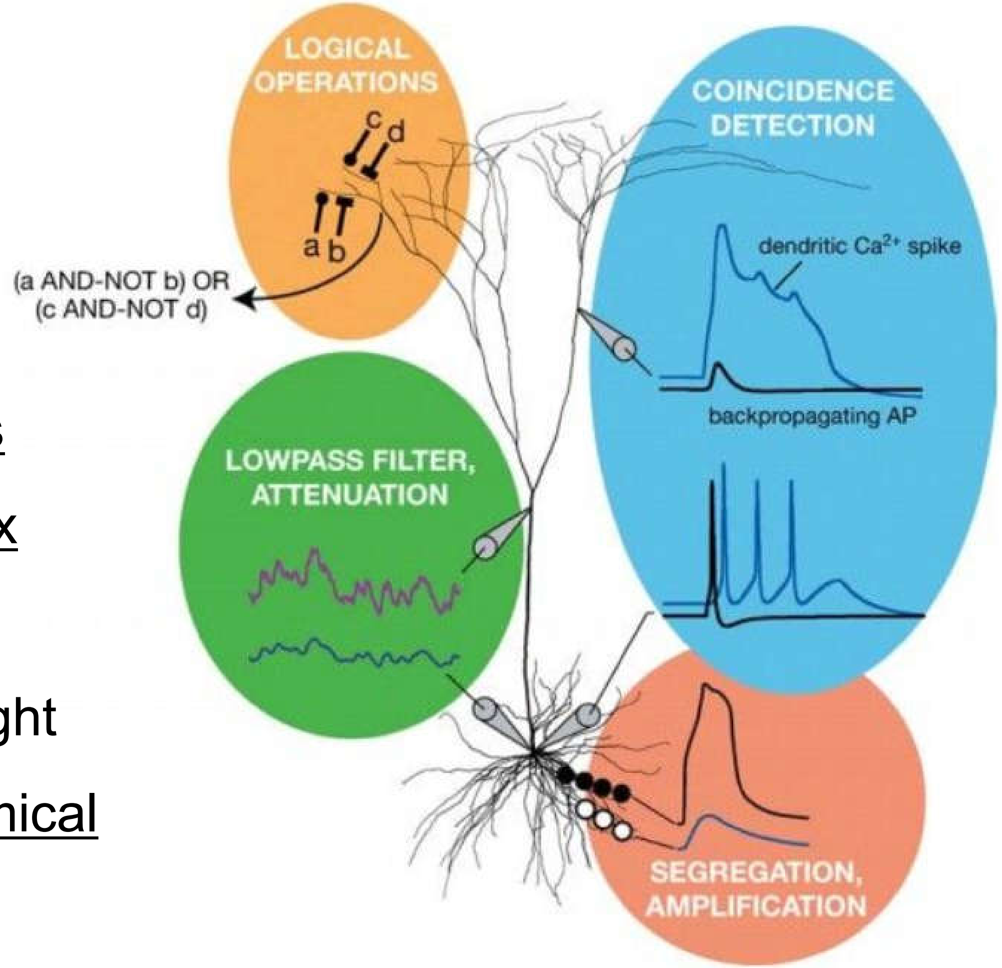
Biological Neuron

Be very careful with your Brain analogies:

Biological Neurons:

- Many different types of neurons
- **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]

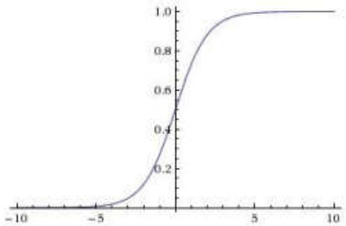
Activation Functions

- Historically people use **Sigmoid and tanh**
- From 2012 **ReLu** became quite popular (default recommendation)
- A few kind of hipster activation functions: **Leaky Relu**, **Maxout,** and **ELU**

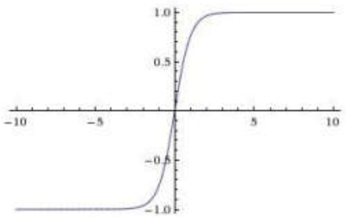
Question #2: why we need activation function?

Sigmoid

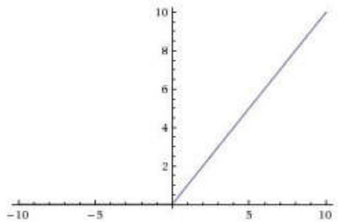
$$\sigma(x) = 1/(1+e^{-x})$$



tanh tanh(x)

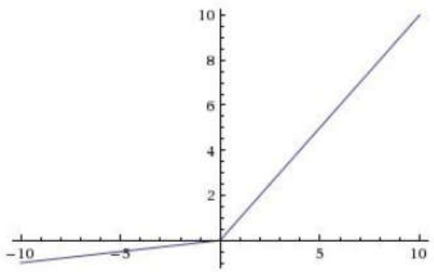


ReLU max(0,x)



Leaky ReLU

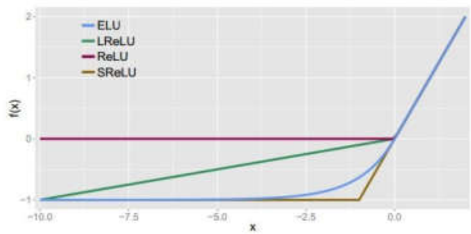
max(0.1x, x)



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

ELU

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \le 0 \end{cases}$$



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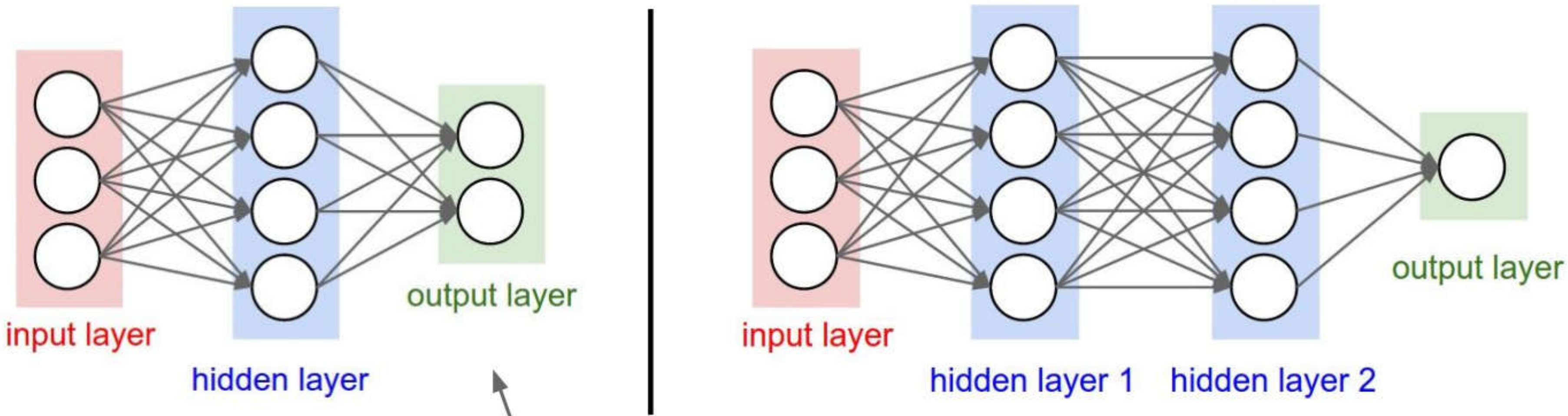
Neural Networks: Architectures



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

“Fully-connected” layers

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

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Example Feed-Forward Computation of a Neural Network

- Assume inputs and weights are 1-D numpy arrays and bias is a number

```
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
```

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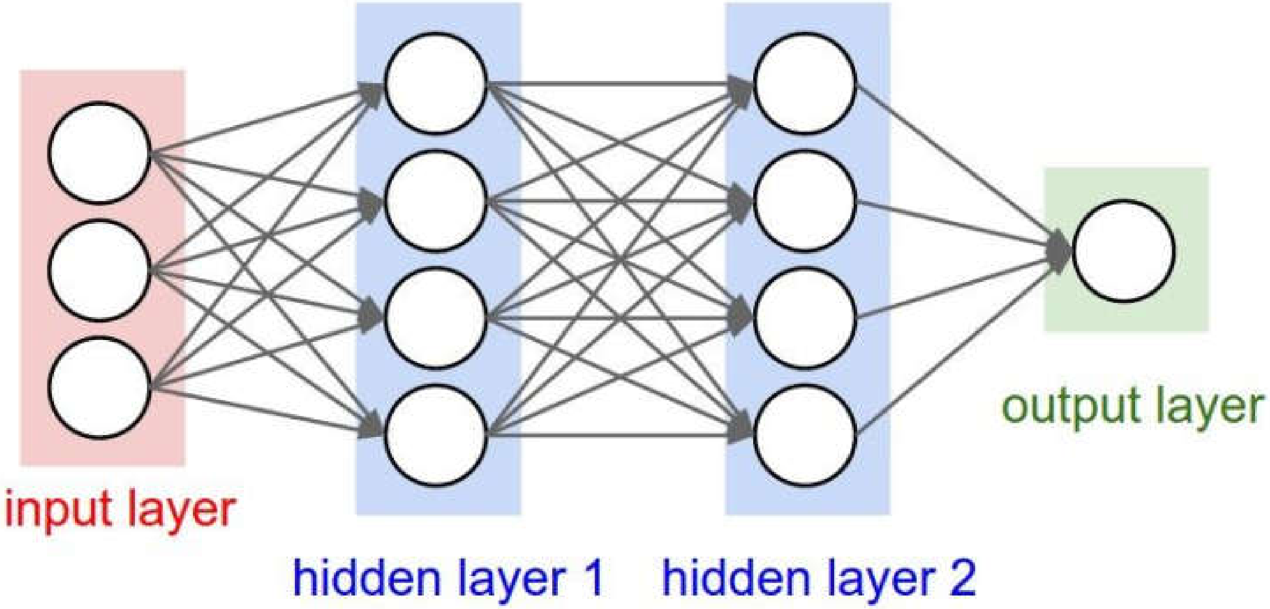
Example Feed-Forward Computation of a Neural Network

- We can compute an entire set of neurons in a single hidden layer using **a single time matrix multiplication**




```
# 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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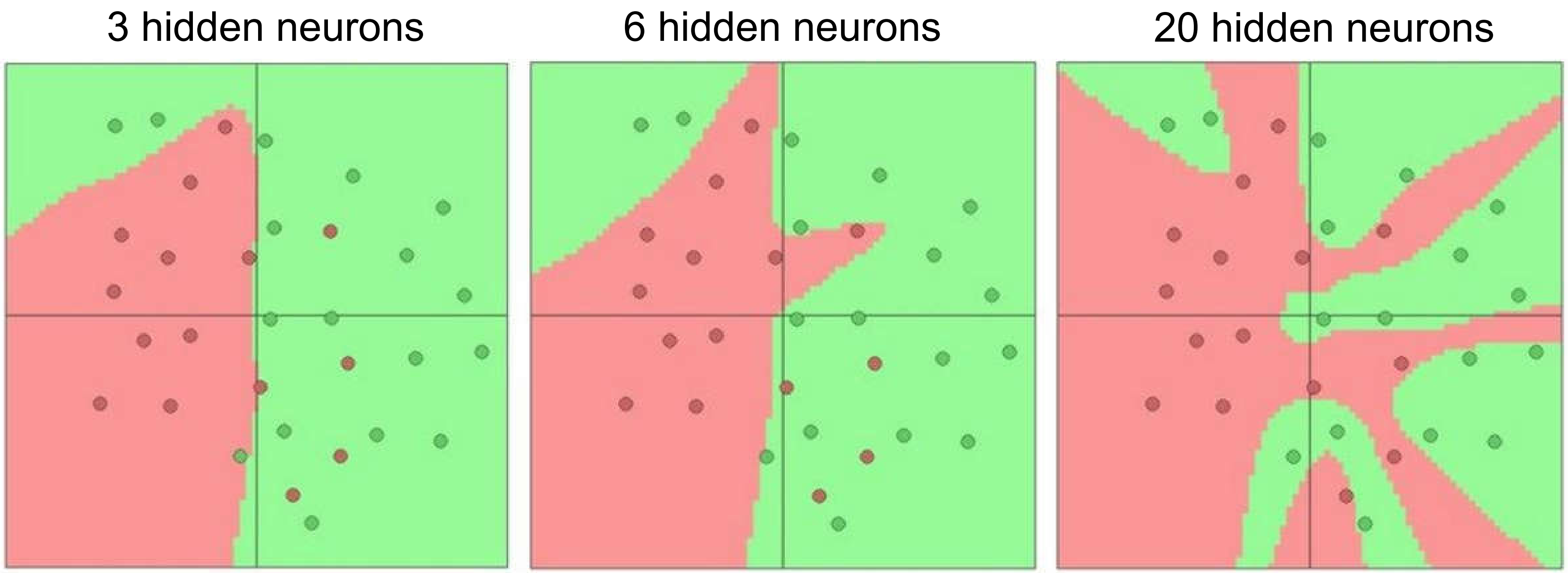
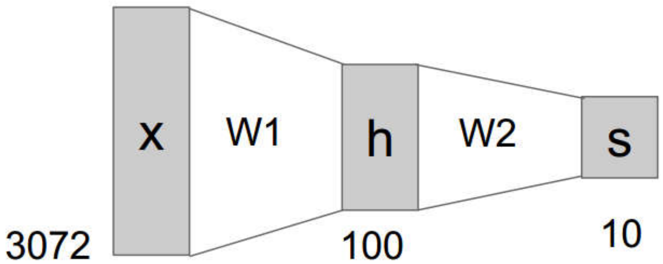
Example of 2-Layer Neural Network

- Setting the **number of neurons** in the hidden layer
- h is **a hyperparameter**

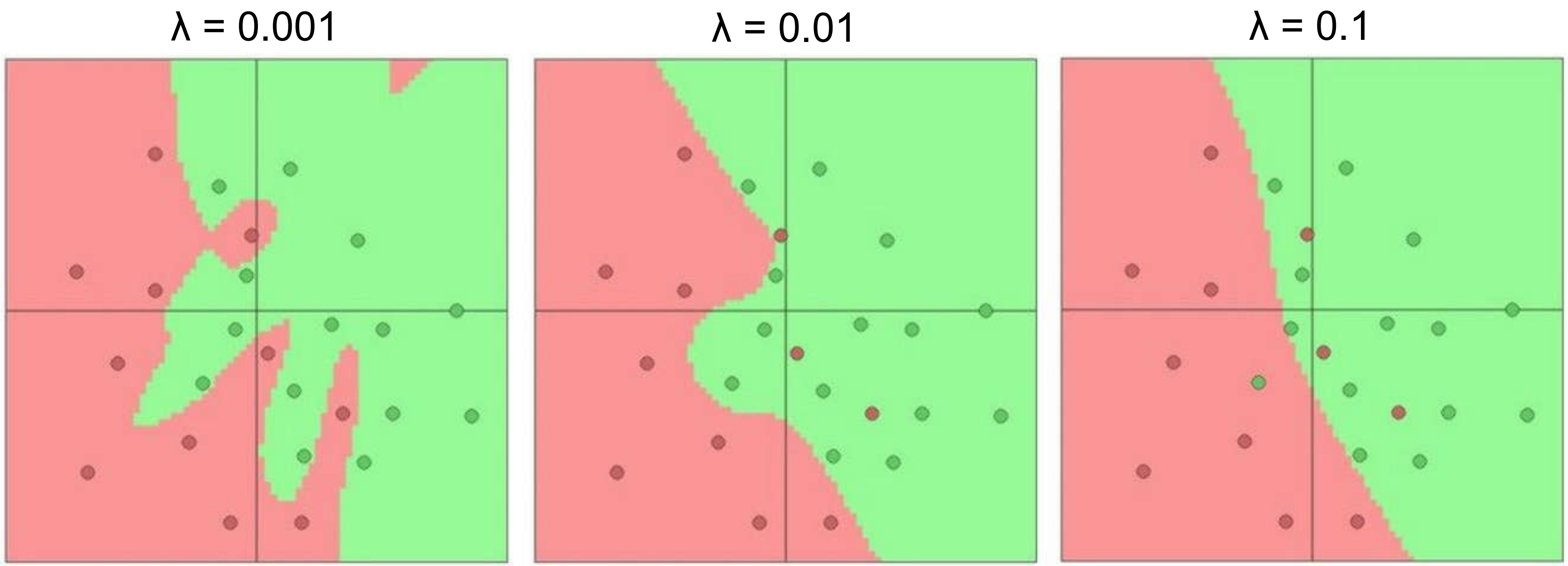




> More neurons = more capacity

Example of 2-Layer Neural Network

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



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

You can play with this demo over at ConvNetJs:
http://cs.Stanford.edu/people/karpathy/convnetjs/demo/classify2d.html

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Summary

- We arrange neurons into **fully-connected layers**
- The abstraction of a layer has the nice property that it allows us to use efficient **vectorized code** (e.g. **matrix multiplies**)
- Neural networks are **not really neural**
- Neural networks: **bigger = better** (<u>but might have to regularize more strongly</u>)

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Next Lecture

More than you ever wanted to know about

Neural Networks and **how to train them**.

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Thank you for your attention!