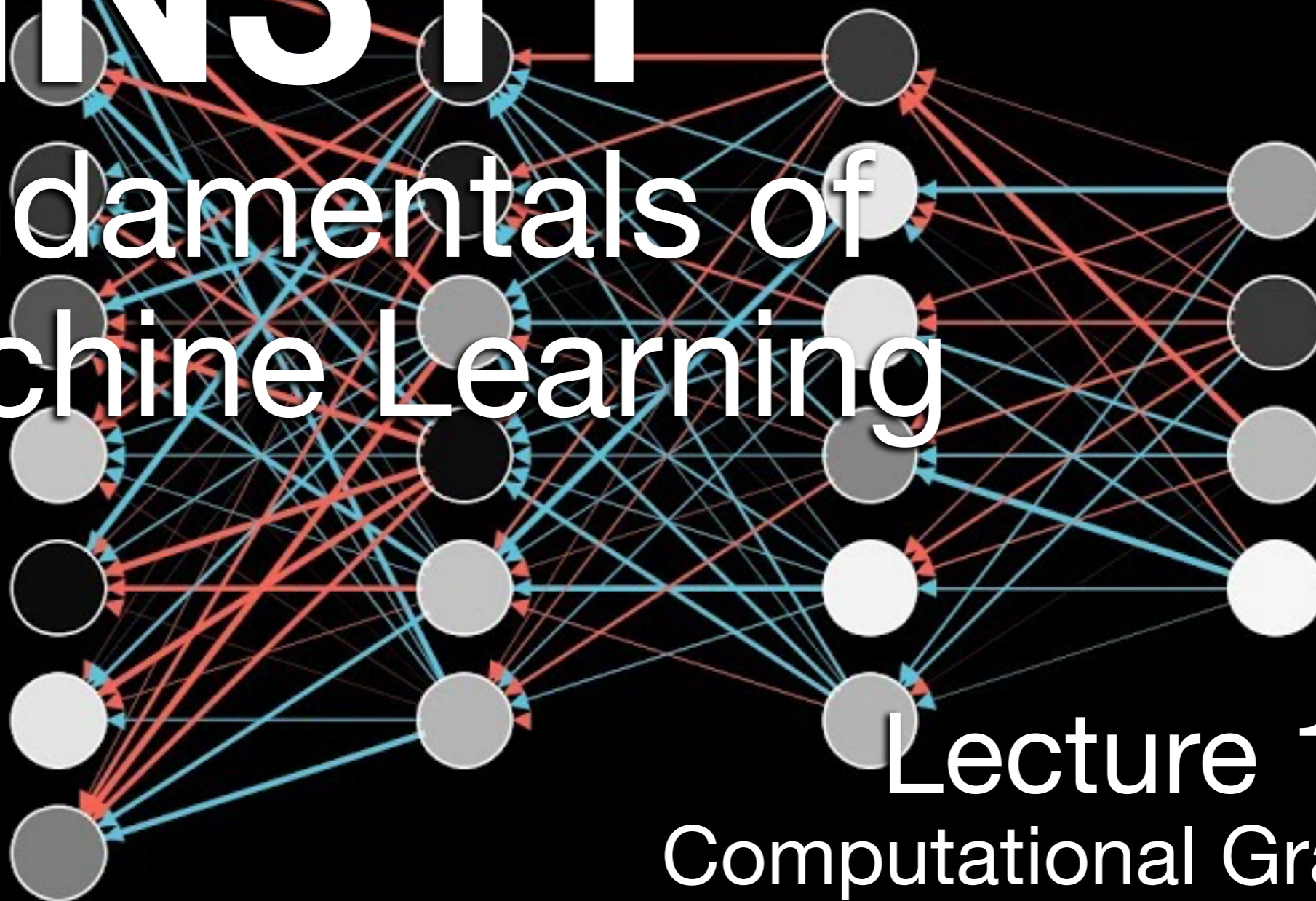


# AIN311



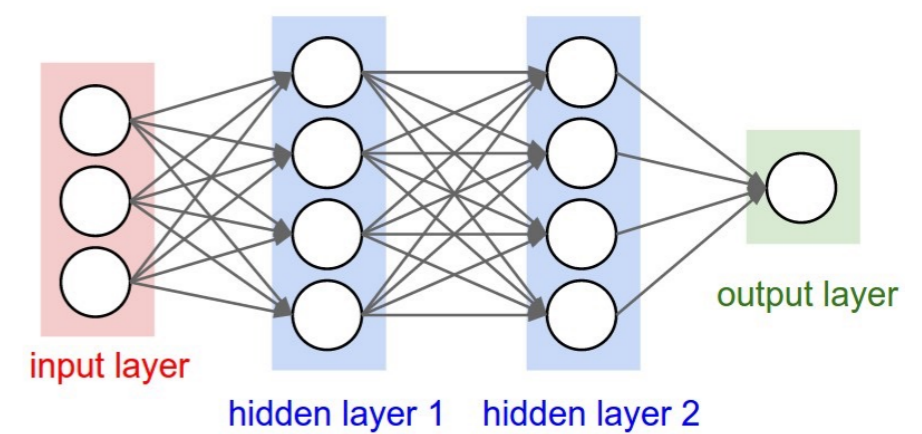
## Fundamentals of Machine Learning



## Lecture 12: Computational Graph Backpropagation

# Last time...

# Multilayer Perceptron

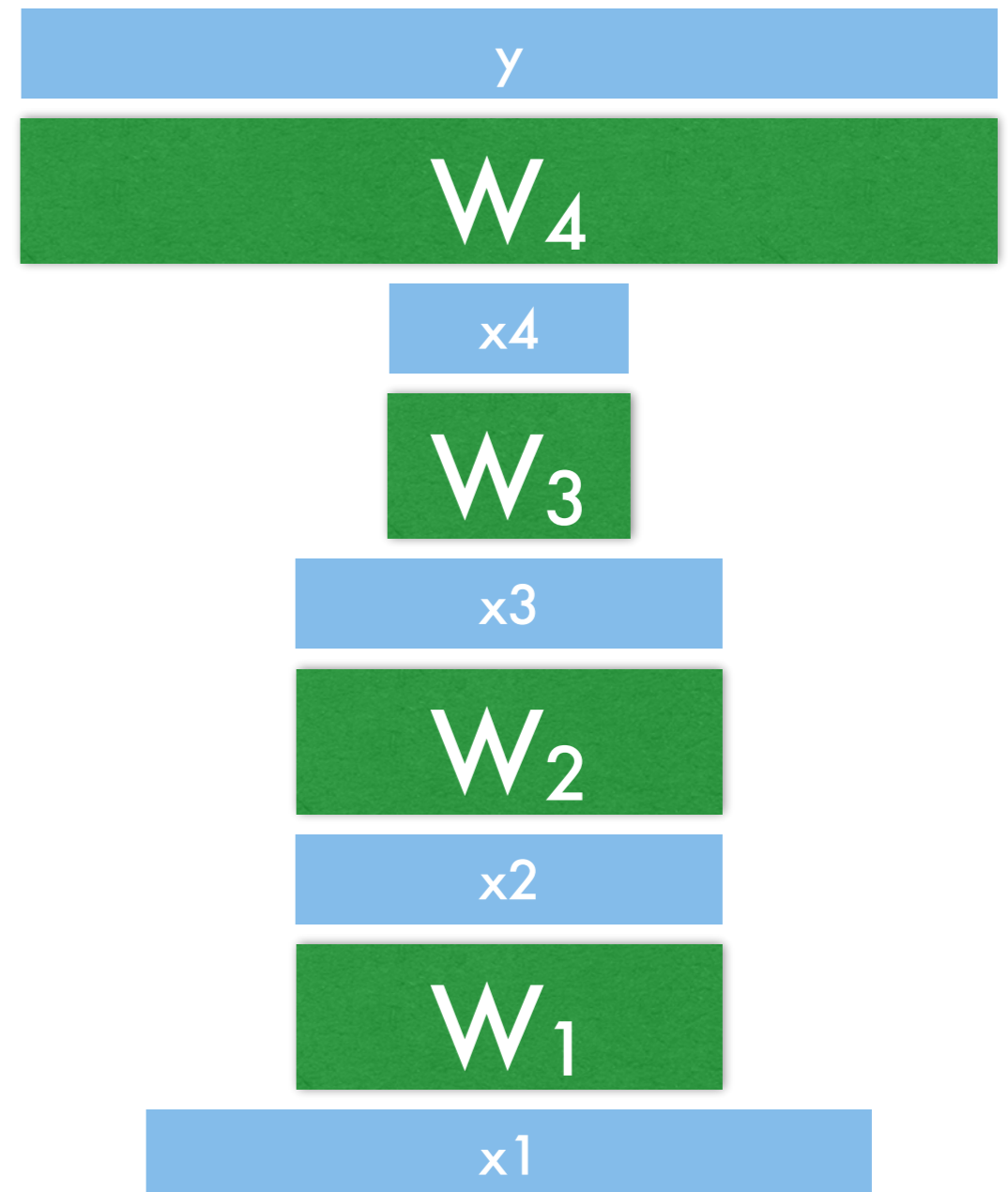


- Layer Representation

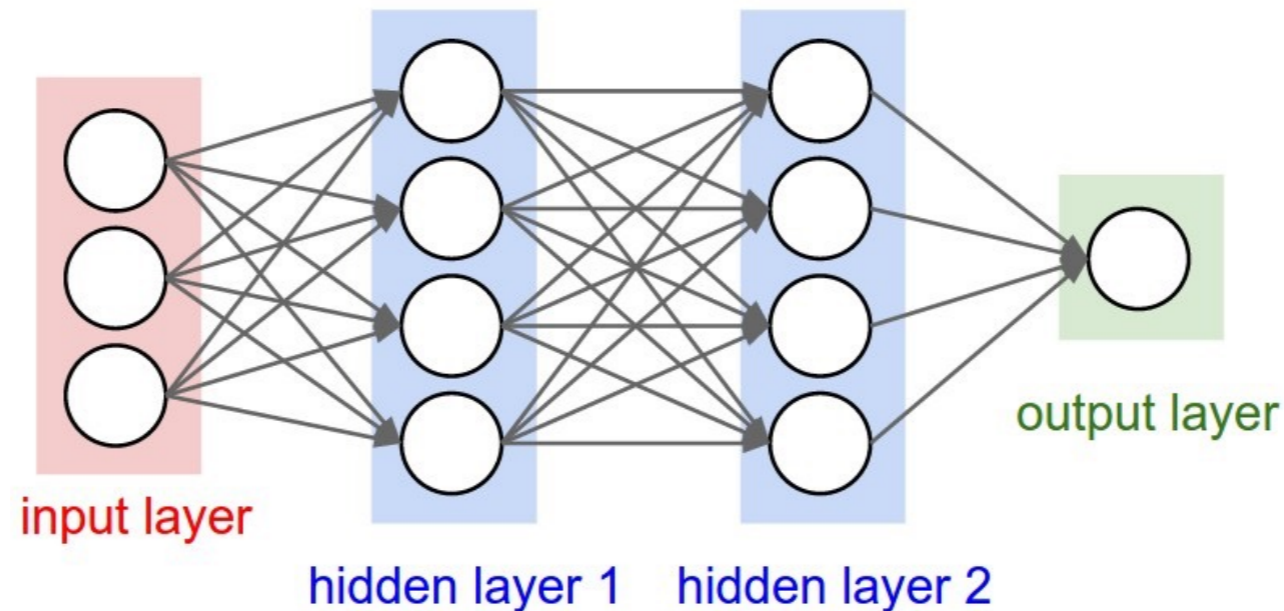
$$y_i = W_i x_i$$

$$x_{i+1} = \sigma(y_i)$$

- (typically) iterate between linear mapping  $Wx$  and nonlinear function
- Loss function  $l(y, y_i)$  to measure quality of estimate so far



# Last time... Forward Pass



- Output of the network can be written as:

$$h_j(\mathbf{x}) = f\left(v_{j0} + \sum_{i=1}^D x_i v_{ji}\right)$$

$$o_k(\mathbf{x}) = g\left(w_{k0} + \sum_{j=1}^J h_j(\mathbf{x}) w_{kj}\right)$$

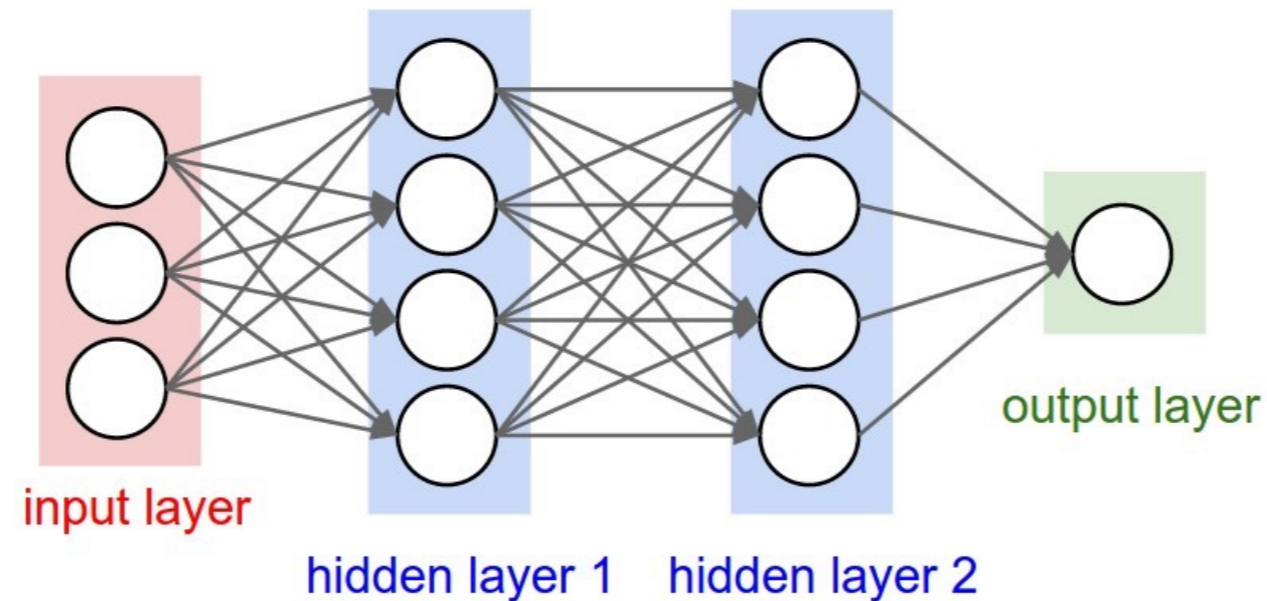
(j indexing hidden units, k indexing the output units, D number of inputs)

- Activation functions  $f$ ,  $g$  : sigmoid/logistic, tanh, or rectified linear (ReLU)

$$\sigma(z) = \frac{1}{1 + \exp(-z)}, \quad \tanh(z) = \frac{\exp(z) - \exp(-z)}{\exp(z) + \exp(-z)}, \quad \text{ReLU}(z) = \max(0, z)$$

# Last time... Forward Pass in Python

- Example code for a forward pass for a 3-layer network in Python:



```
# 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)
```

- Can be implemented efficiently using matrix operations
- Example above:  $W_1$  is matrix of size  $4 \times 3$ ,  $W_2$  is  $4 \times 4$ . What about biases and  $W_3$ ?

# Backpropagation

# Recap: Loss function/Optimization



airplane	-3.45	-0.51	3.42
automobile	-8.87	<b>6.04</b>	4.64
bird	0.09	5.31	2.65
cat	<b>2.9</b>	-4.22	5.1
deer	4.48	-4.19	2.64
dog	8.02	3.58	5.55
frog	3.78	4.49	<b>-4.34</b>
horse	1.06	-4.37	-1.5
ship	-0.36	-2.09	-4.79
truck	-0.72	-2.93	6.14

## TODO:

1. Define a **loss function** that quantifies our unhappiness with the scores across the training data.
2. Come up with a way of efficiently finding the parameters that minimize the loss function. (**optimization**)

We defined a (linear) **score function**:

$$f(x_i, W, b) = Wx_i + b$$

# Softmax Classifier (Multinomial Logistic Regression)



cat  
car  
frog

**3.2**

**5.1**

**-1.7**

# Softmax Classifier (Multinomial Logistic Regression)



scores = unnormalized log probabilities of the classes.

$$s = f(x_i; W)$$

cat  
car  
frog

3.2

5.1

-1.7



# Softmax Classifier (Multinomial Logistic Regression)



scores = unnormalized log probabilities of the classes.

$$P(Y = k | X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}} \quad \text{where } s = f(x_i; W)$$

cat	3.2
car	5.1
frog	-1.7

# Softmax Classifier (Multinomial Logistic Regression)



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Softmax function

cat            **3.2**

car            **5.1**

frog           **-1.7**

# Softmax Classifier (Multinomial Logistic Regression)



**scores = unnormalized log probabilities of the classes.**

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}} \quad \text{where} \quad s = f(x_i; W)$$

Want to maximize the log likelihood, or (for a loss function) to minimize the negative log likelihood of the correct class:

$$L_i = -\log P(Y = y_i|X = x_i)$$

cat

3.2

car

5.1

frog

-1.7

# Softmax Classifier (Multinomial Logistic Regression)



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$$L_i = -\log P(Y = y_i|X = x_i)$$

---

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

cat  
car  
frog

3.2

5.1

-1.7

# Softmax Classifier (Multinomial Logistic Regression)



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

cat

**3.2**

car

5.1

frog

-1.7

unnormalized log probabilities

# Softmax Classifier (Multinomial Logistic Regression)



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

unnormalized probabilities

cat  
car  
frog

3.2  
5.1  
-1.7

exp

24.5  
164.0  
0.18

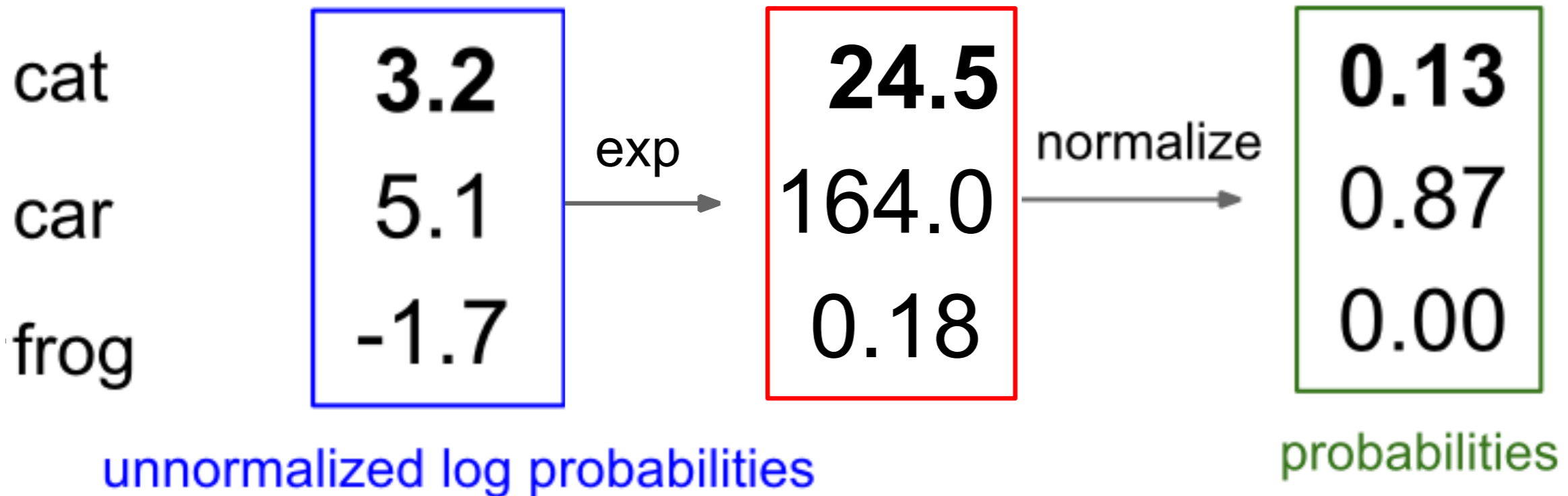
unnormalized log probabilities

# Softmax Classifier (Multinomial Logistic Regression)



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

unnormalized probabilities



# Softmax Classifier (Multinomial Logistic Regression)



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

unnormalized probabilities

cat  
car  
frog

3.2  
5.1  
-1.7

exp

24.5  
164.0  
0.18

normalize

0.13  
0.87  
0.00

$$L_i = -\log(0.13) = 0.89$$

unnormalized log probabilities

probabilities



# Optimization

# Gradient Descent

```
# Vanilla Gradient Descent
```

```
while True:
```

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

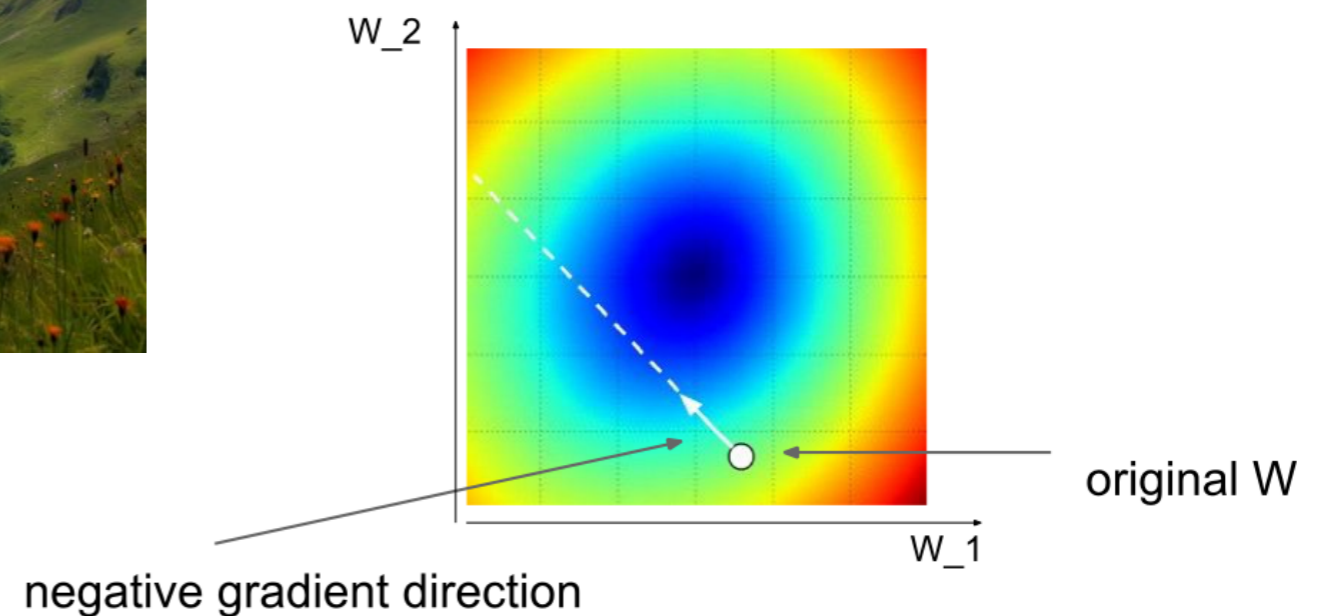
```
    weights += - step_size * weights_grad # perform parameter update
```



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).



# Mini-batch Gradient Descent

- only use a small portion of the training set to compute the gradient

```
# 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
```

# Mini-batch Gradient Descent

- only use a small portion of the training set to compute the gradient

```
# Vanilla Minibatch Gradient Descent
```

```
while True:
```

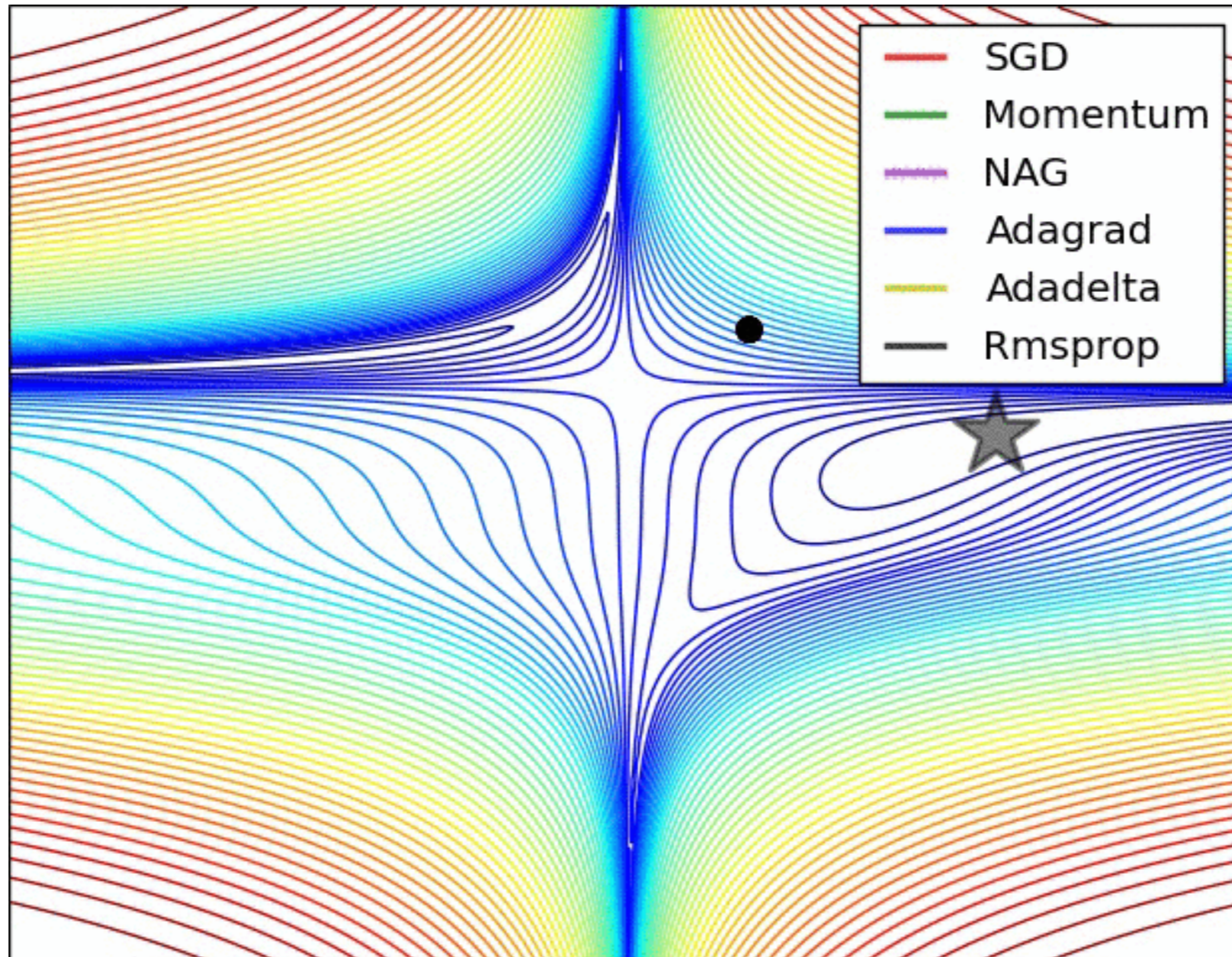
```
    data_batch = sample_training_data(data, 256) # sample 256 examples
```

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

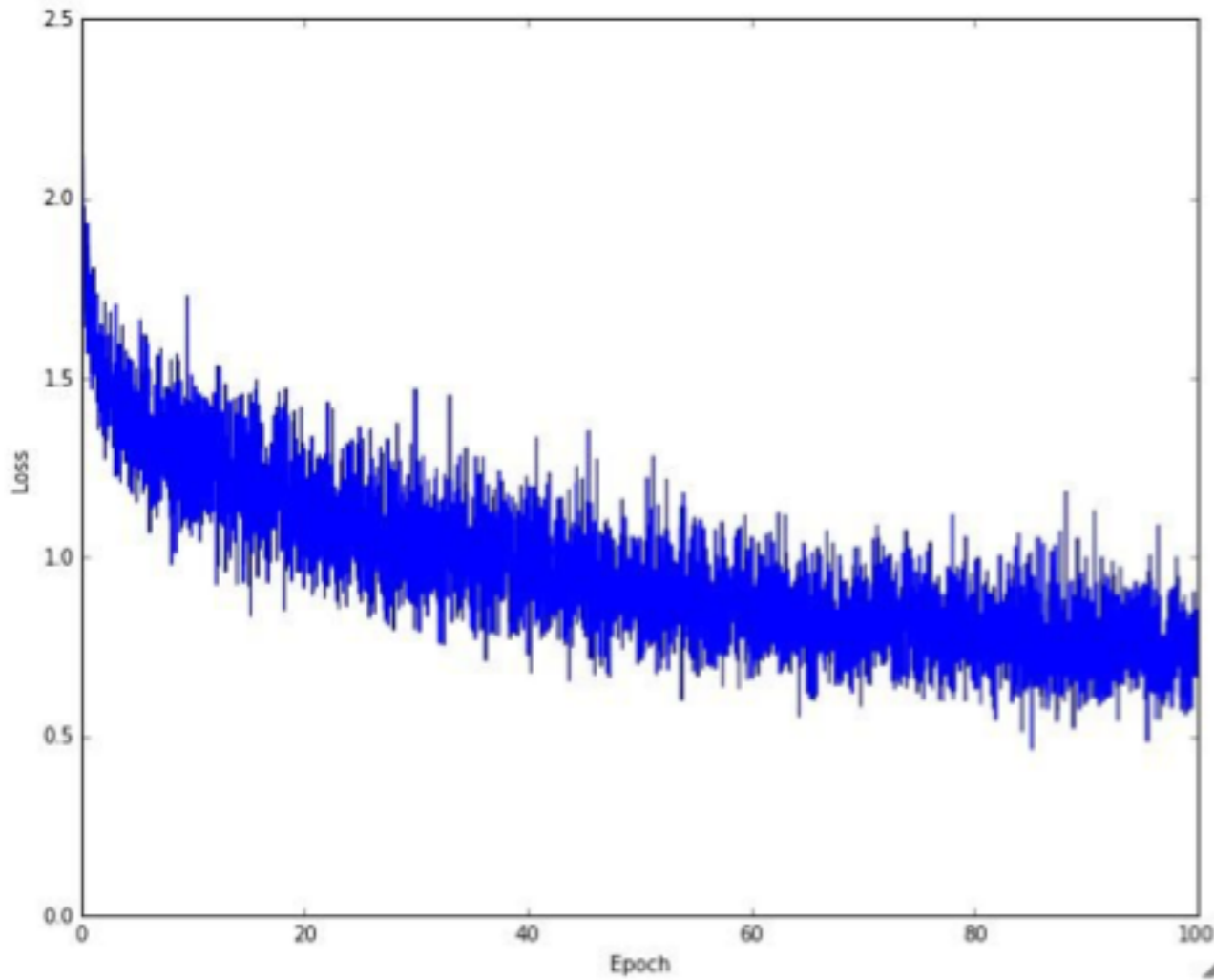
```
    weights += - step_size * weights_grad # perform parameter update
```

there are also more fancy update formulas (momentum, Adagrad, RMSProp, Adam, ...)

# The effects of different update form formulas

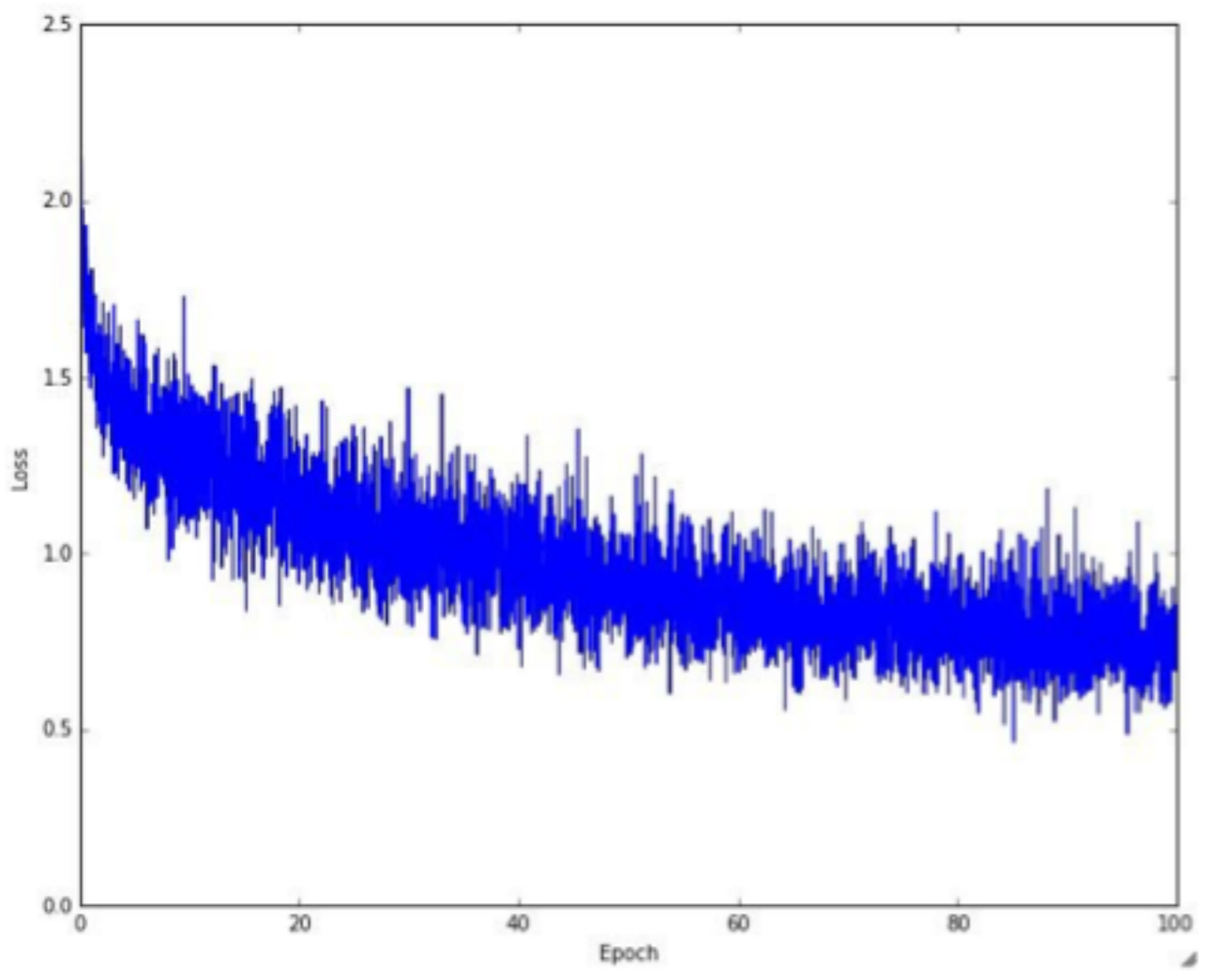


(image credits to Alec Radford)

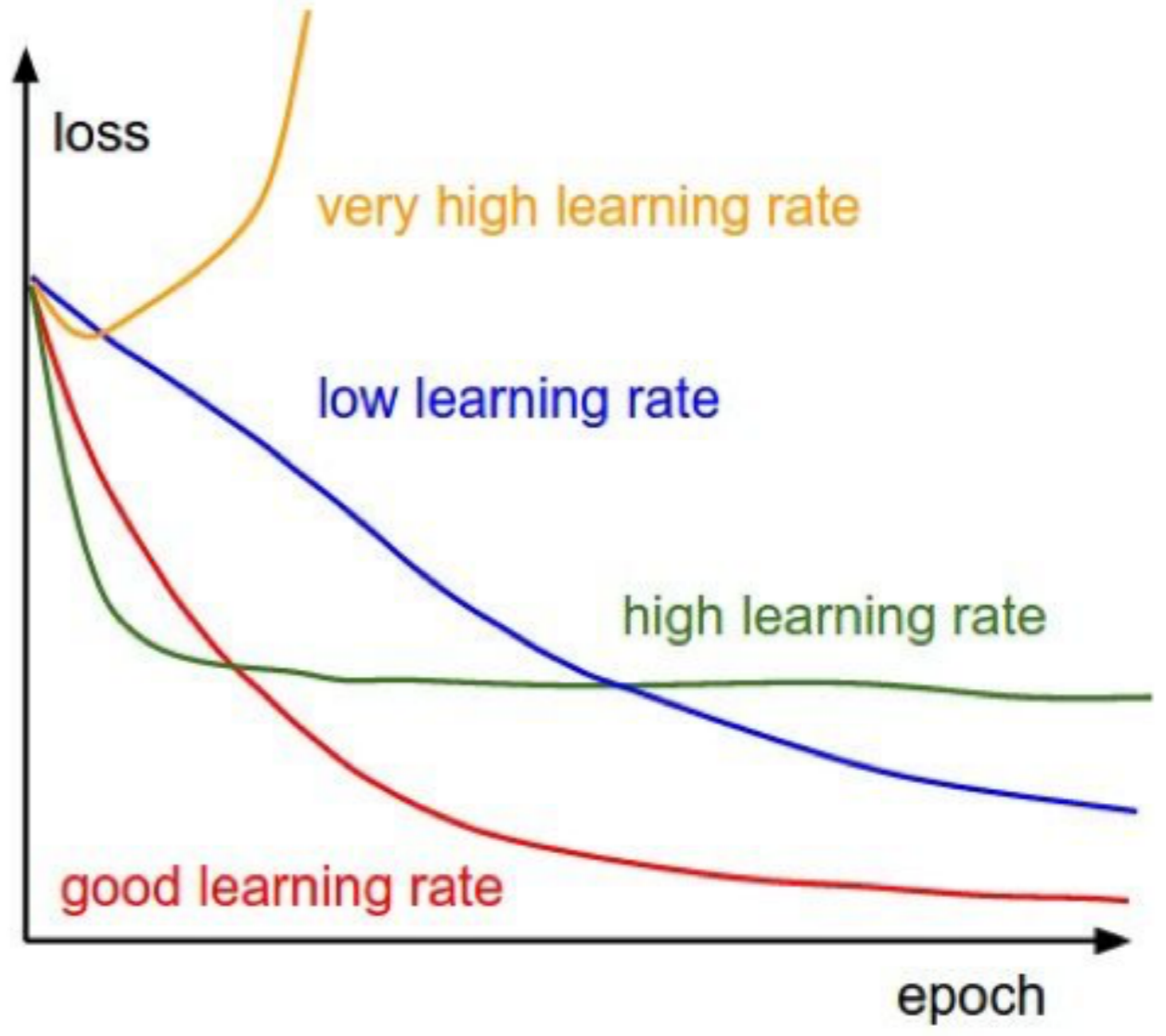


Example of optimization progress while training a neural network.

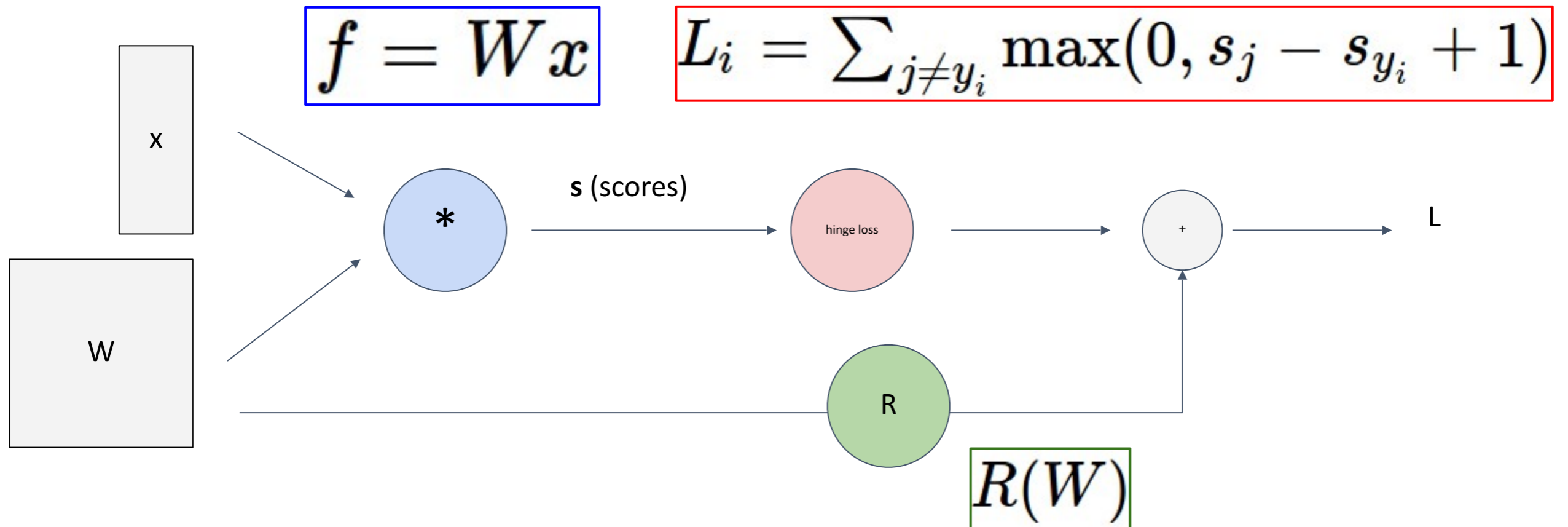
(Loss over mini-batches goes down over time.)



The effects of step size (or “learning rate”)



# Computational Graph



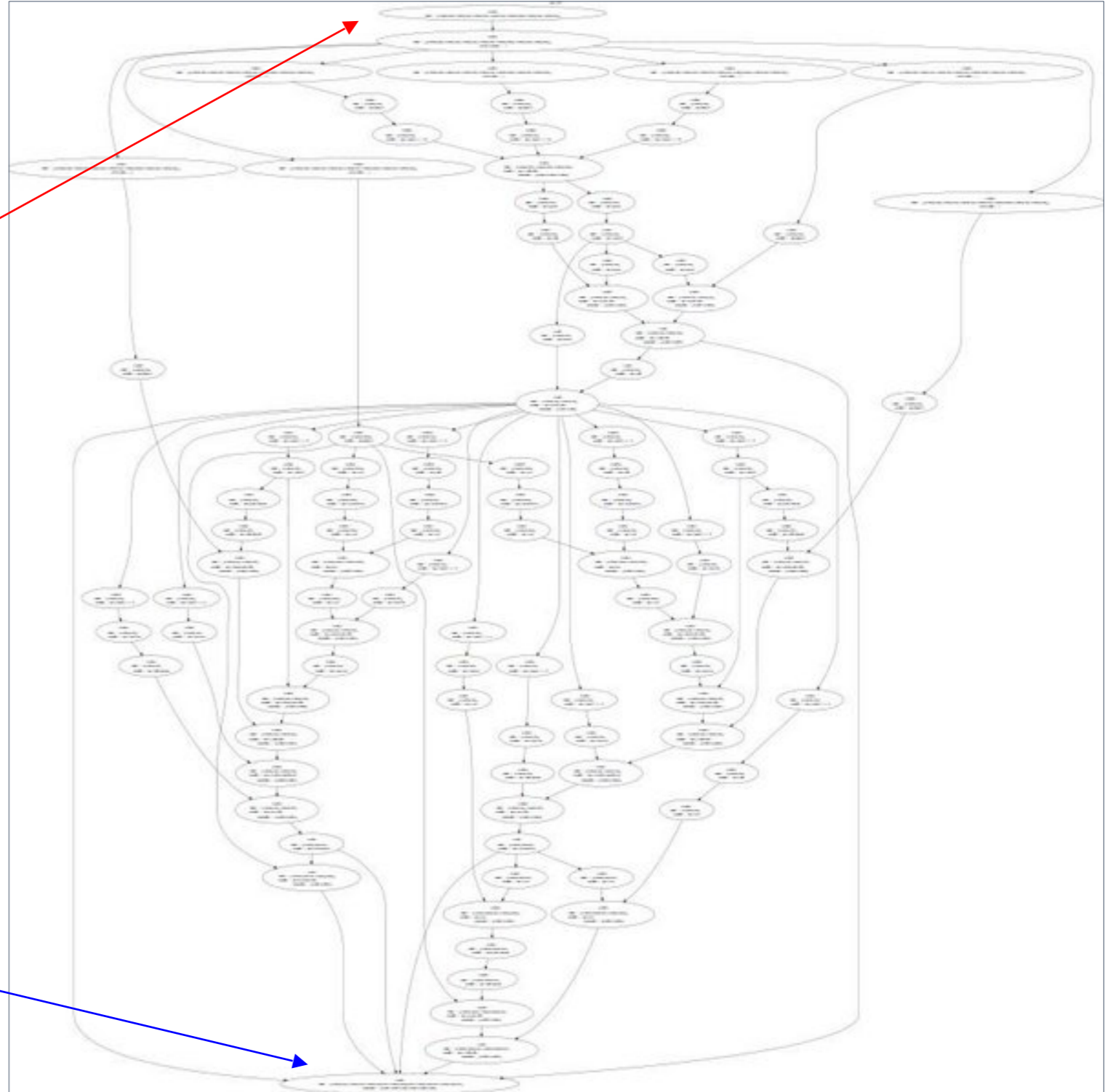




# Neural Turing Machine

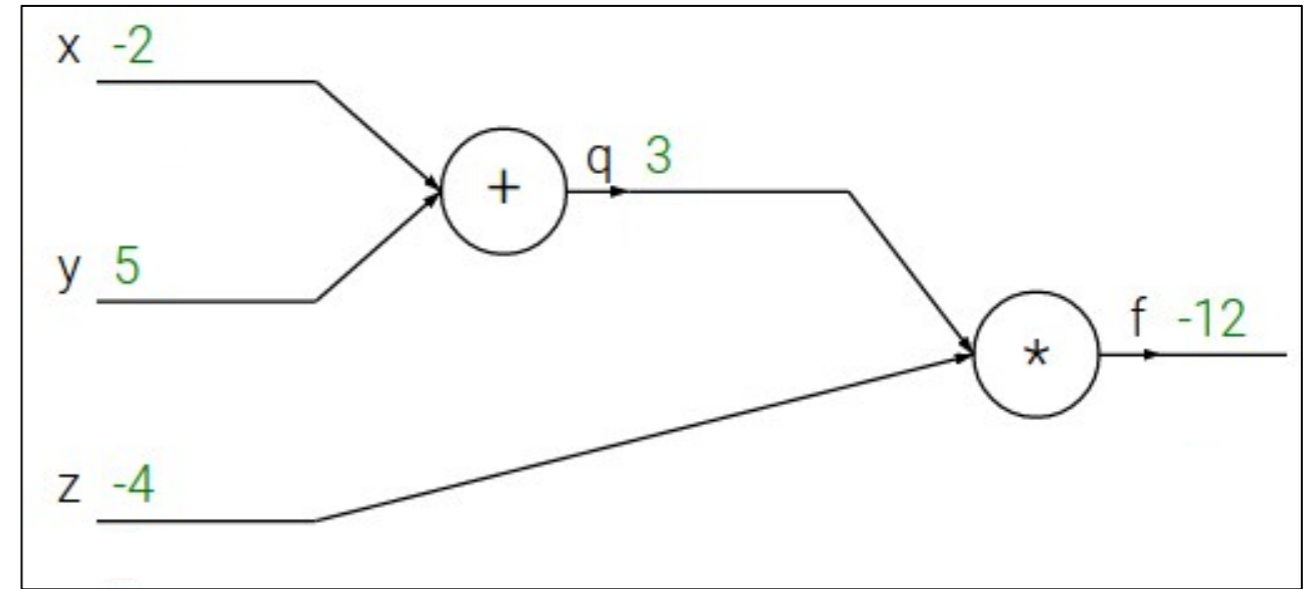
input tape

loss



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

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



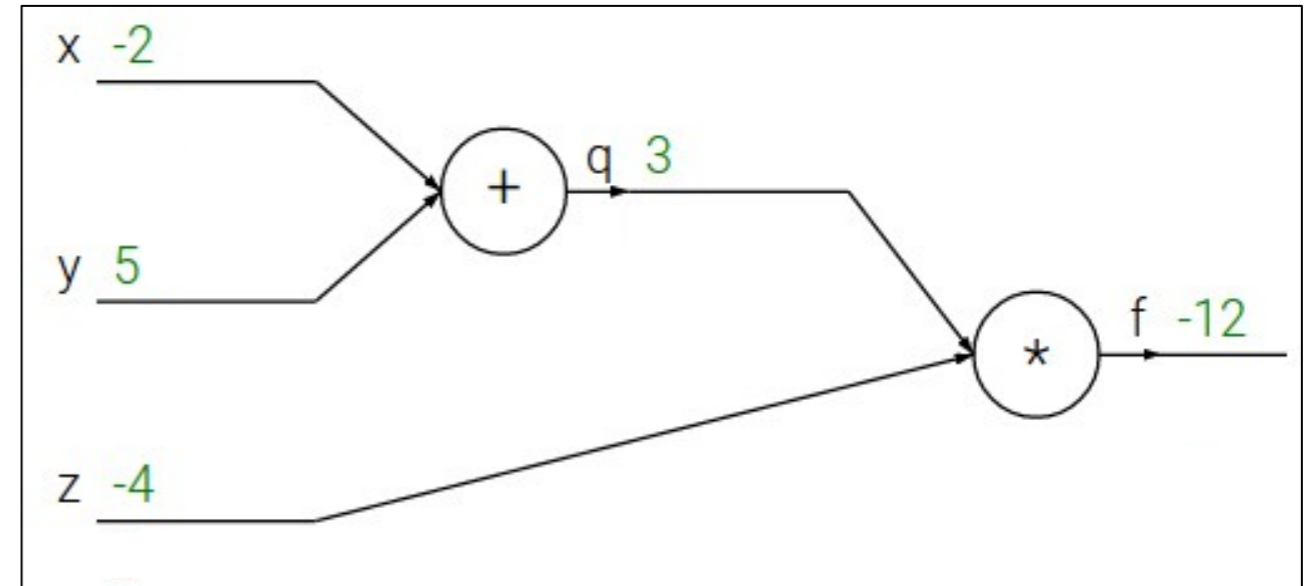
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$$q = x + y \quad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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

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



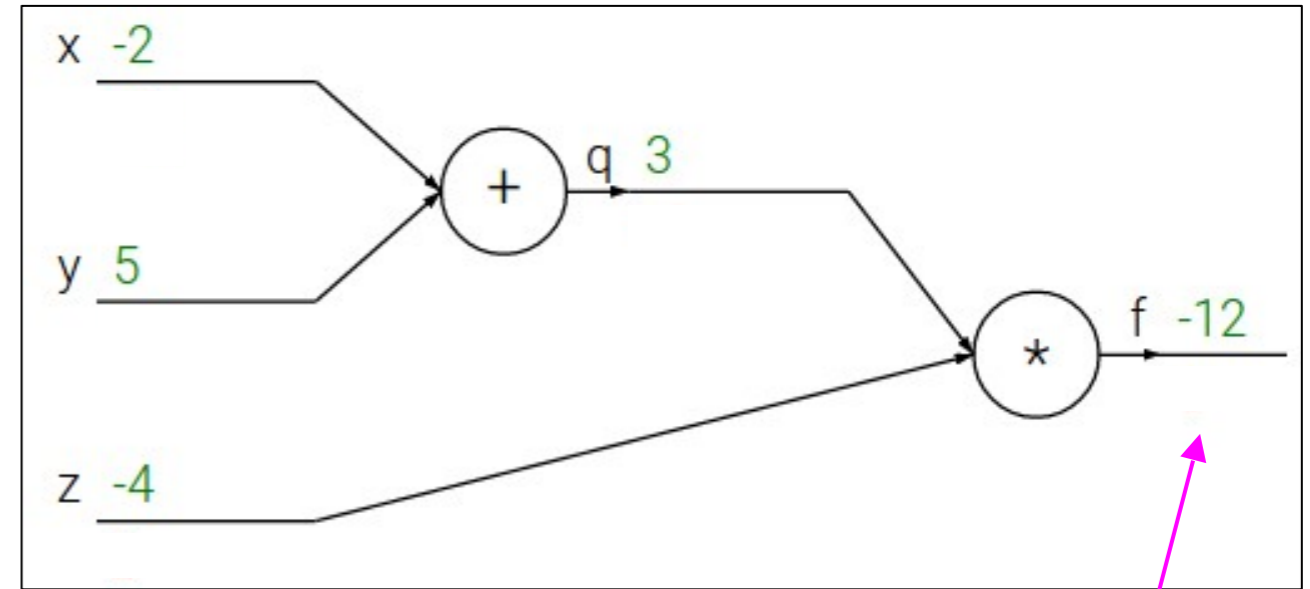
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$$\frac{\partial f}{\partial f}$$

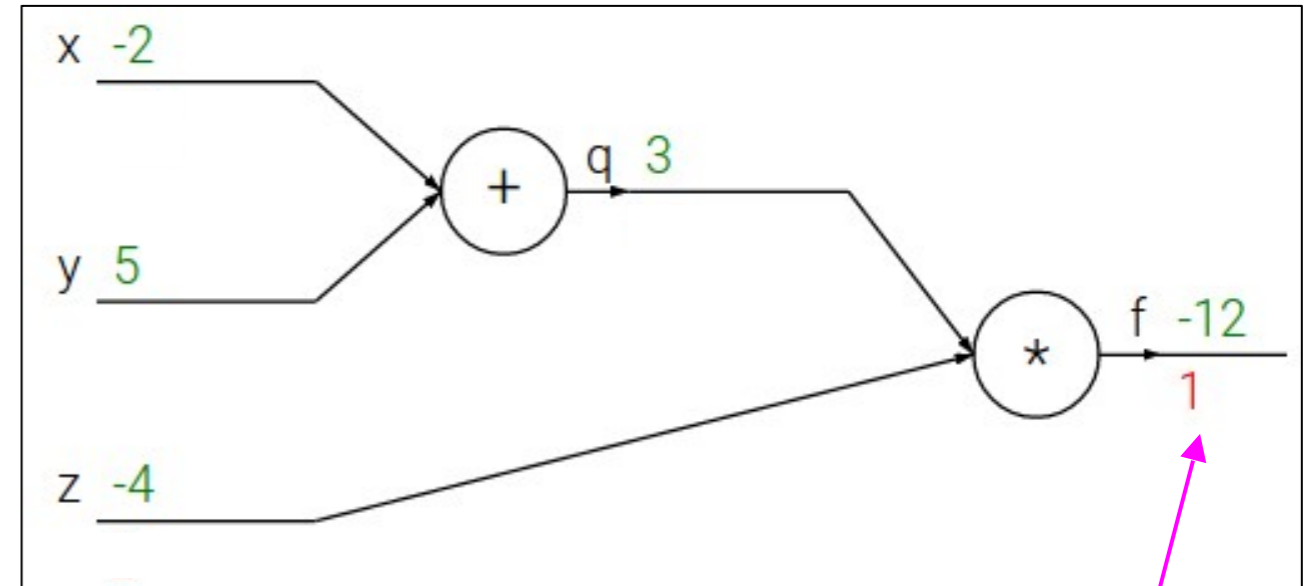
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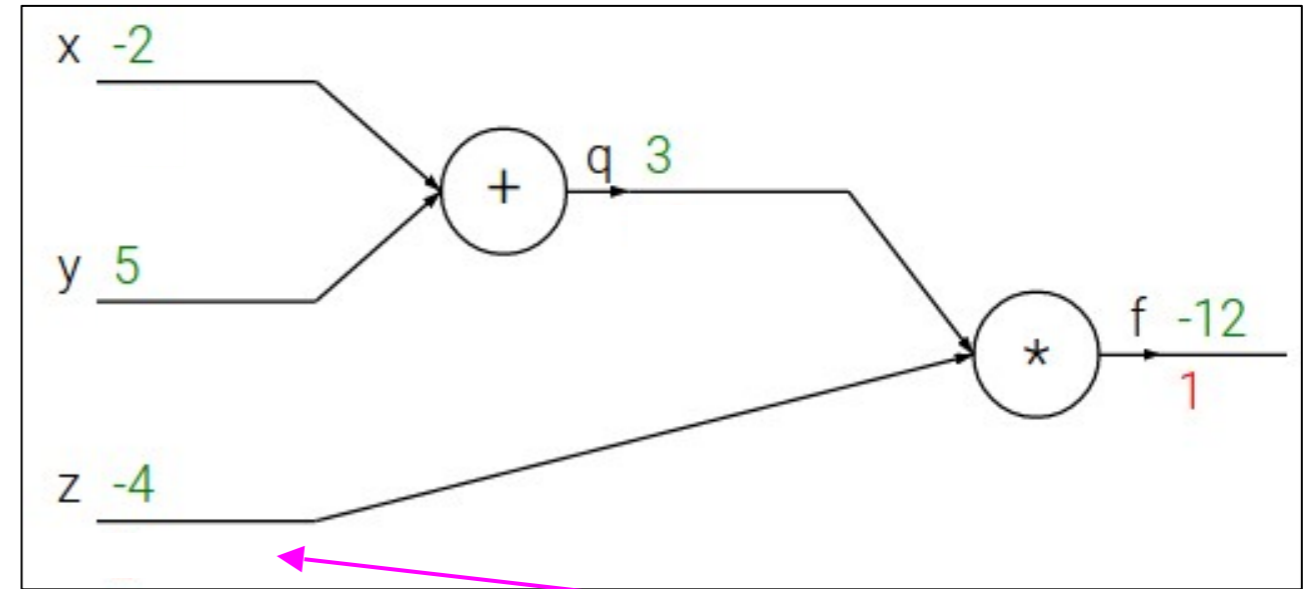
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Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

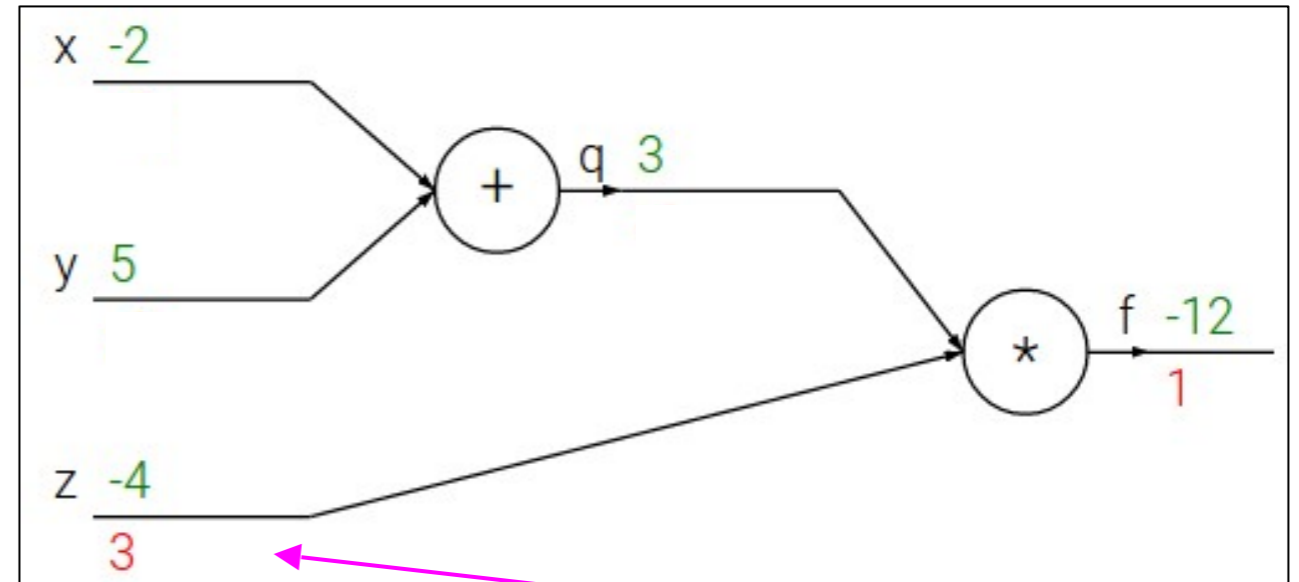
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$$\frac{\partial f}{\partial z}$$



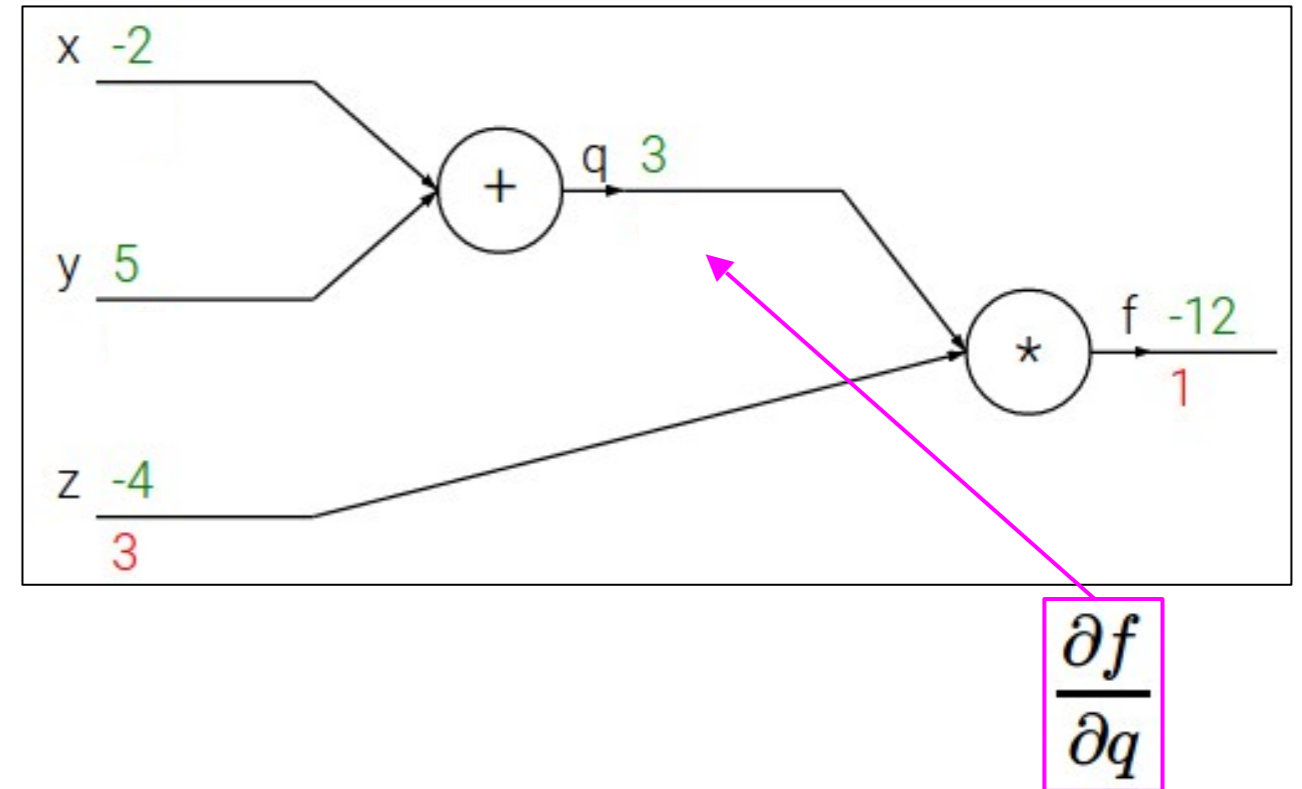
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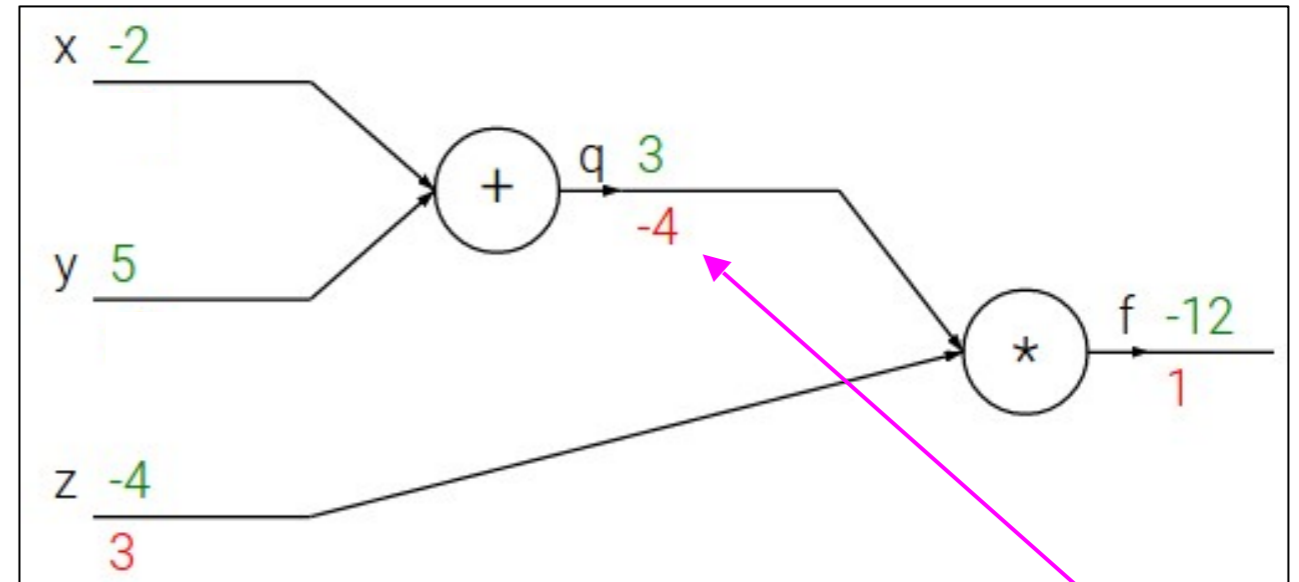
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Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

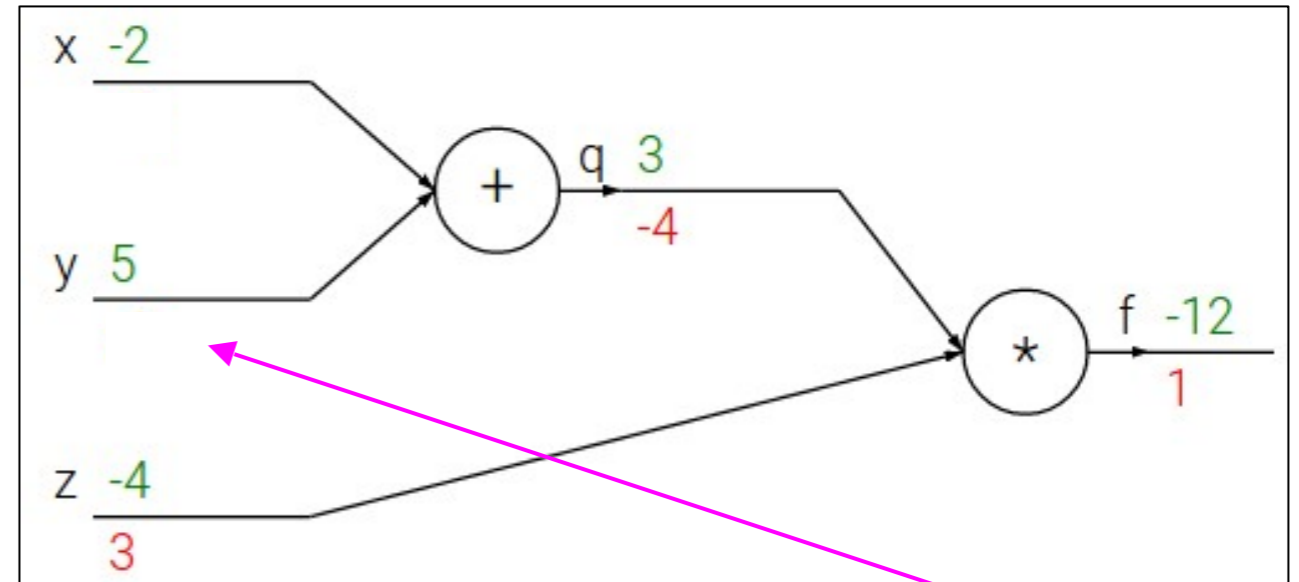
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Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

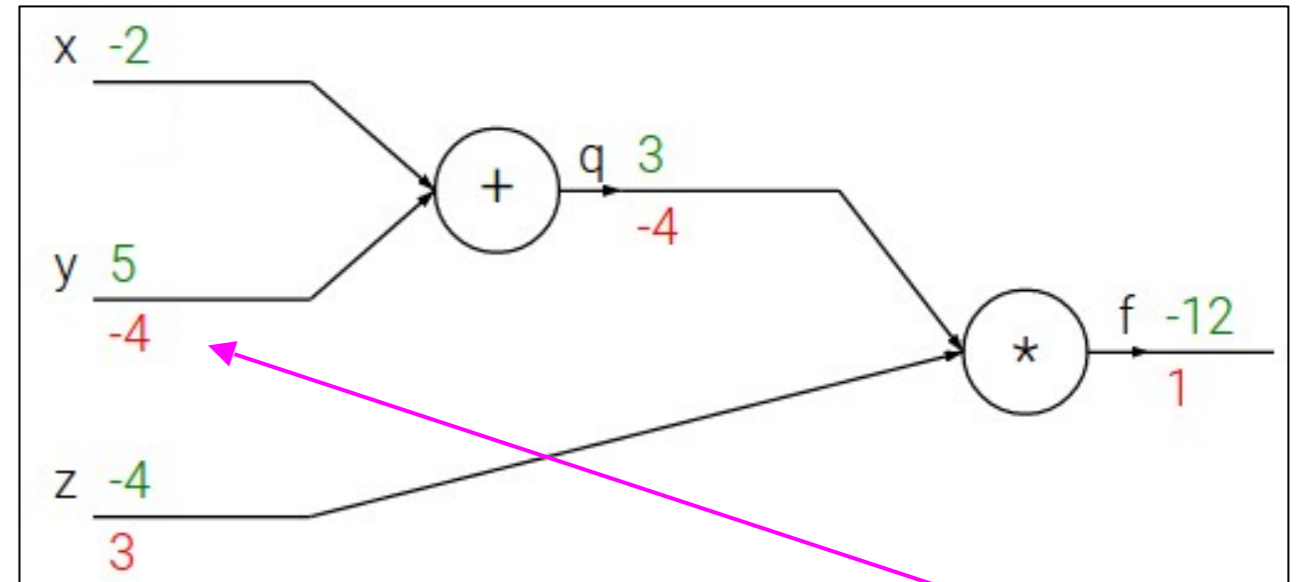
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$$\frac{\partial f}{\partial y}$$

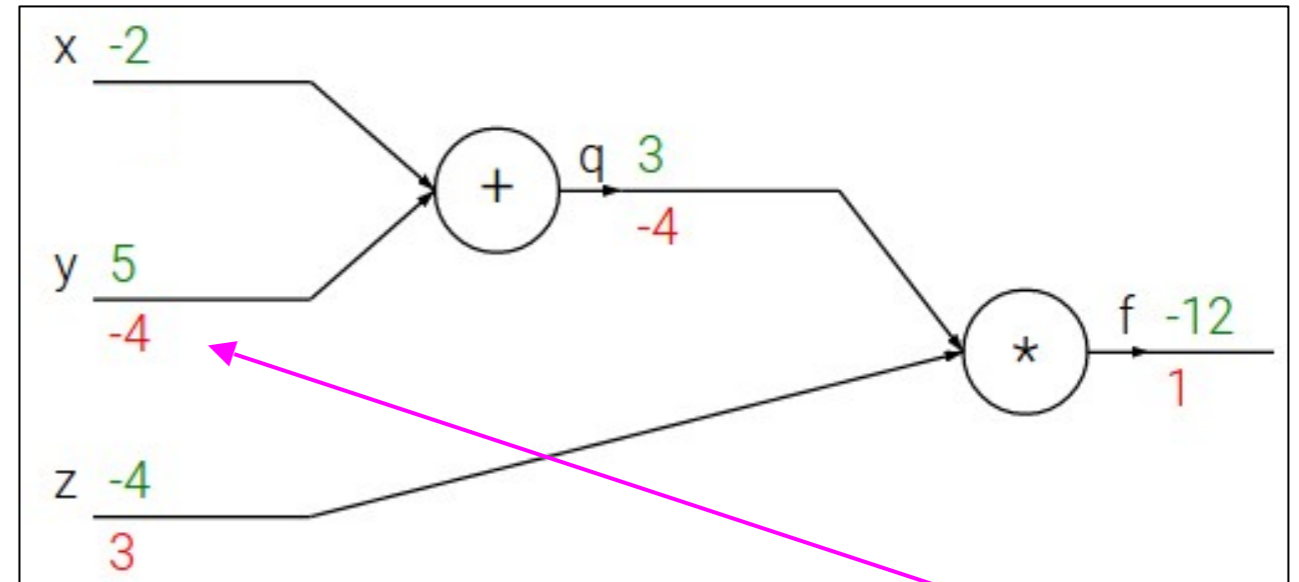
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Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Chain rule:

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

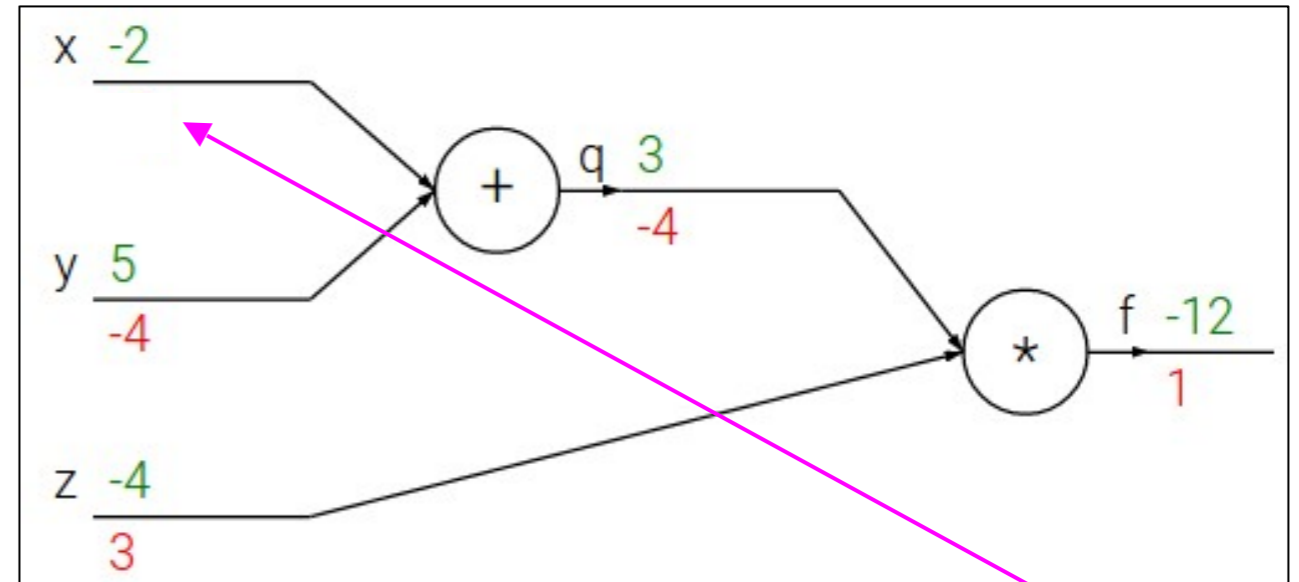
$$f(x, y, z) = (x + y)z$$

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



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

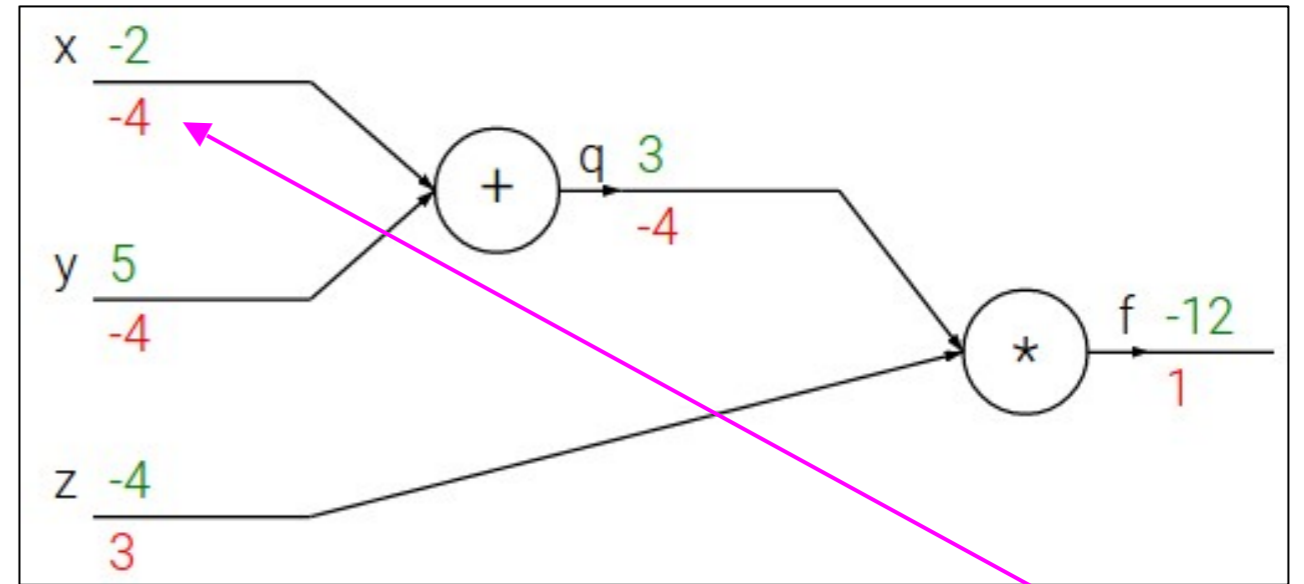
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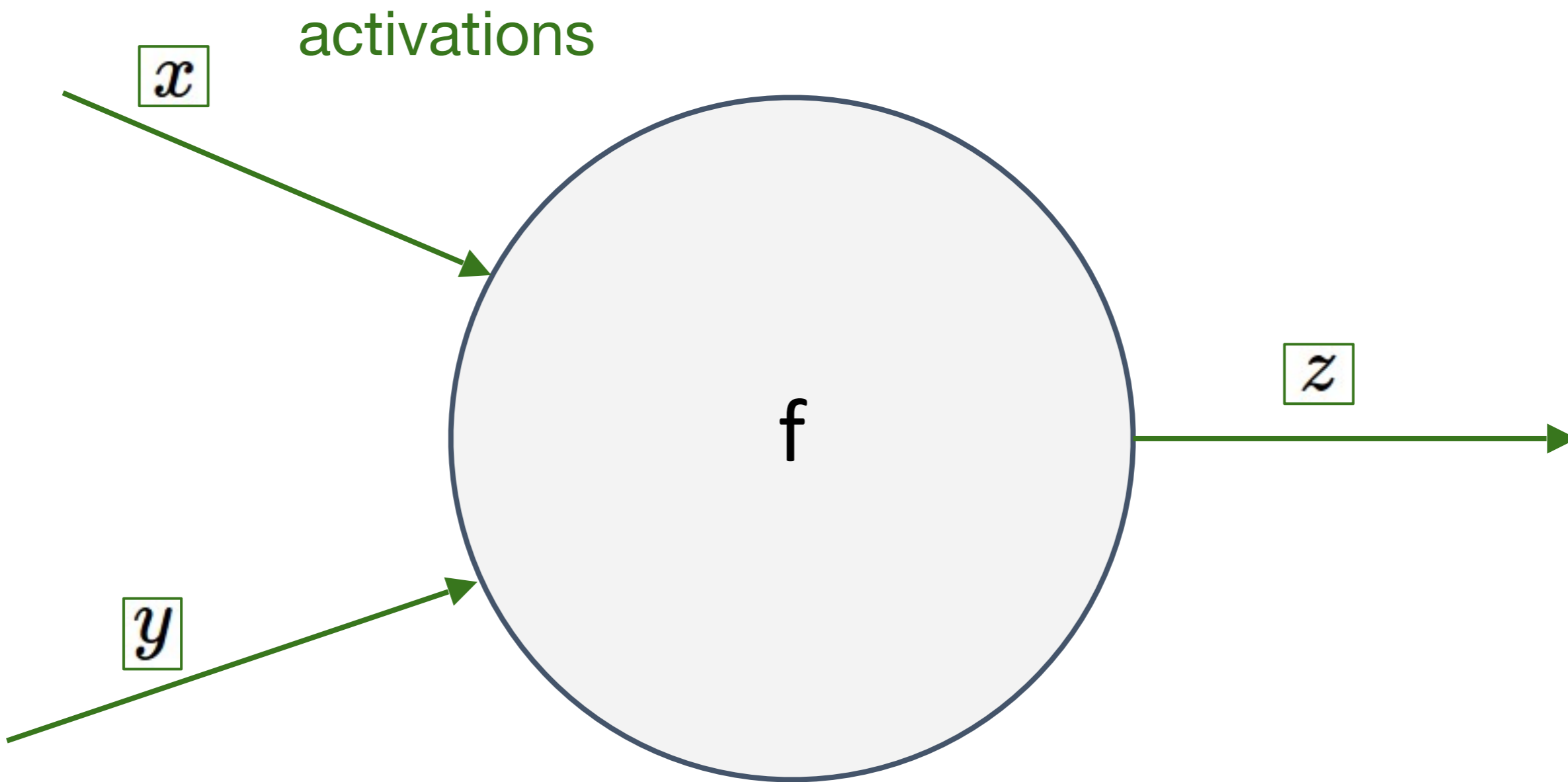
Want:  $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



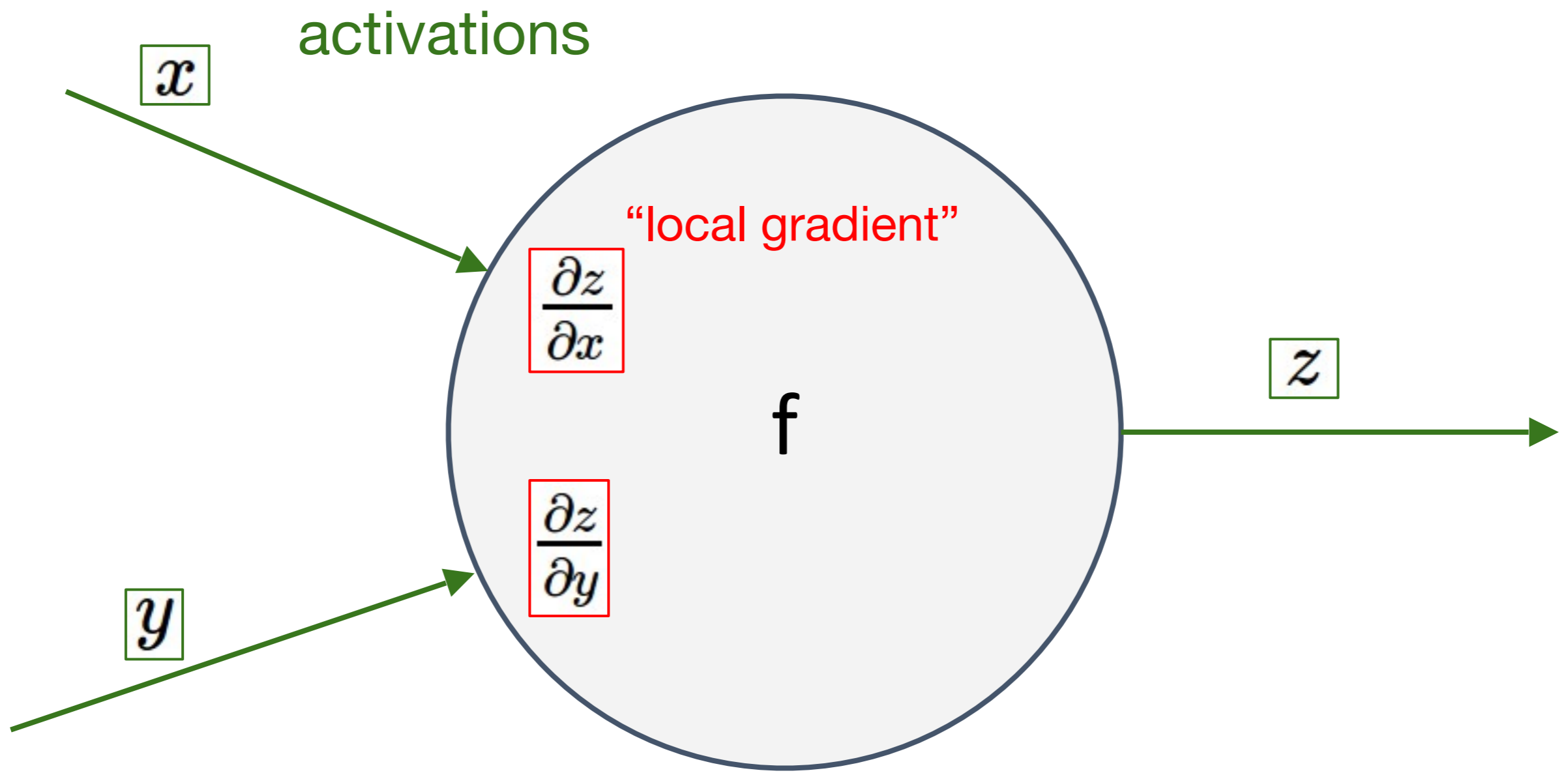
$$\frac{\partial f}{\partial x}$$

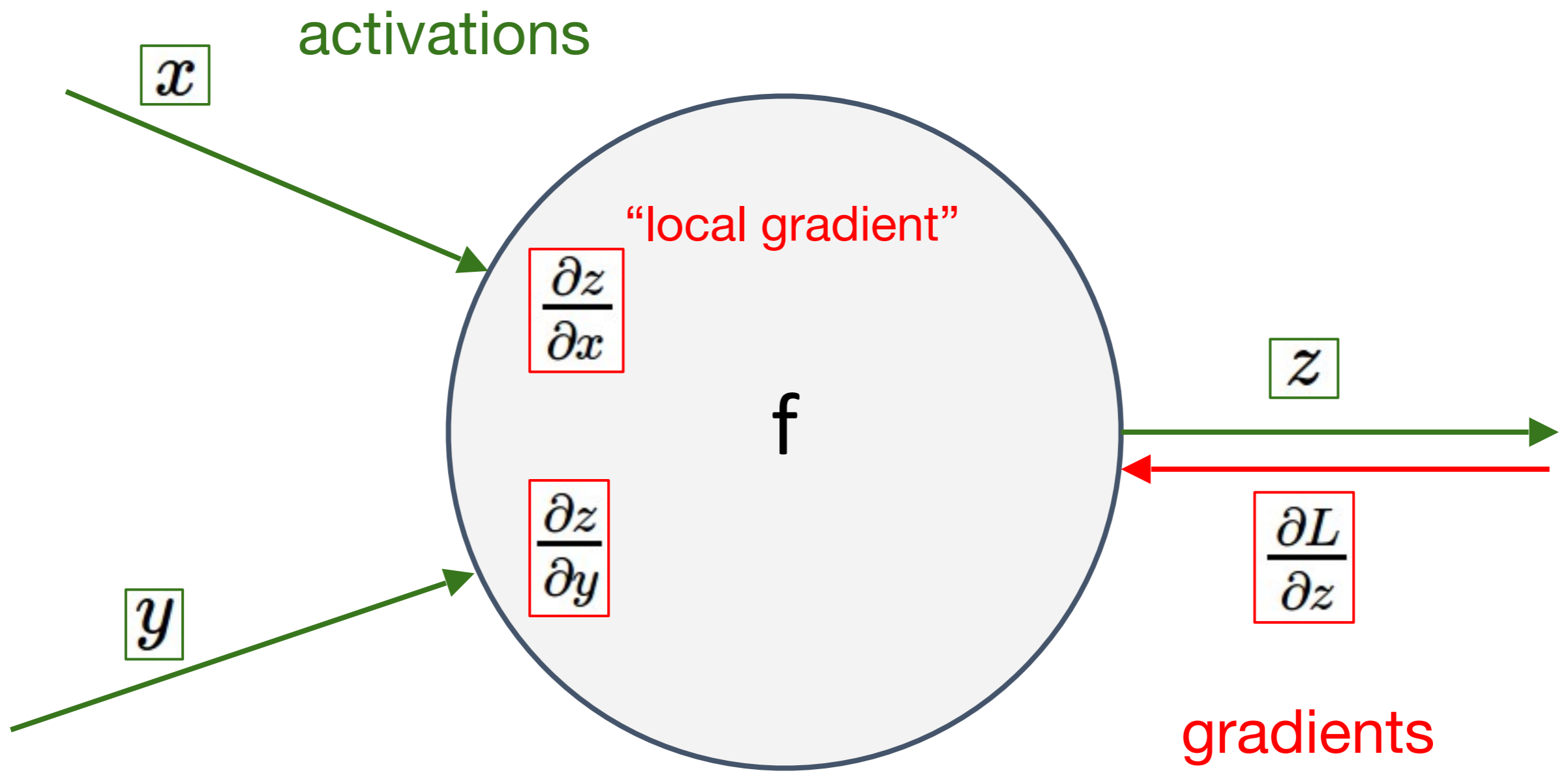
Chain rule:

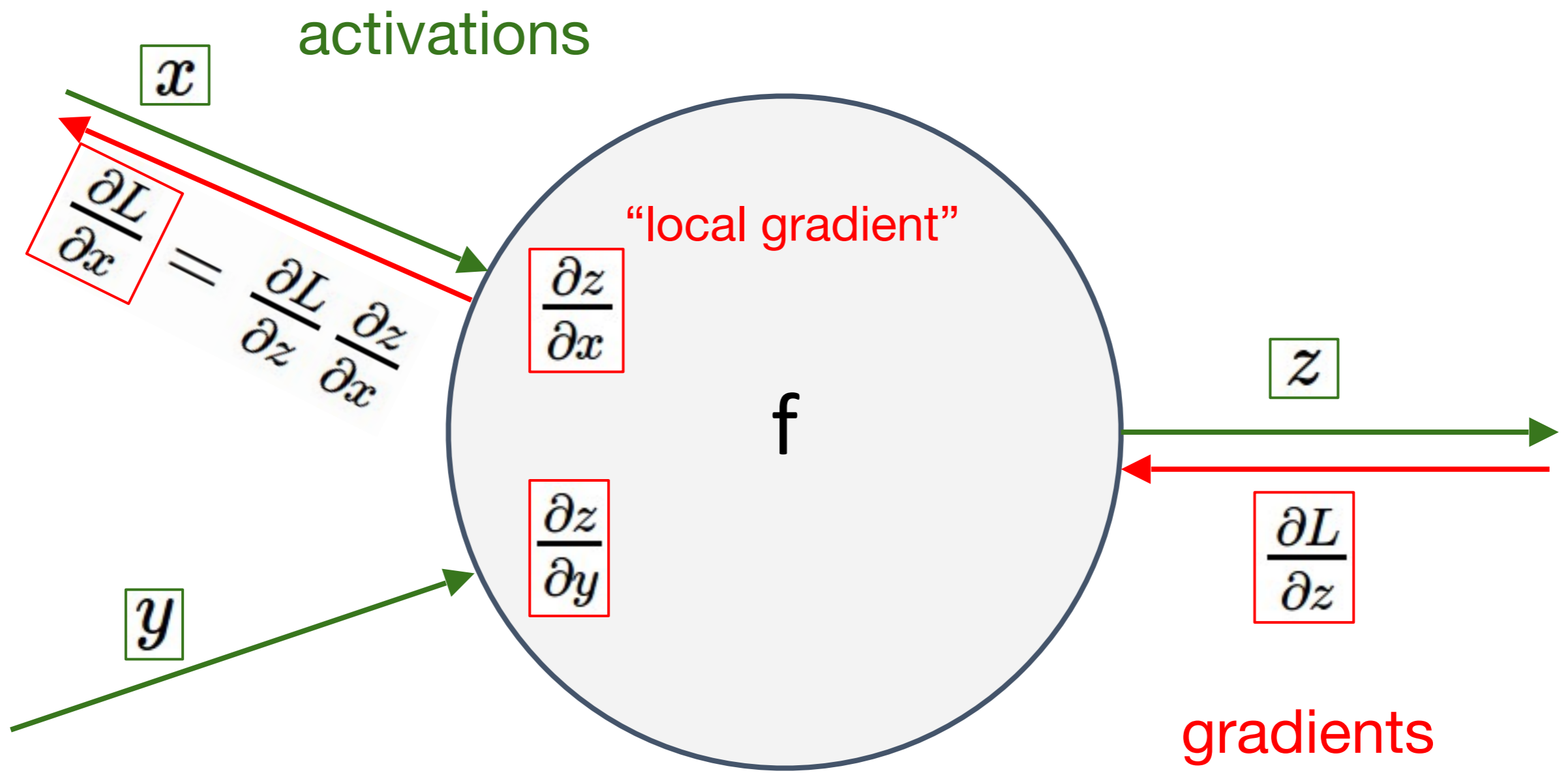
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

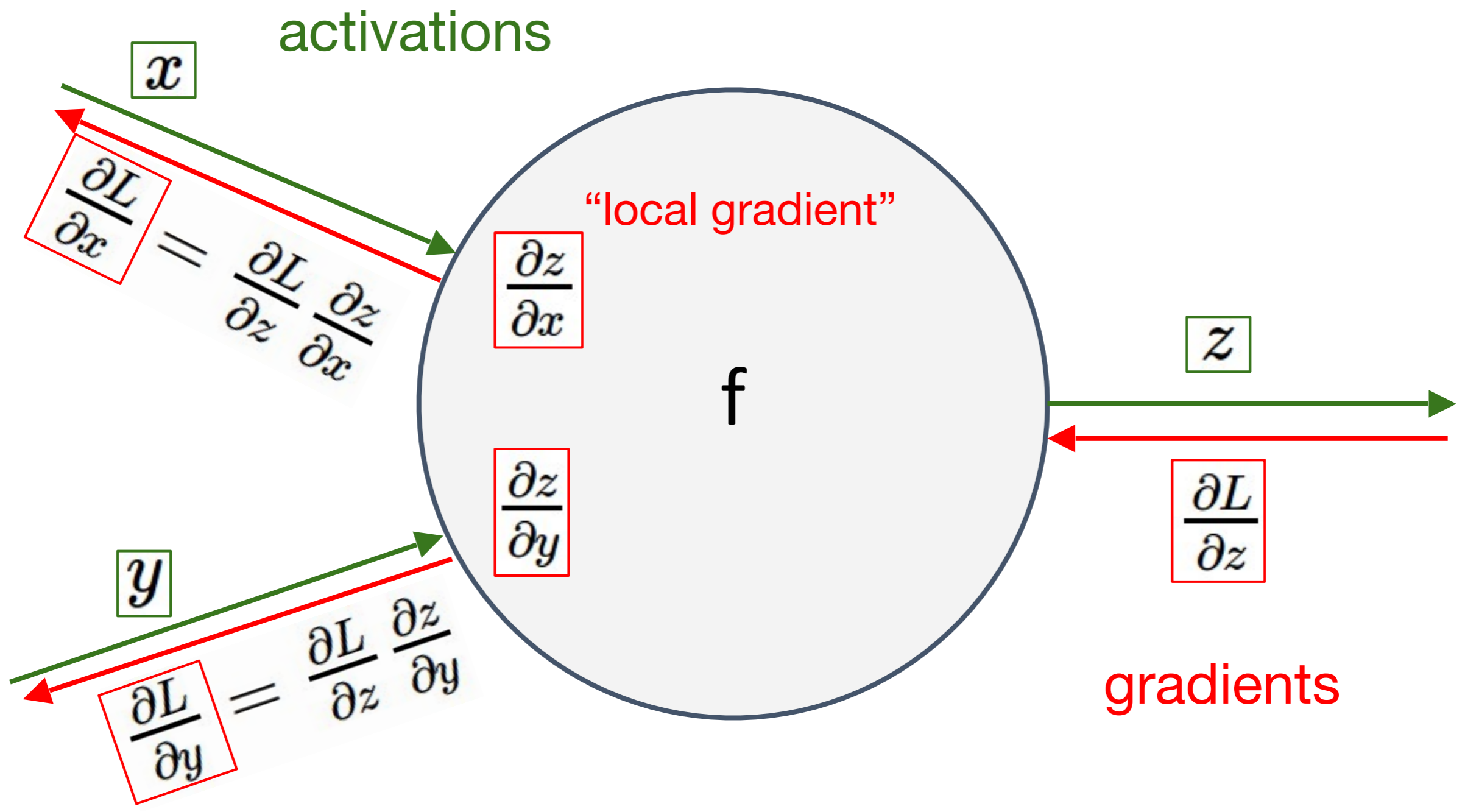


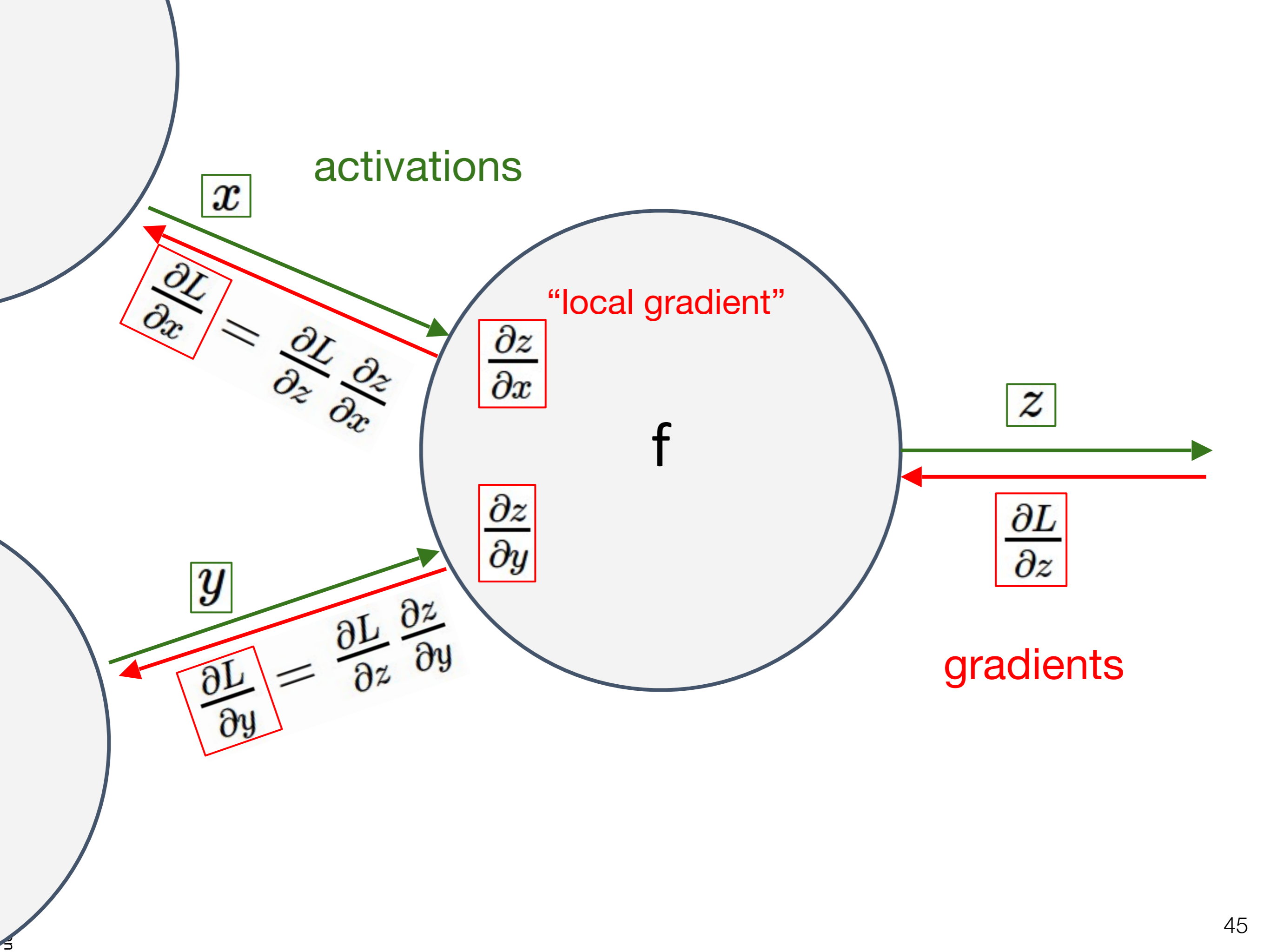




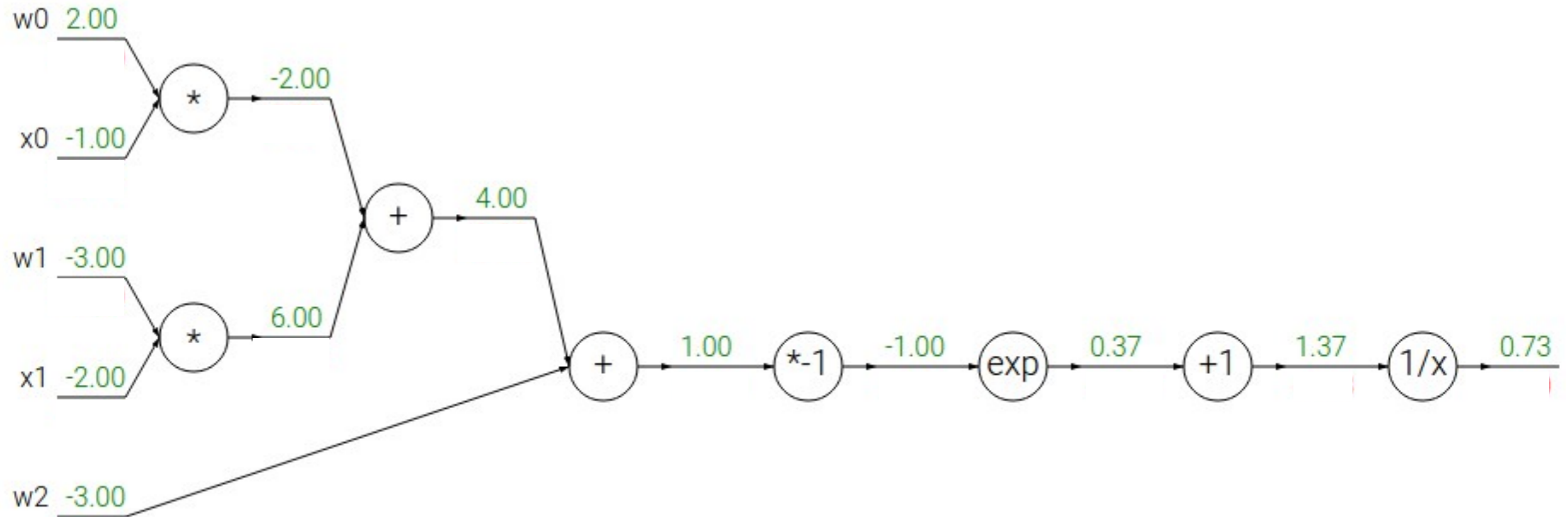




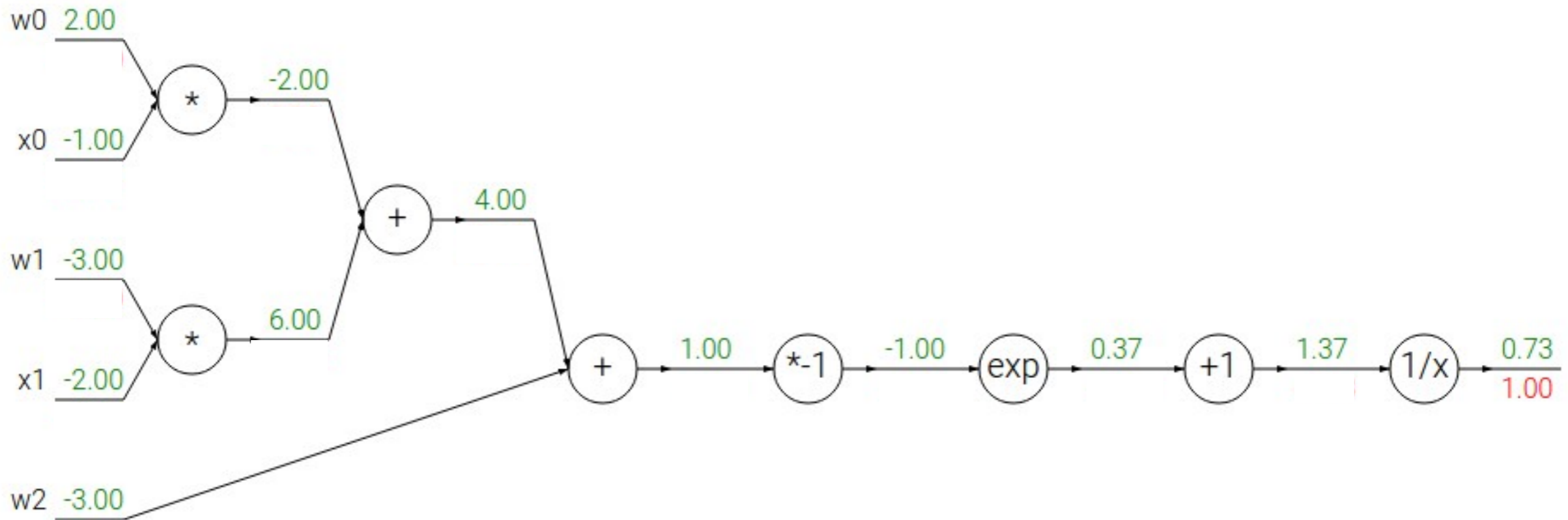




Another example:  $f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$

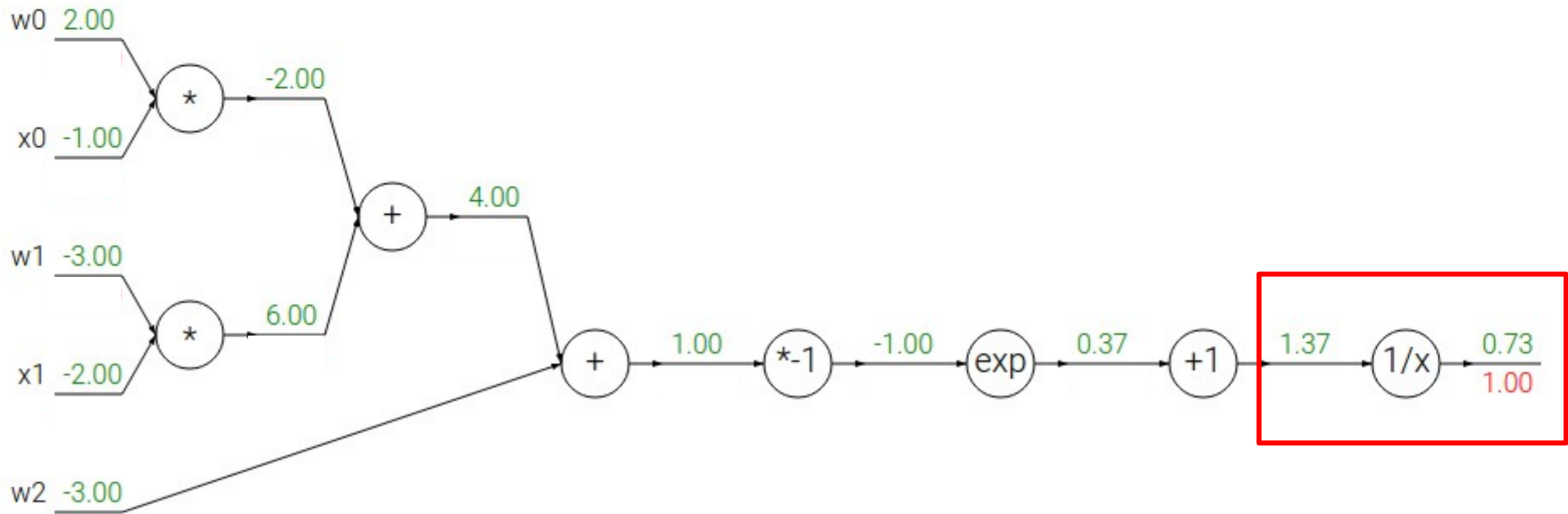


Another example:  $f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$



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

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



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

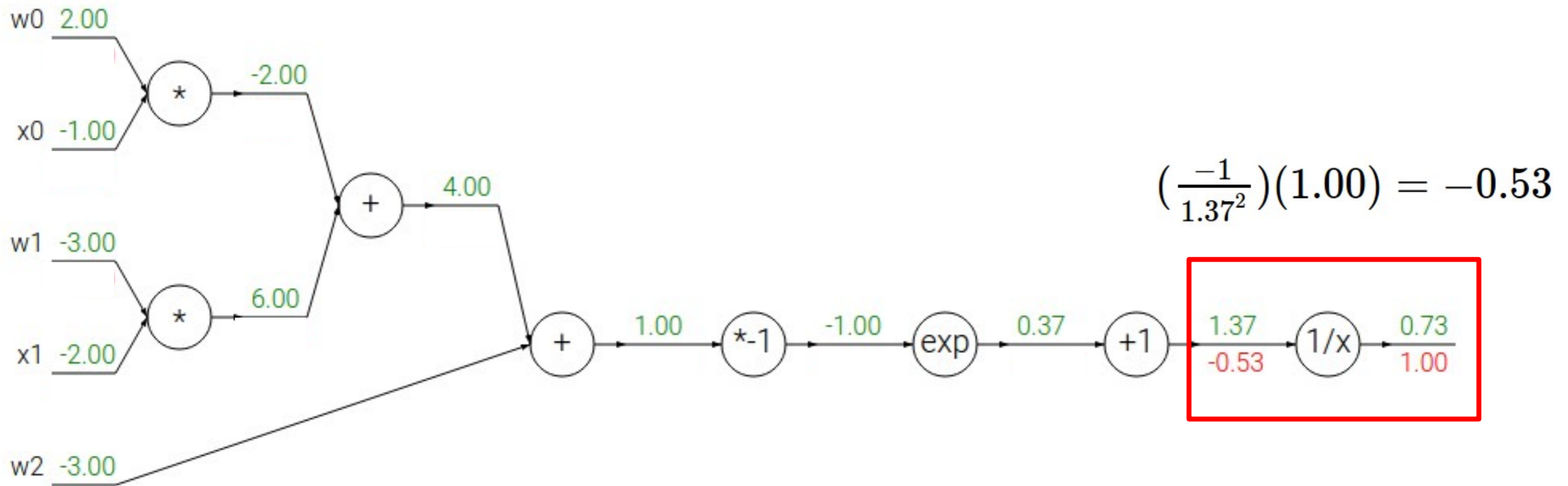
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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



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



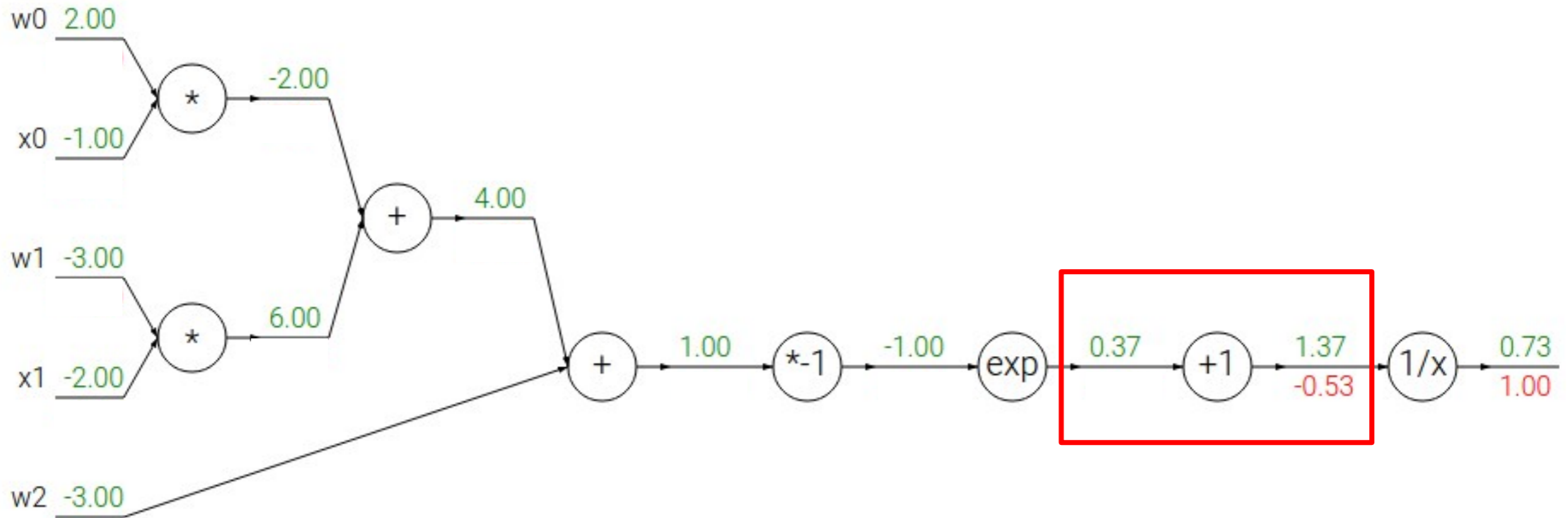
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$$f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$$

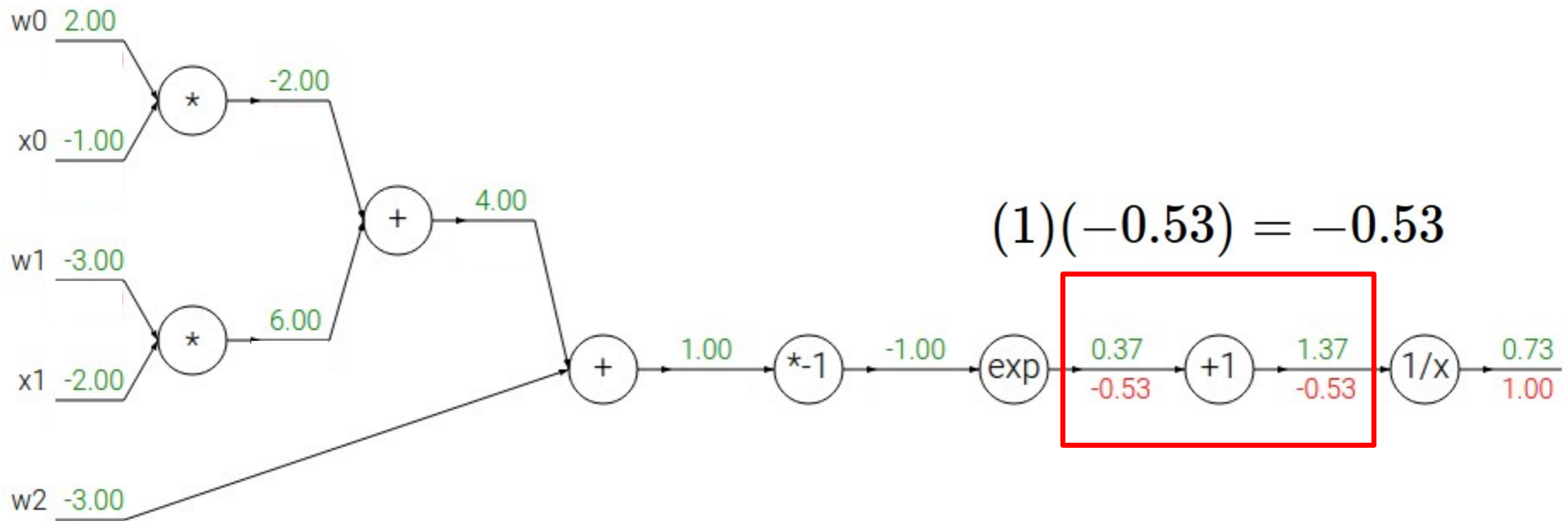
$$f_c(x) = c + x \rightarrow \frac{df}{dx} = 1$$

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



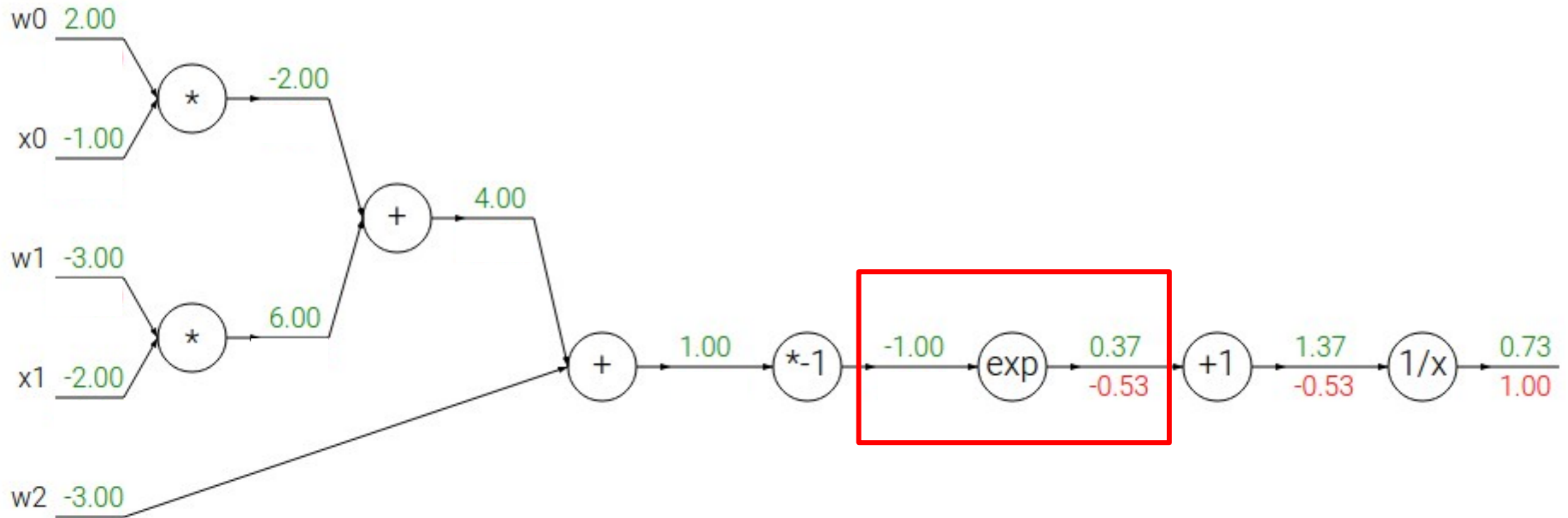
$f(x) = e^x$	$\rightarrow$	$\frac{df}{dx} = e^x$		$f(x) = \frac{1}{x}$	$\rightarrow$	$\frac{df}{dx} = -1/x^2$
$f_a(x) = ax$	$\rightarrow$	$\frac{df}{dx} = a$		$f_c(x) = c + x$	$\rightarrow$	$\frac{df}{dx} = 1$

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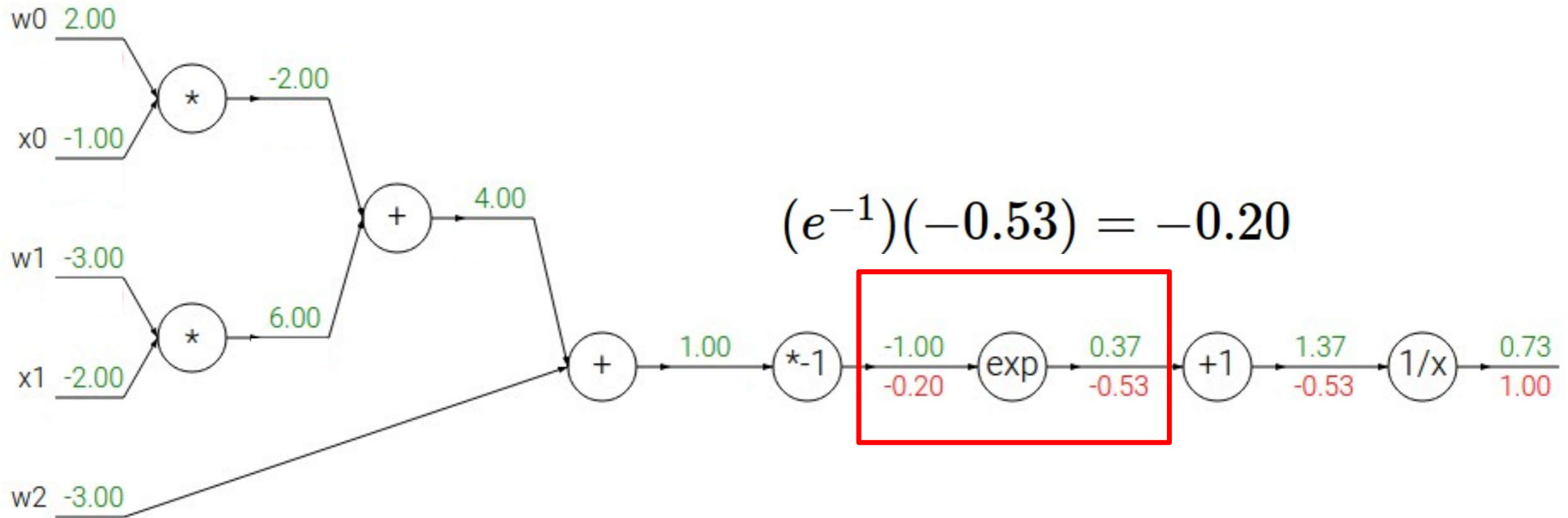
$$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$$

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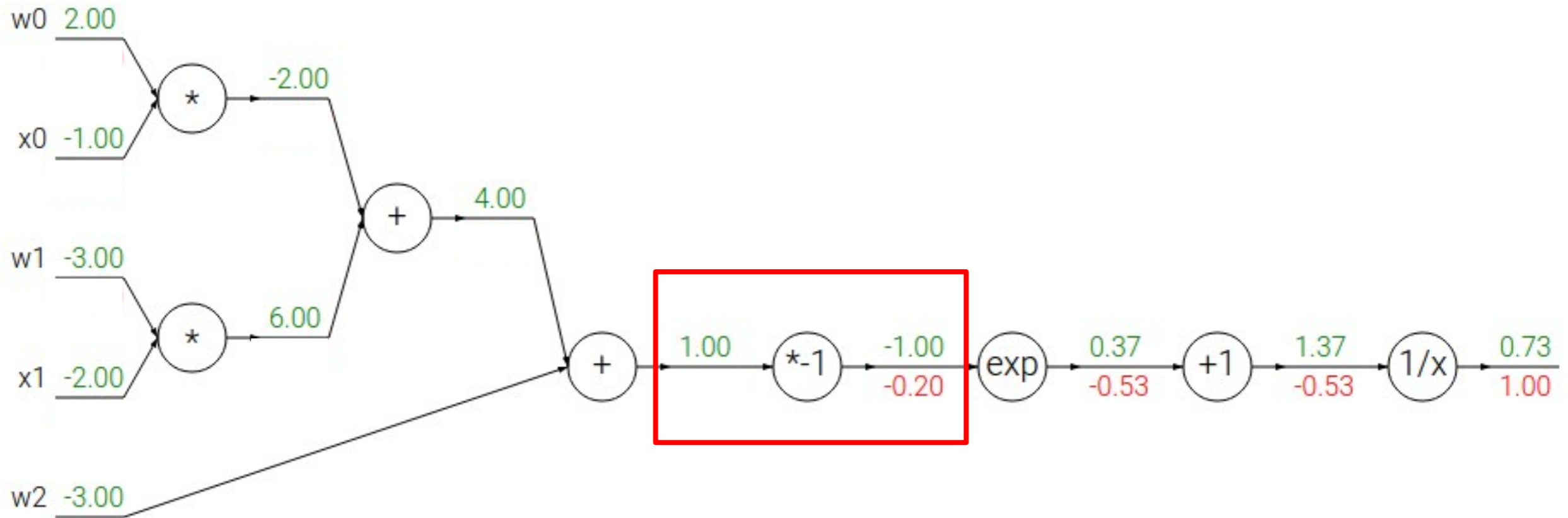
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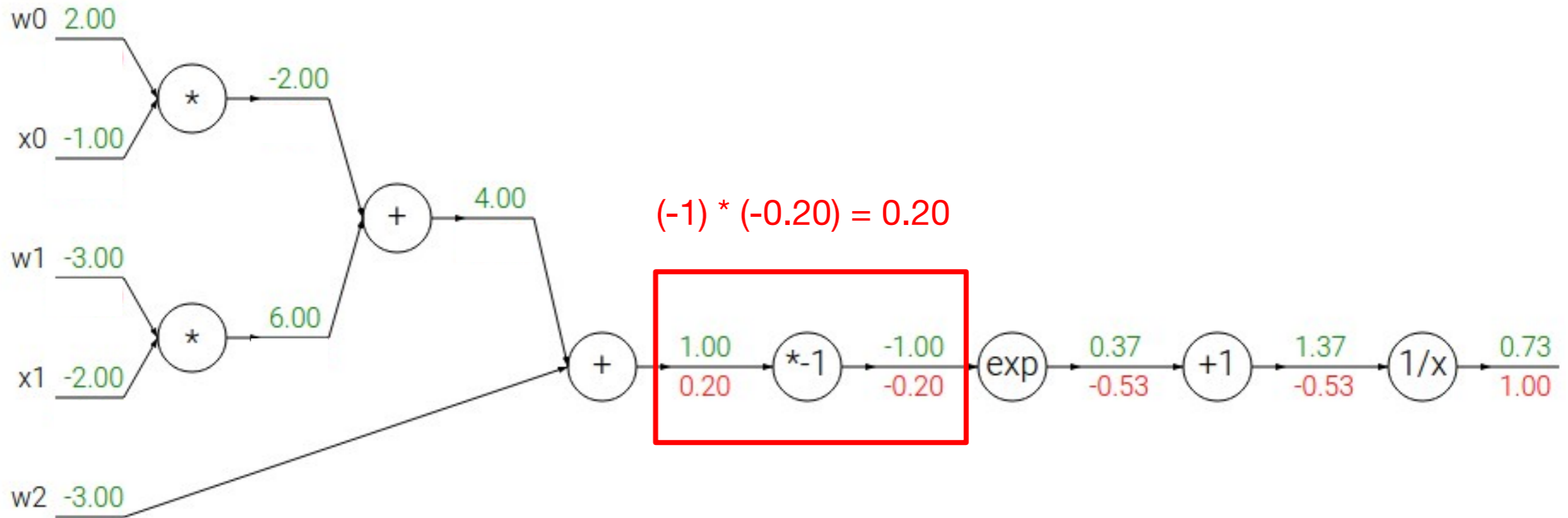
$\rightarrow$

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

$\rightarrow$

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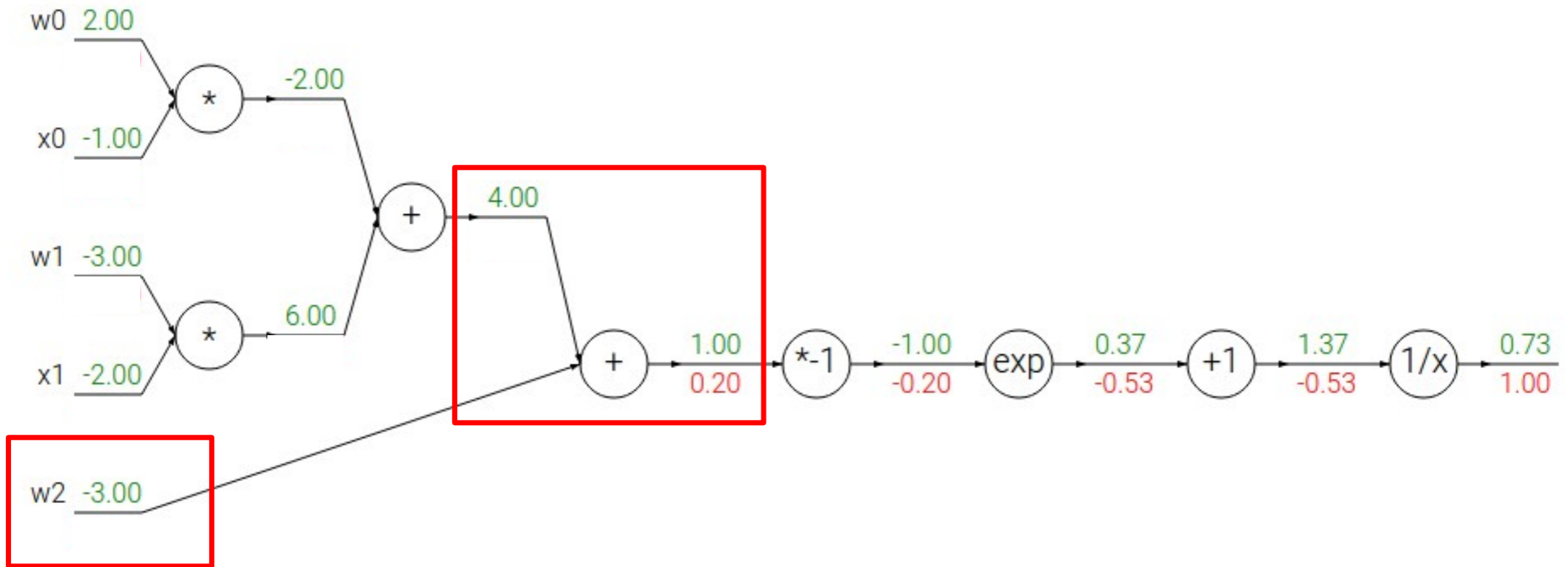
$\rightarrow$

$\rightarrow$

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

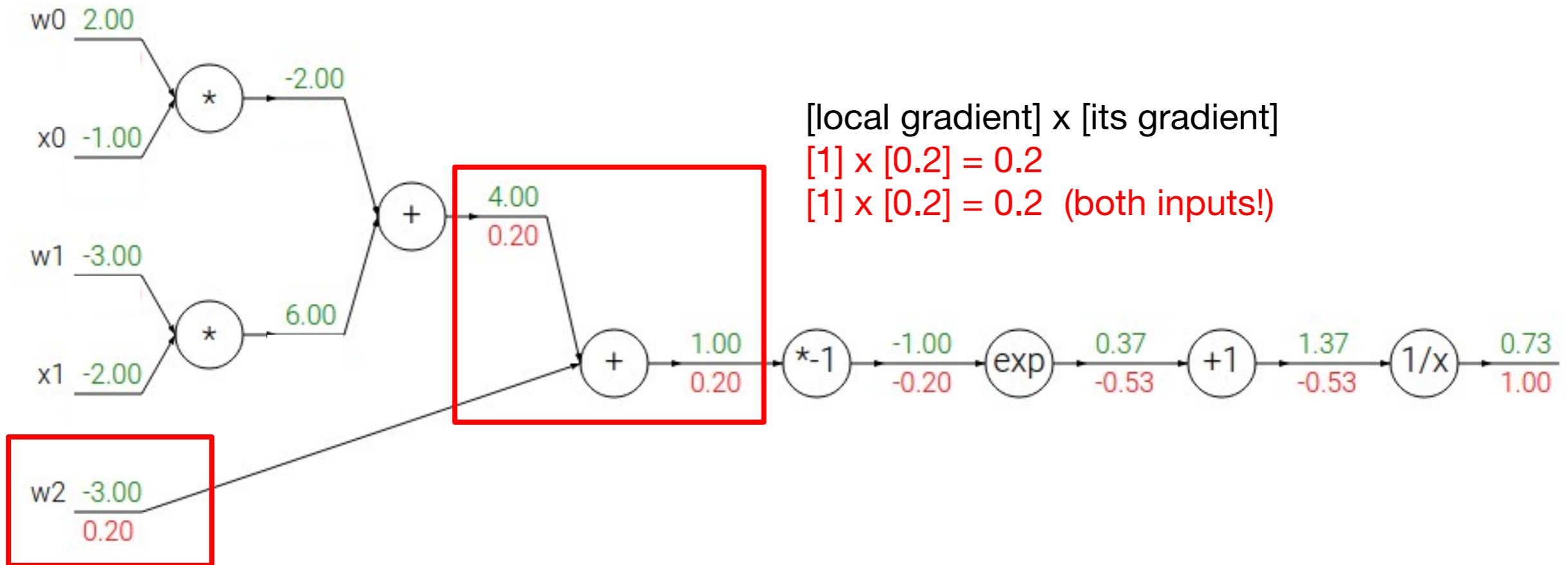
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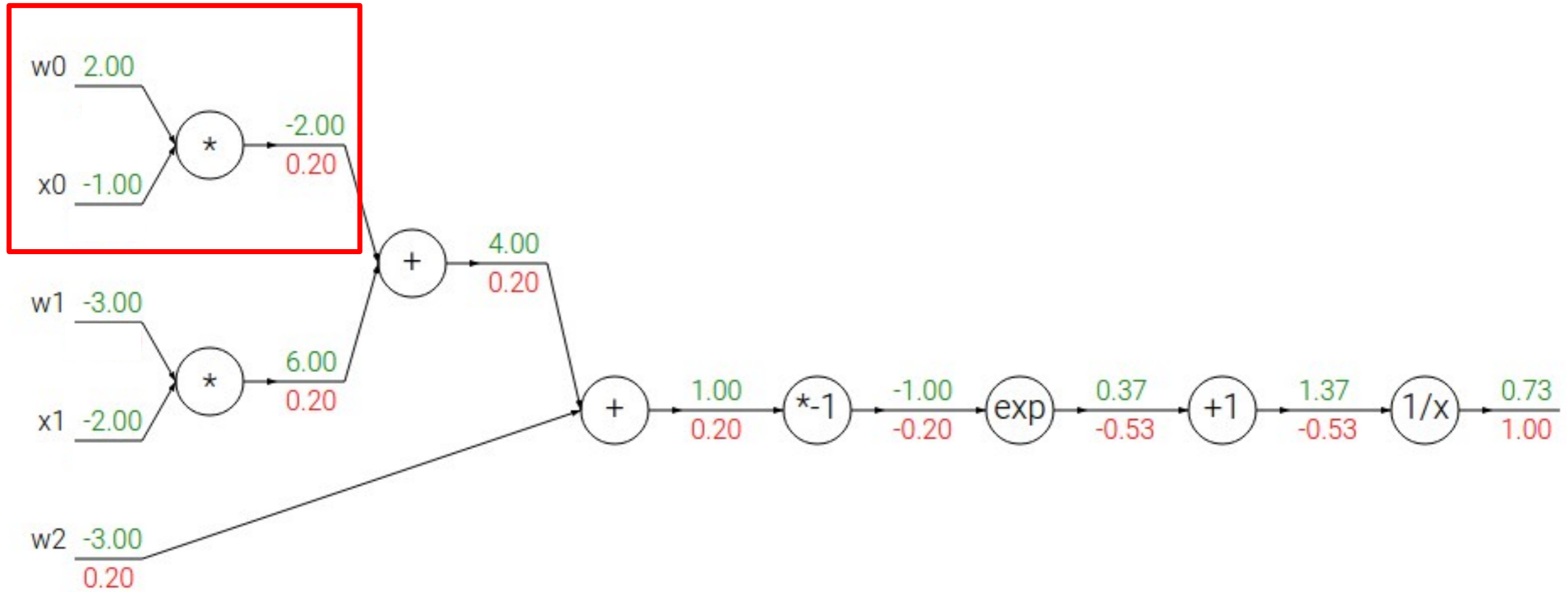


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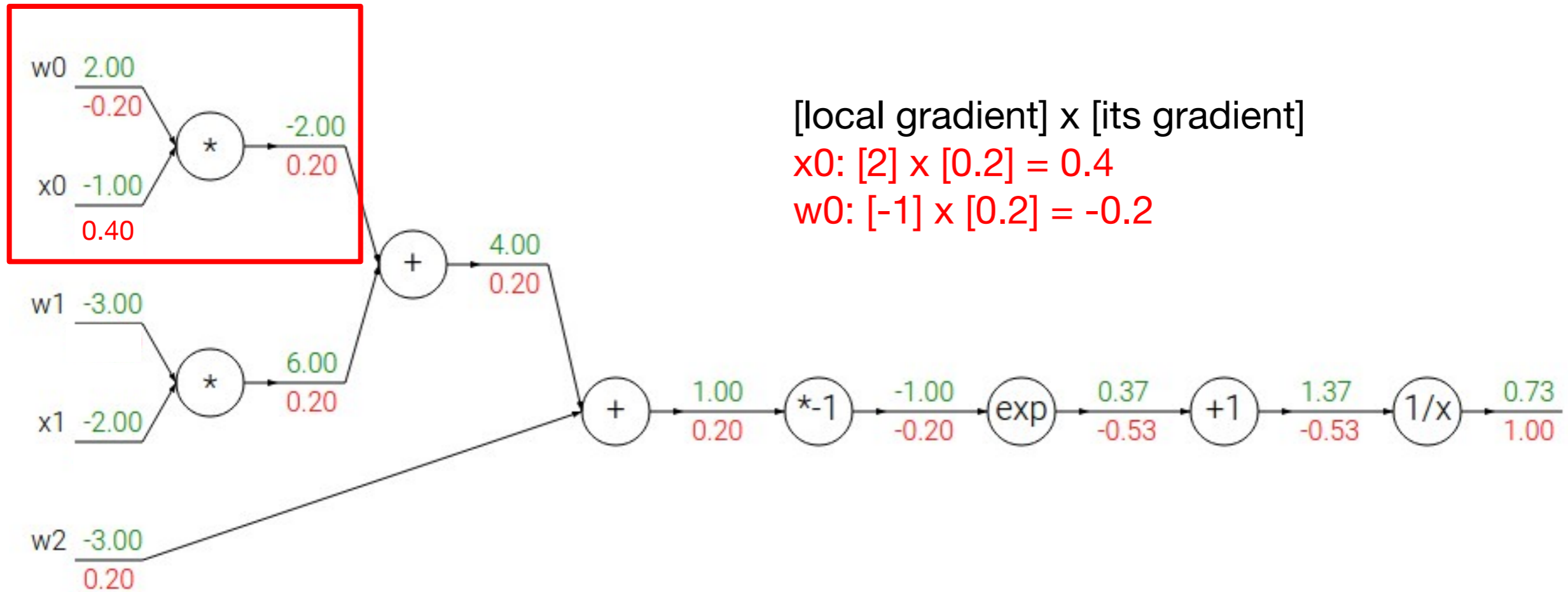
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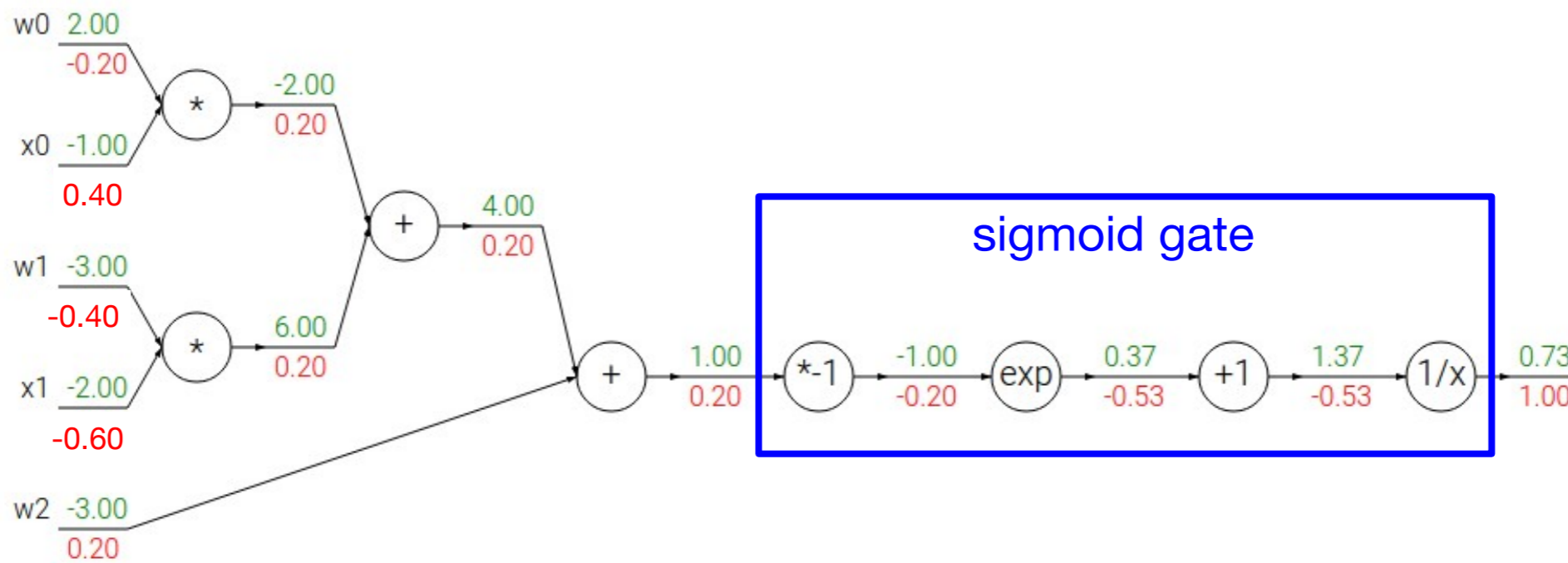
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$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$

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

sigmoid function

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

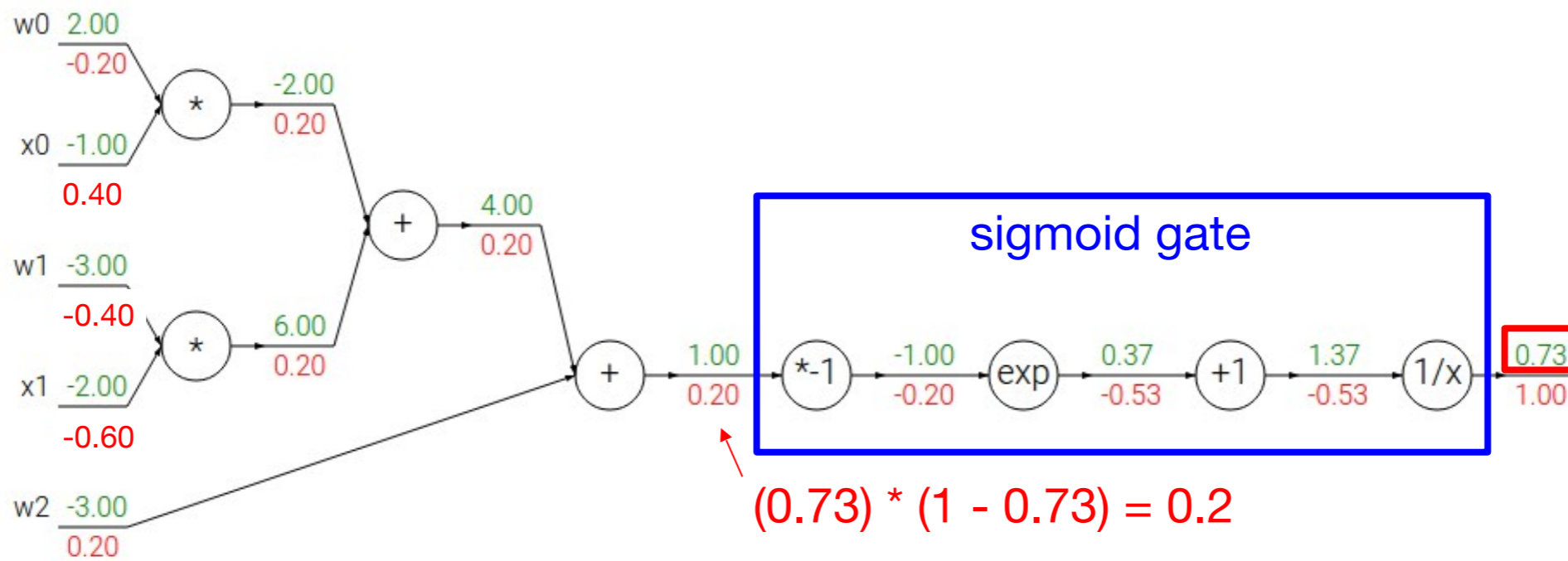


$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$

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

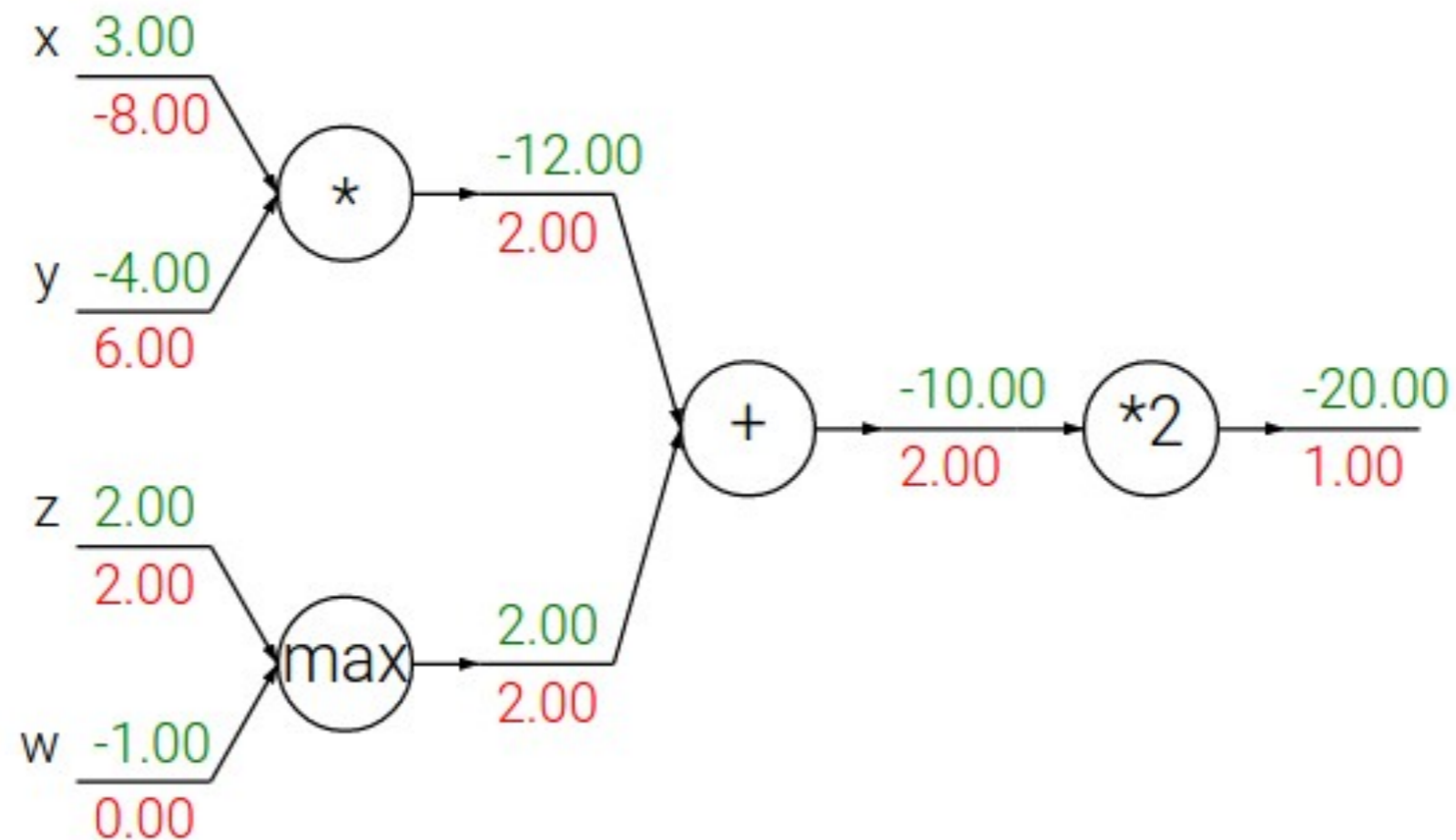
sigmoid function

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

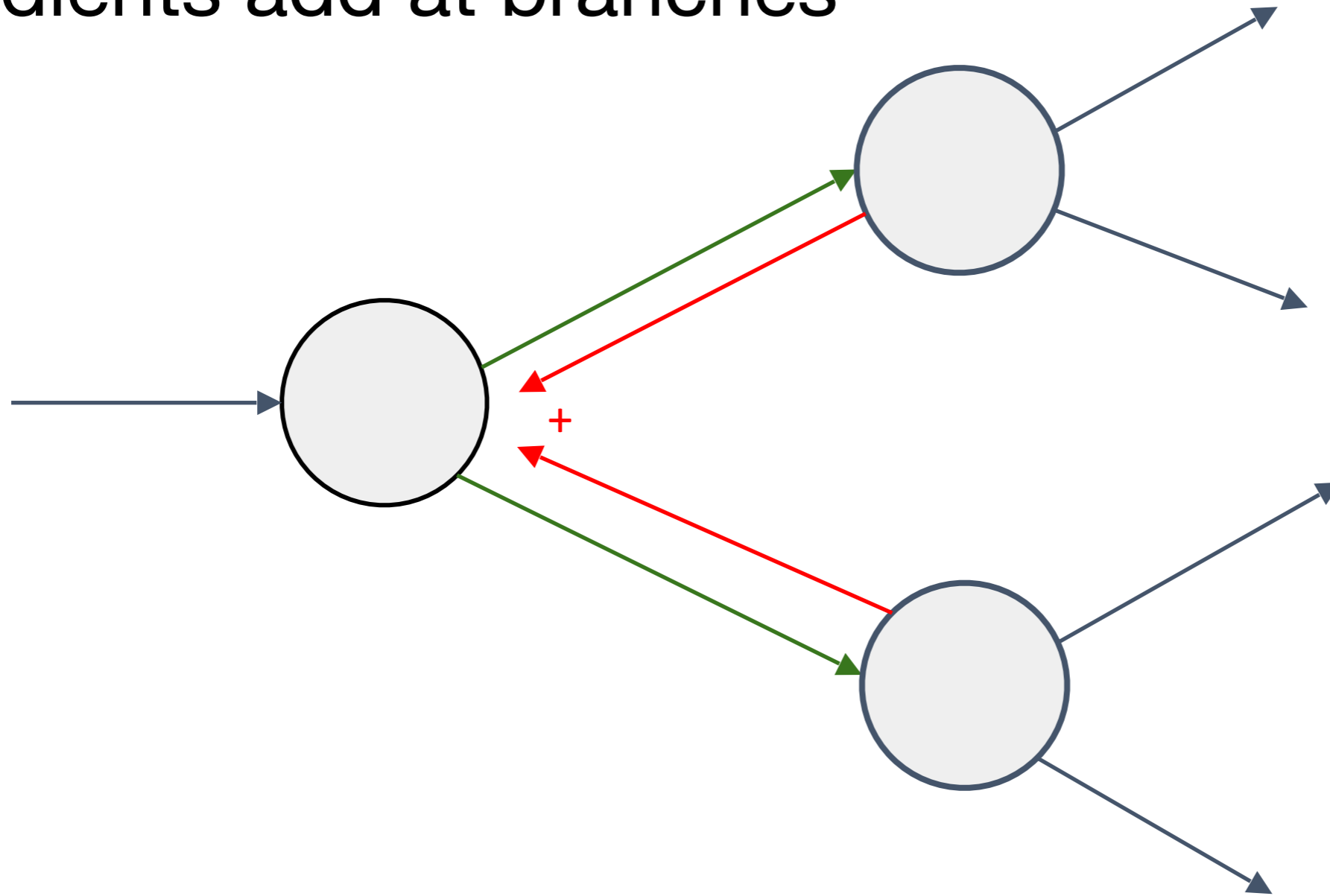


# Patterns in backward flow

- **add** gate: gradient distributor
- **max** gate: gradient router
- **mul** gate: gradient... “switcher”?



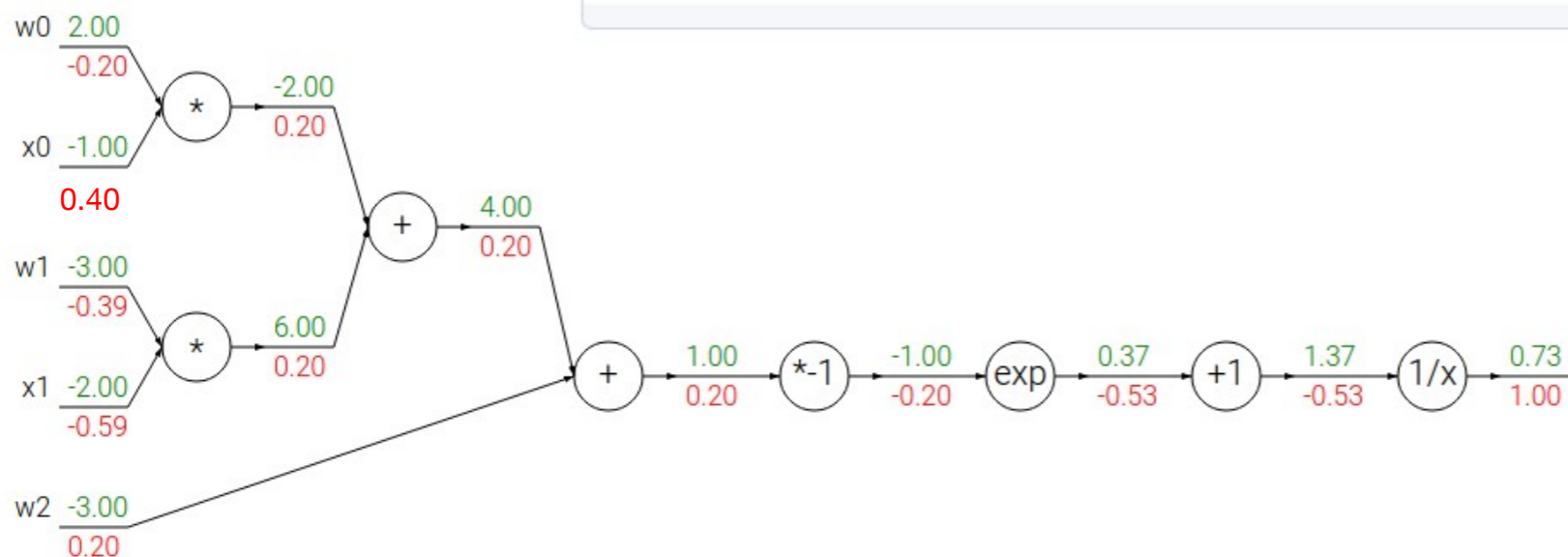
# Gradients add at branches



# Implementation: forward/backward API

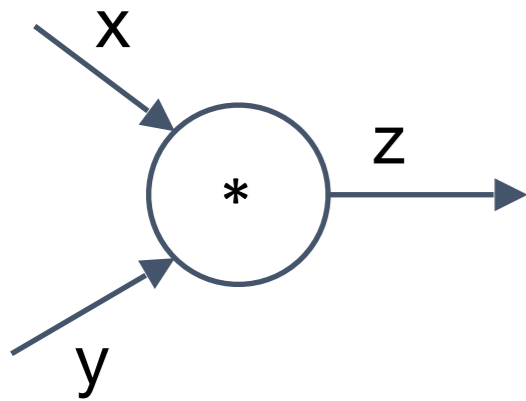
Graph (or Net) object.  
(Rough pseudo code)

```
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
```





# Implementation: forward/backward API



(x,y,z are scalars)

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

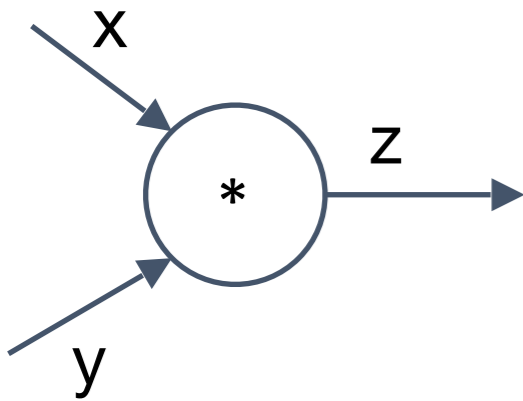
$$\frac{\partial L}{\partial z}$$

An arrow points from this box to the `dz` parameter in the `backward` method of the code block above.

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

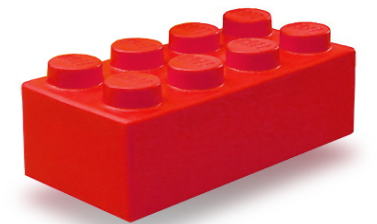
An arrow points from this box to the `dx` element in the `return [dx, dy]` statement of the code block above.

# Implementation: forward/backward API



(x,y,z are scalars)

```
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]
```



# Summary

- 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.

# Where are we now...

## Mini-batch SGD

Loop:

- 1. Sample** a batch of data
- 2. Forward** prop it through the graph, get loss
- 3. Backprop** to calculate the gradients
- 4. Update** the parameters using the gradient

**Next Lecture:**

Introduction to Deep Learning