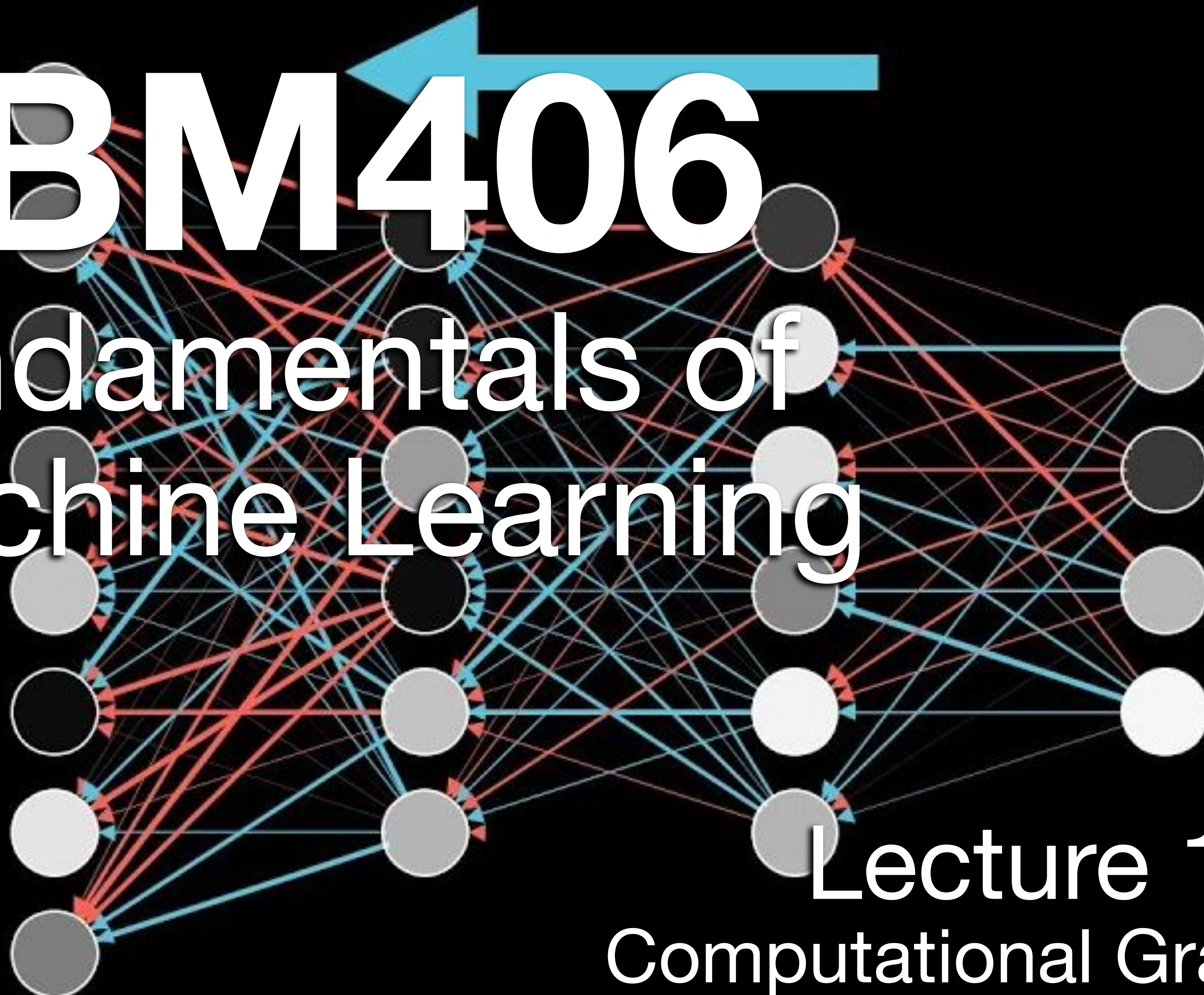
Illustration: 3Blue1Brown



BBM406

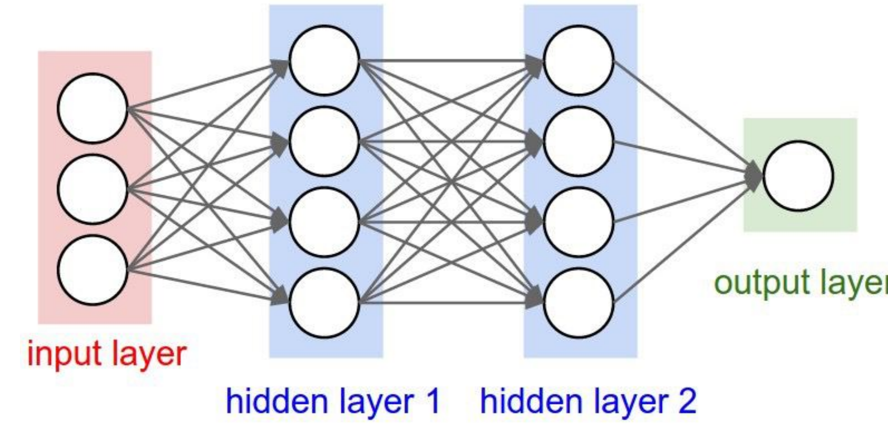
Fundamentals of Machine Learning

Lecture 12:
Computational Graph
Backpropagation

HACETTEPE UNIVERSITY COMPUTER VISION LAB

Erkut Erdem // Hacettepe University // Fall 2021

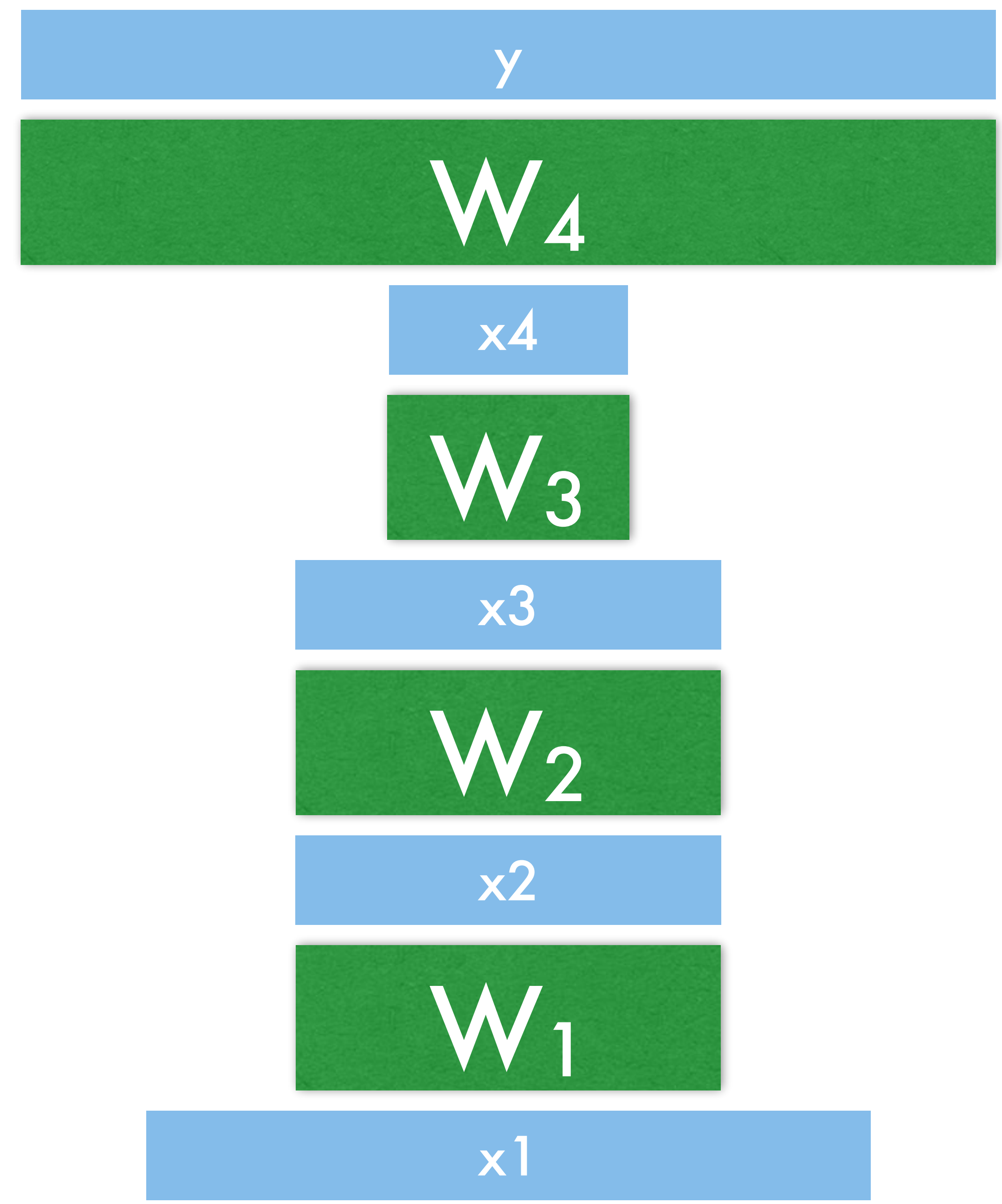
Last time...
Multilayer Perceptron



- Layer Representation

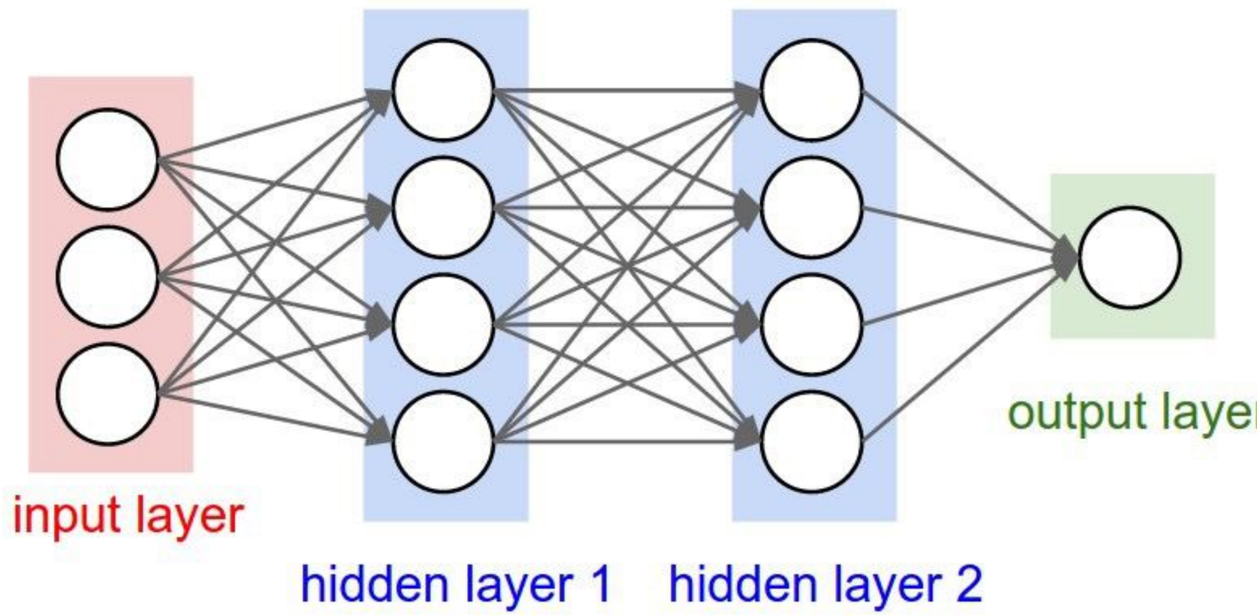
$$y_i = W_i x_i$$
$$x_{i+1} = \sigma(y_i)$$

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



slide by Alex Smola

Last time… **Forward Pass**



- Output of the network can be written as:

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

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

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

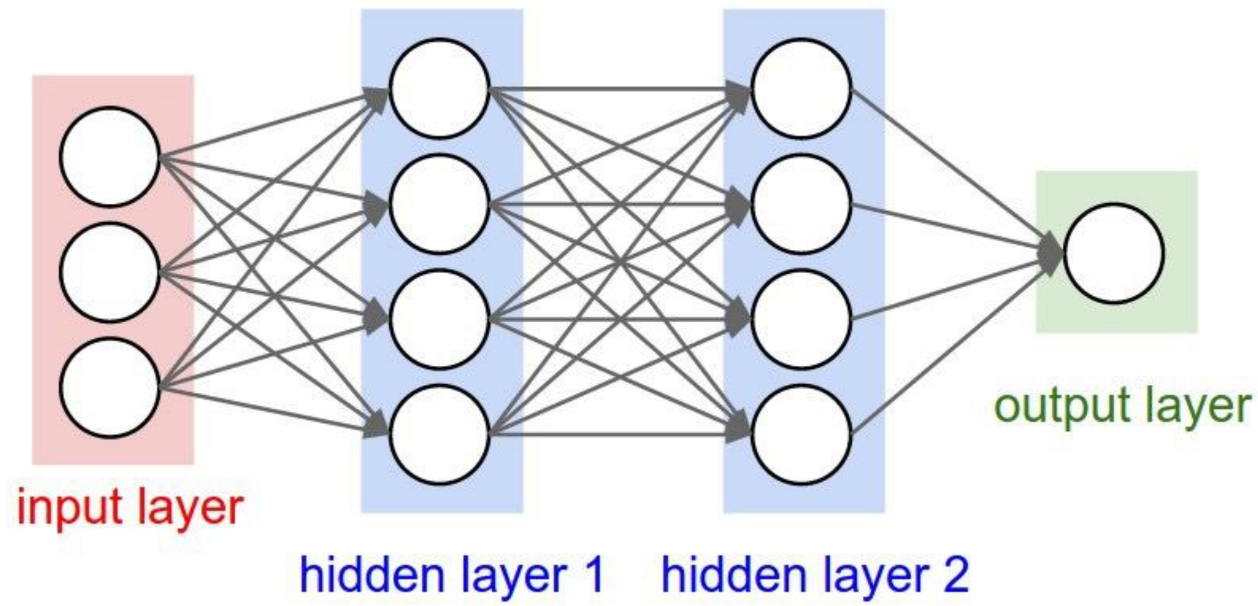
- Activation functions f , g : sigmoid/logistic, tanh, or rectified linear (ReLU)

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

slide by Raquel Urtasun, Richard Zemel, Sanja Fidler

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 × 3, W_2 is 4 × 4. What about biases and W_3?

[http://cs231n.github.io/neural-networks-1/]

slide by Raquel Urtasun, Richard Zemel, Sanja Fidler

Backpropagation

Recap: Loss function/Optimization

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

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

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

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)**

slide by Fei-Fei Li & Andrej Karpathy & Justin Johnson

Softmax Classifier (Multinomial Logistic Regression)

cat	**3.2**
car	5.1
frog	-1.7

slide by Fei-Fei Li & Andrej Karpathy & Justin Johnson

Softmax Classifier (Multinomial Logistic Regression)

scores = unnormalized log probabilities of the classes.

$$\boxed{s = f(x_i; W)}$$

cat	**3.2**
car	5.1
frog	-1.7

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Softmax Classifier (Multinomial Logistic Regression)

scores = unnormalized log probabilities of the classes.

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

cat	**3.2**
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Softmax function

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frog	-1.7

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Softmax Classifier (Multinomial Logistic Regression)

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

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**
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Softmax Classifier (Multinomial Logistic Regression)

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

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

---

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

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Softmax Classifier (Multinomial Logistic Regression)

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cat	**3.2**
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unnormalized log probabilities

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Softmax Classifier (Multinomial Logistic Regression)

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

unnormalized probabilities

		exp	
cat	**3.2**	→	**24.5**
car	5.1	→	164.0
frog	-1.7	→	0.18

unnormalized log probabilities

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Softmax Classifier (Multinomial Logistic Regression)

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

unnormalized probabilities

	unnormalized log probabilities	exp →	unnormalized probabilities	normalize →	probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

unnormalized log probabilities

probabilities

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Softmax Classifier (Multinomial Logistic Regression)

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

	unnormalized log probabilities		unnormalized probabilities		probabilities
cat	**3.2**	exp →	**24.5**	normalize →	**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

L_i = -log(0.13)
= **0.89**

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Optimization

Gradient Descent

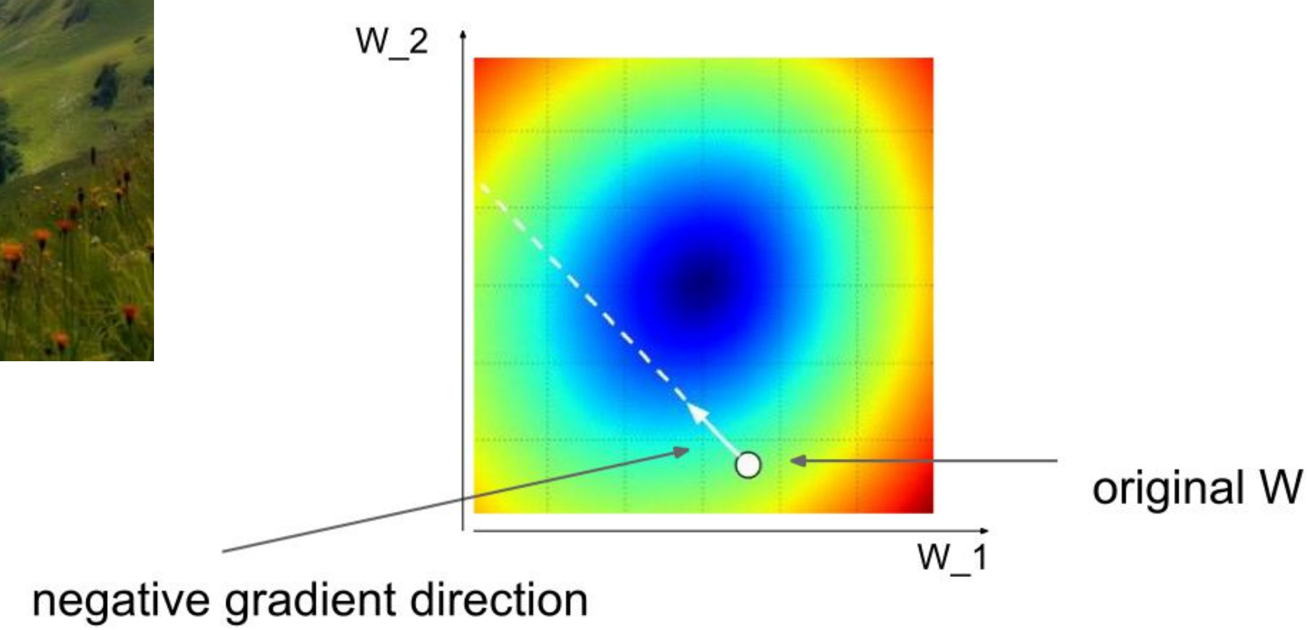
```
# Vanilla Gradient Descent

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:

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

In multiple dimensions, the **gradient** is the vector of (partial derivatives).



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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
```

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

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

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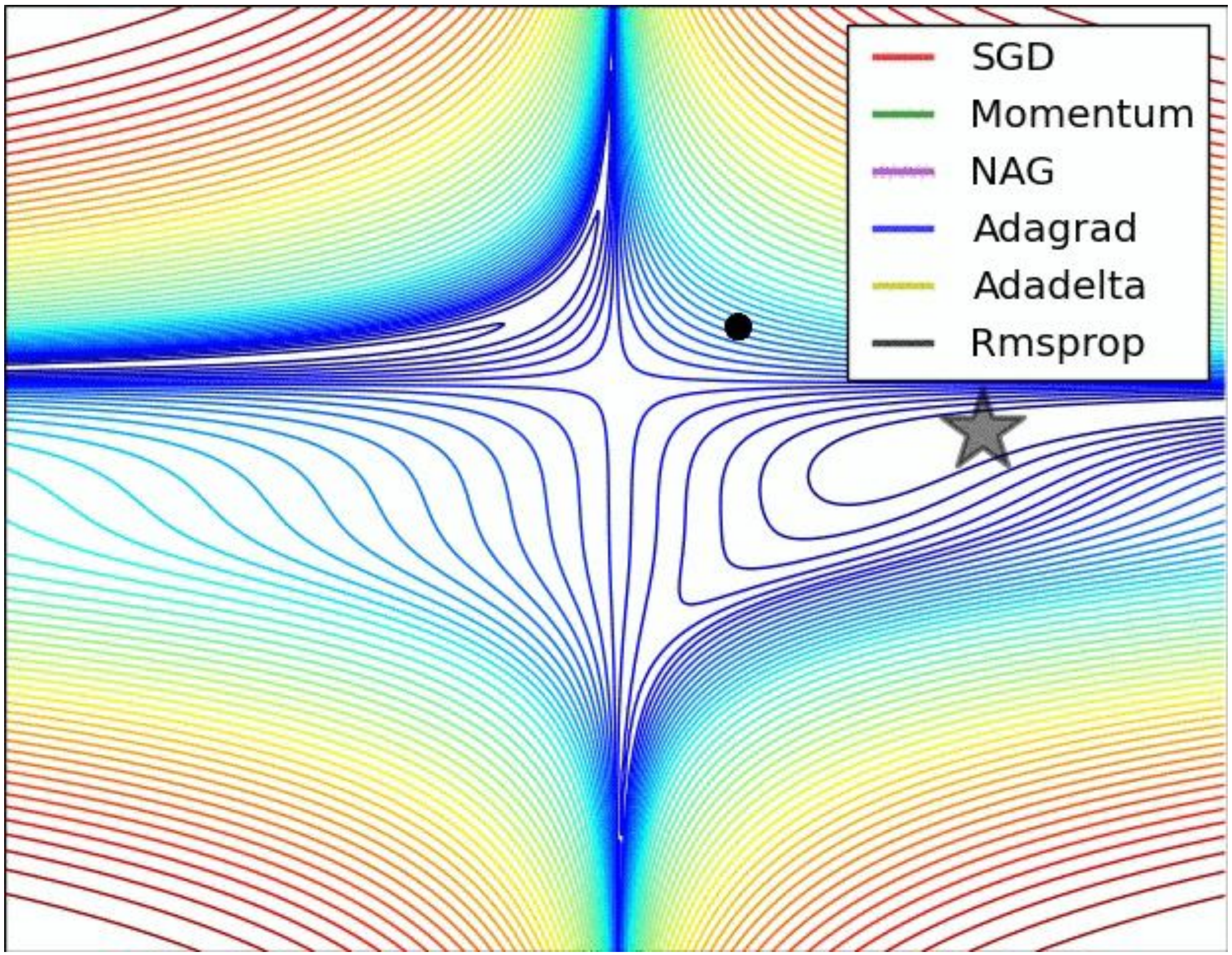
The effects of different update form formulas



(image credits to Alec Radford)

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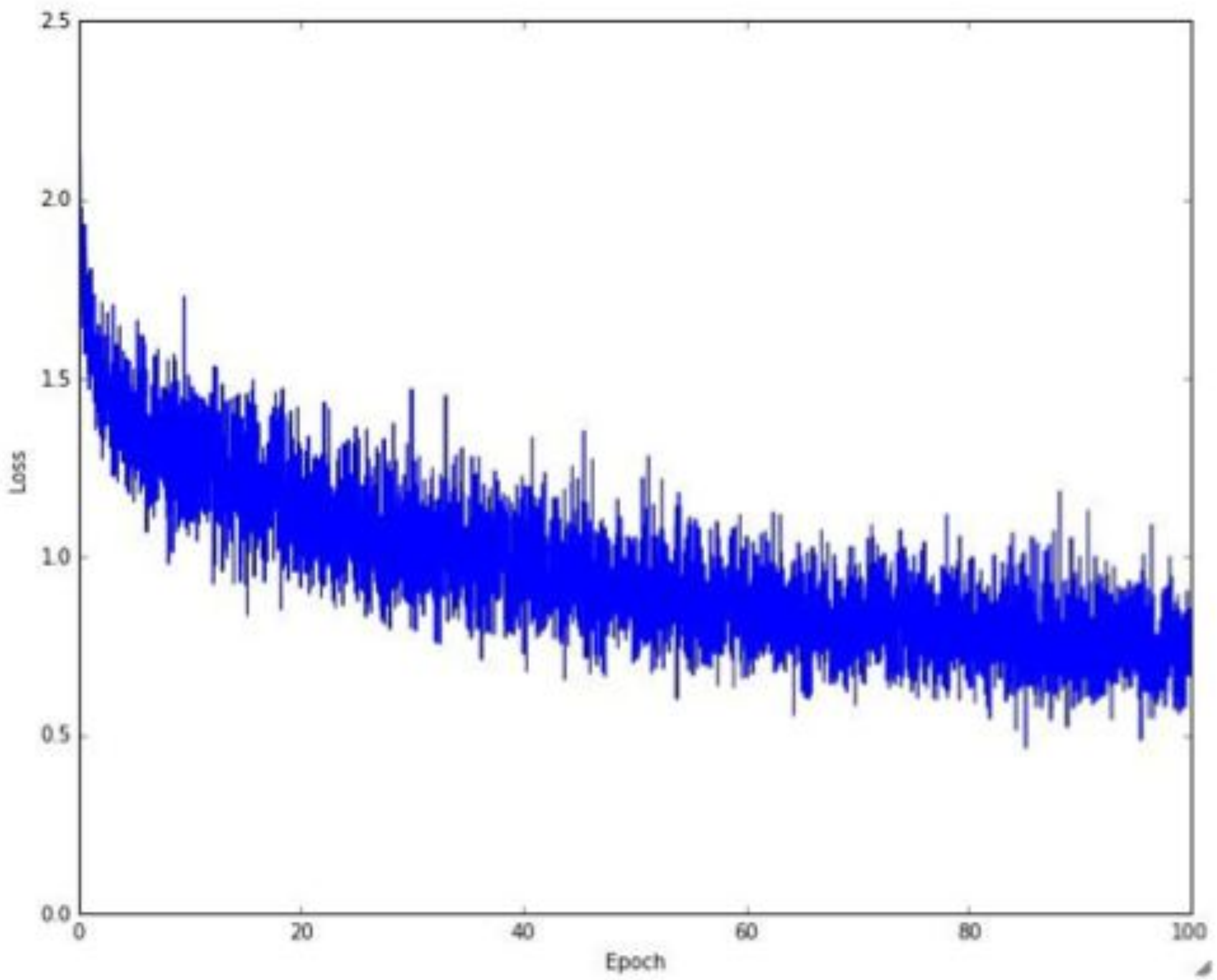
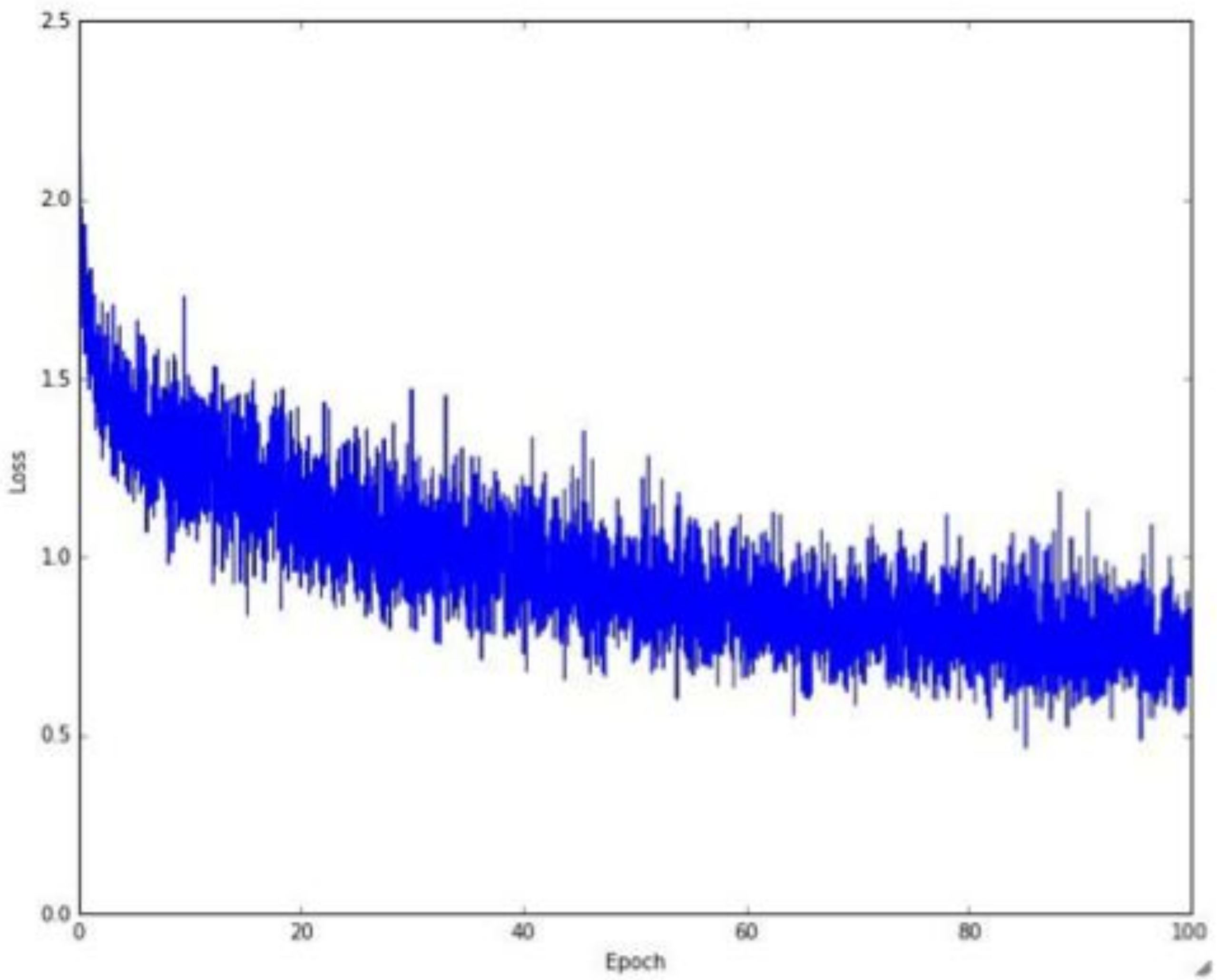
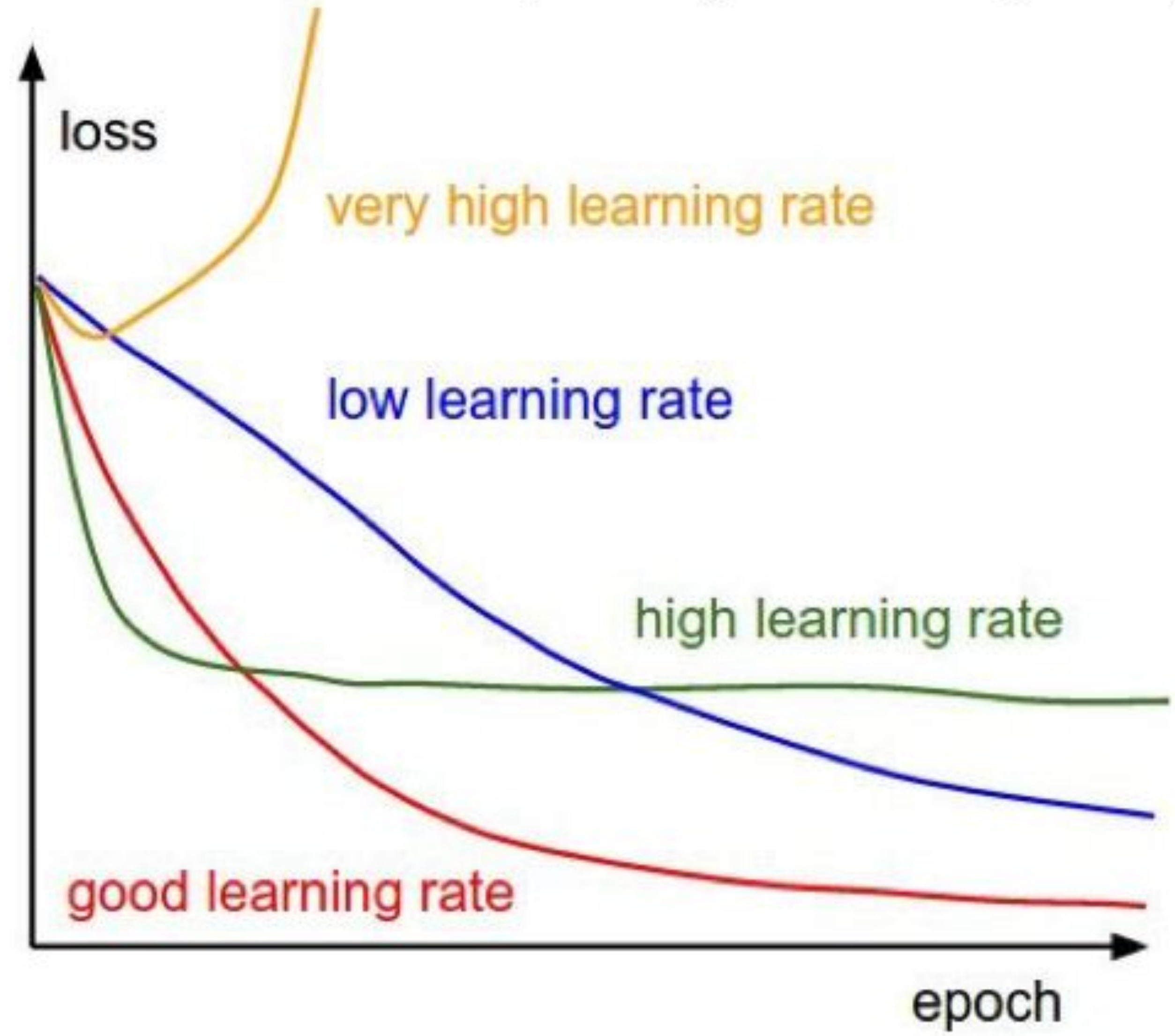


Example of optimization progress while training a neural network.

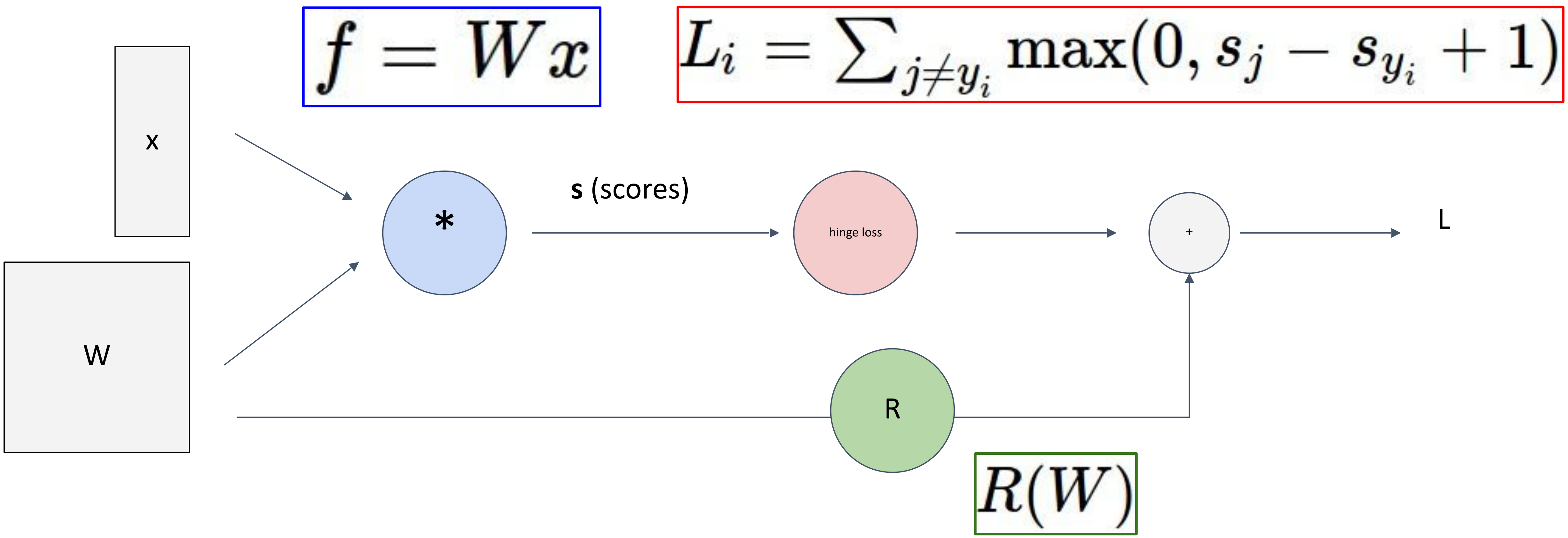
(Loss over mini-batches goes down over time.)



The effects of step size (or "learning rate")



Computational Graph



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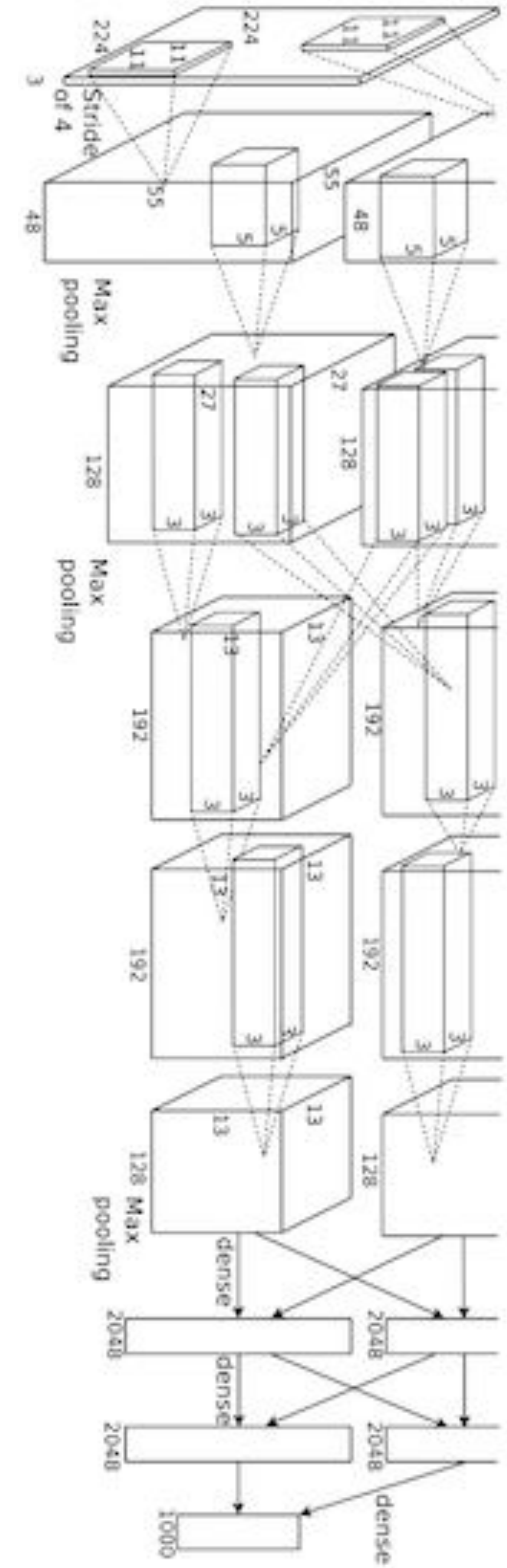
Convolutional Network (AlexNet)

input image

weights

loss



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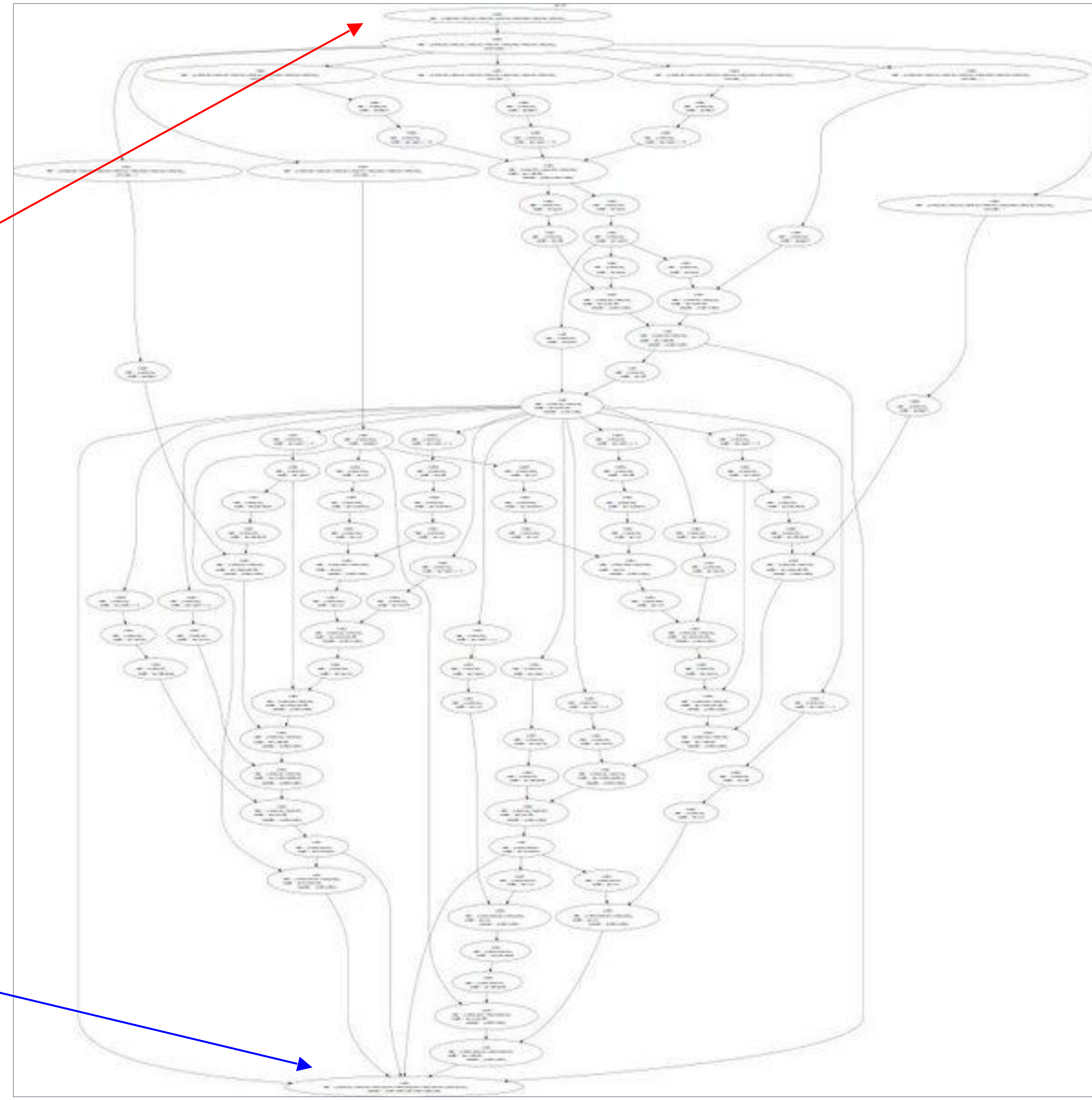
Neural Turing Machine

input tape

loss



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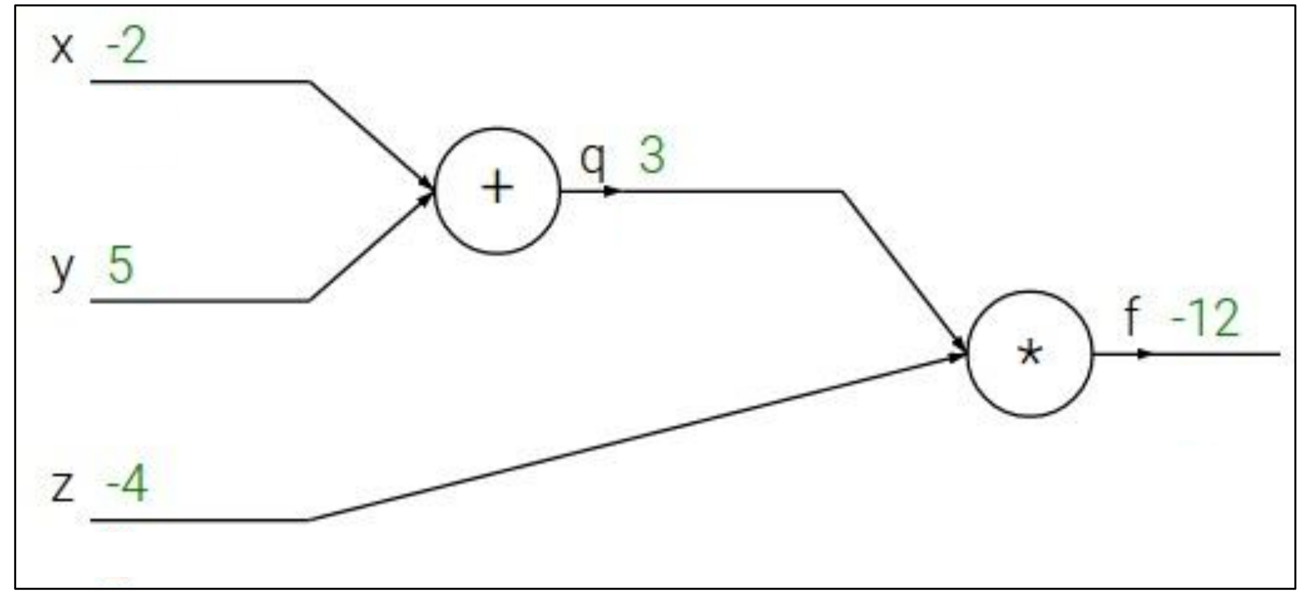
$$f(x, y, z) = (x + y)z$$

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



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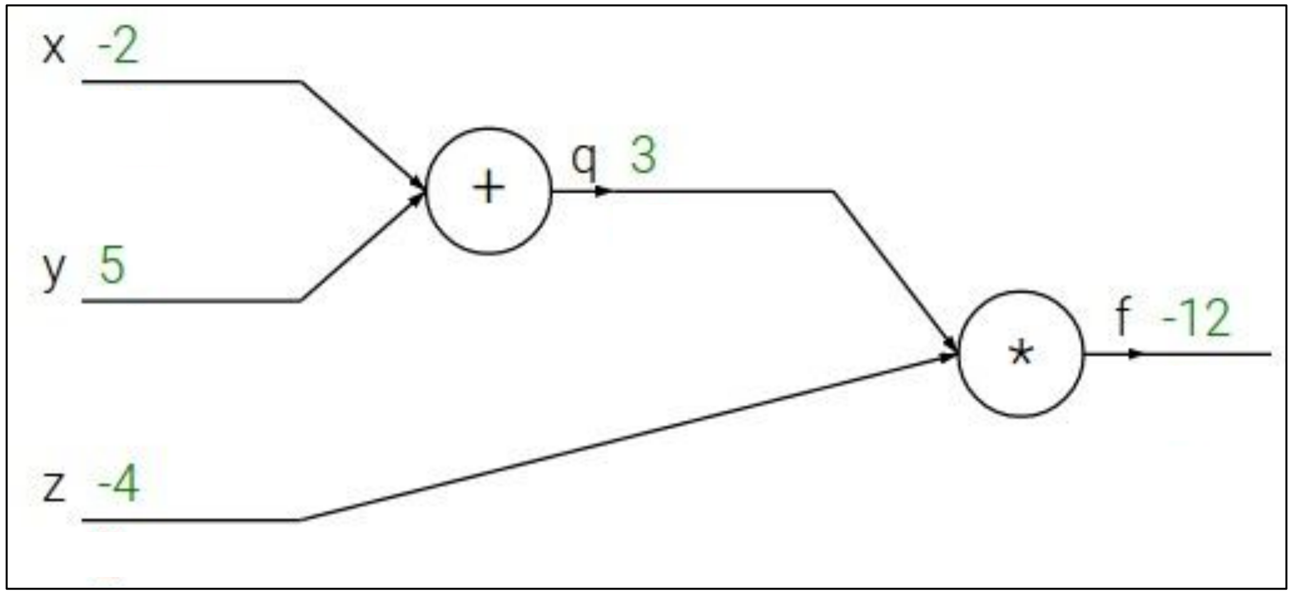

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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

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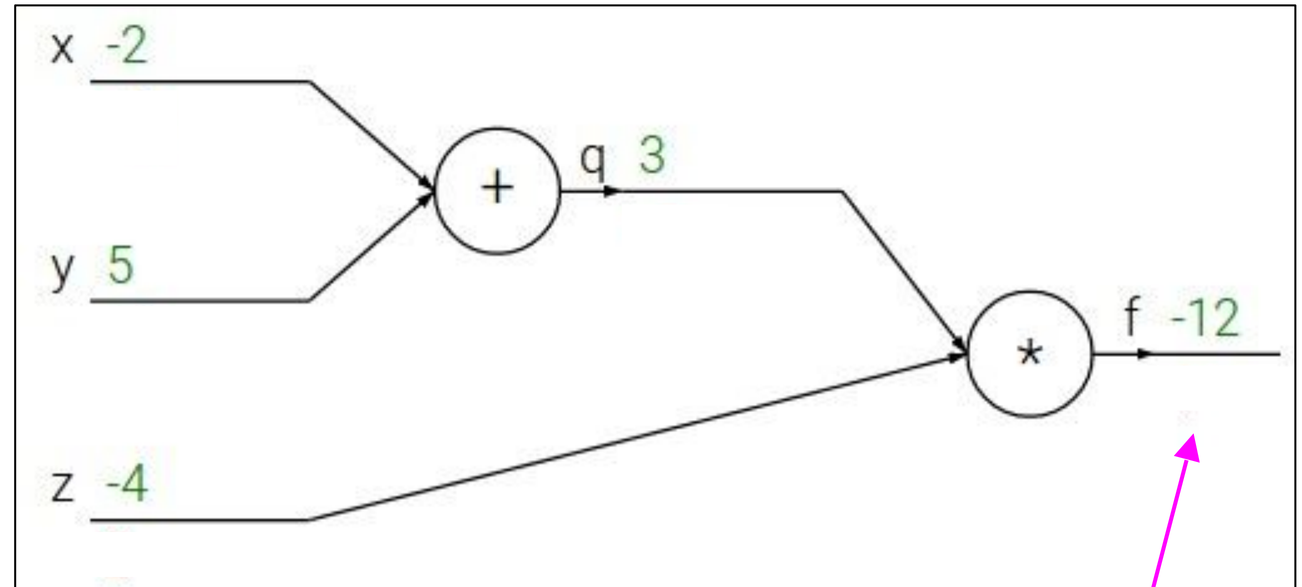

$$\boxed{\frac{\partial f}{\partial f}}$$

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

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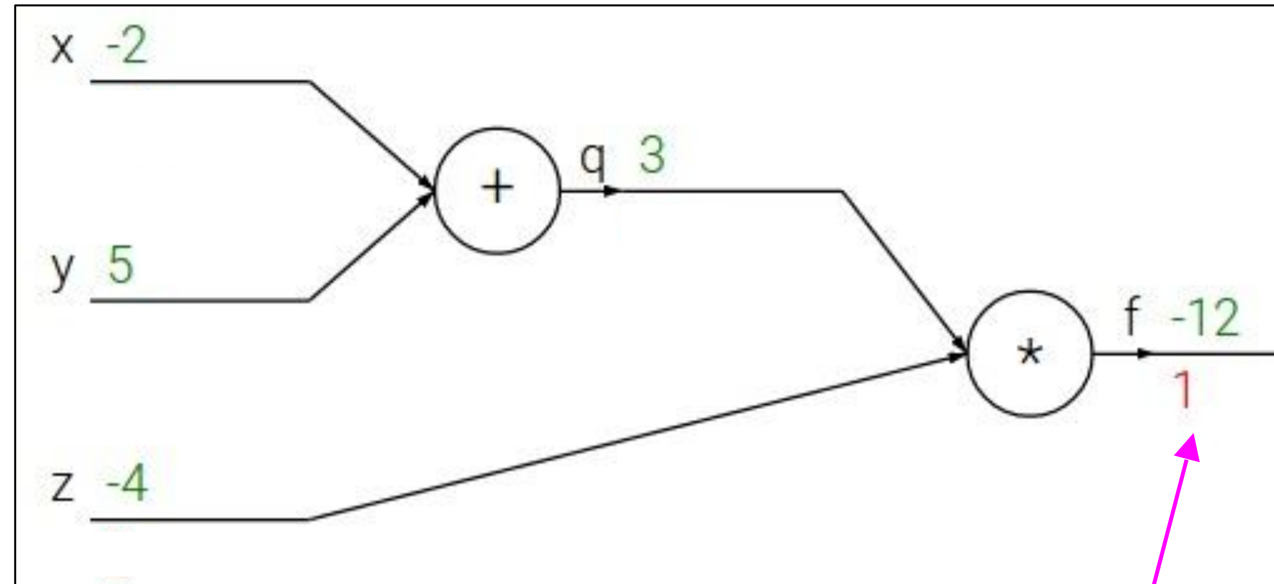

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$$\boxed{\frac{\partial f}{\partial f}}$$

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

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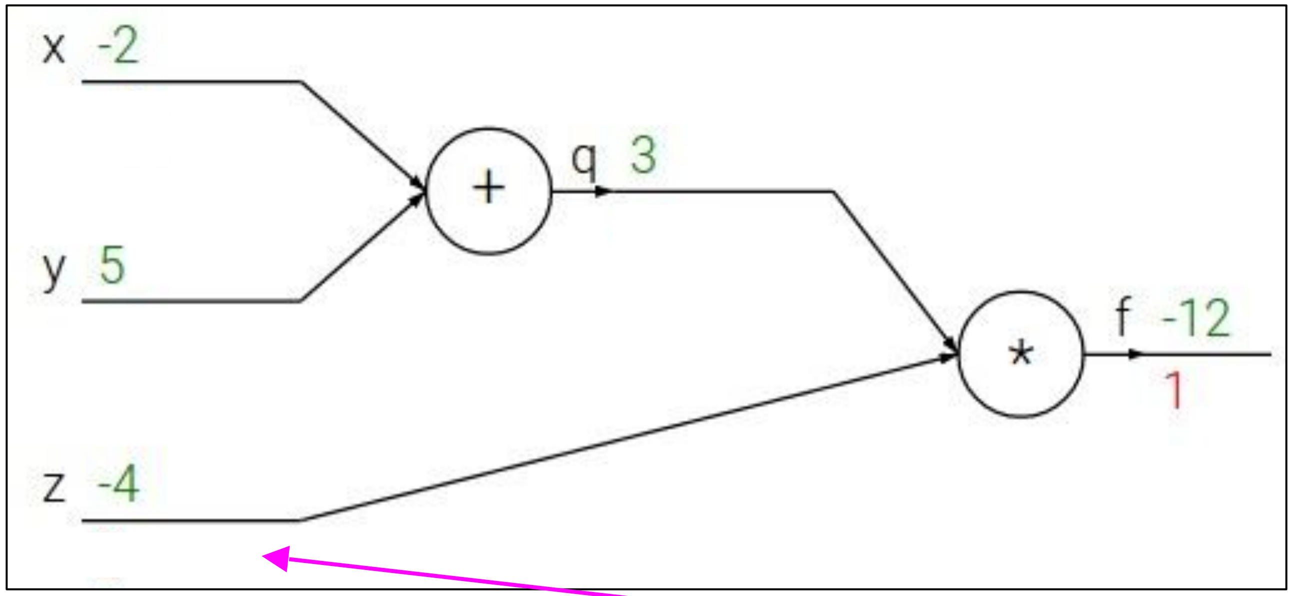

$$\frac{\partial f}{\partial z}$$

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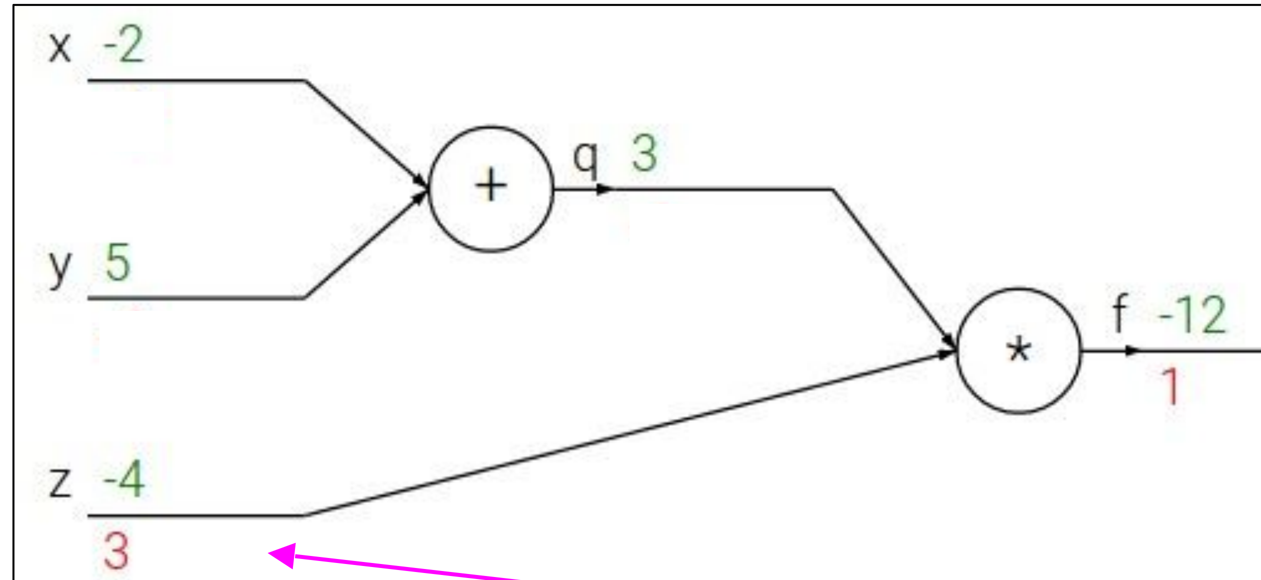

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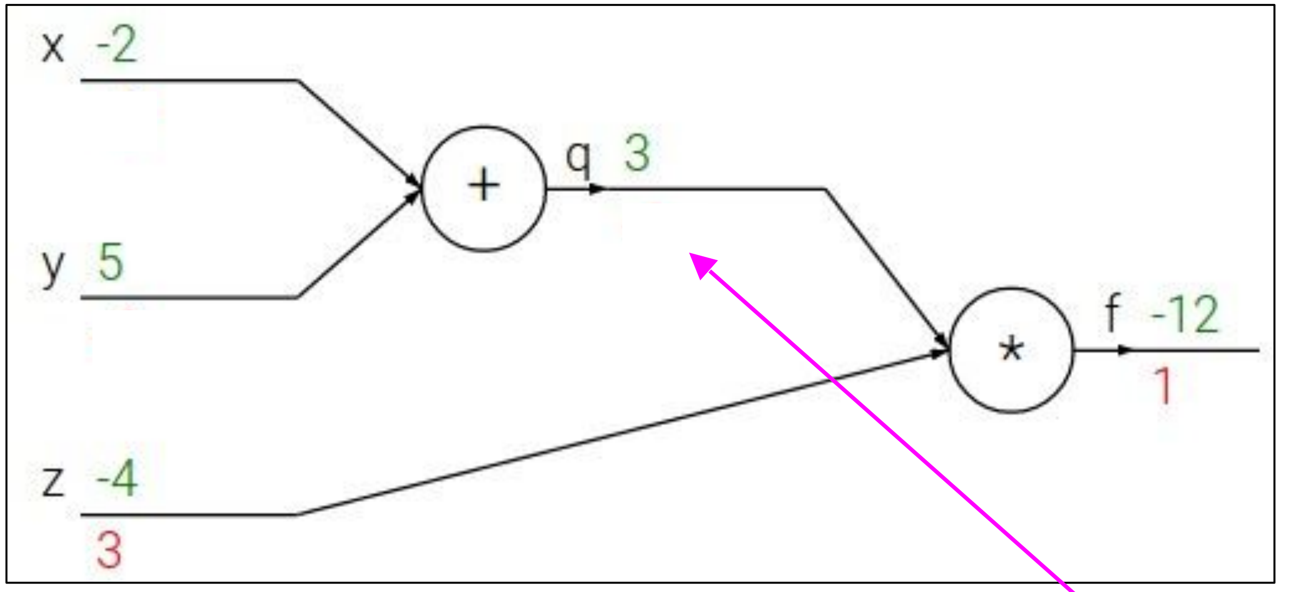

$$\frac{\partial f}{\partial q}$$

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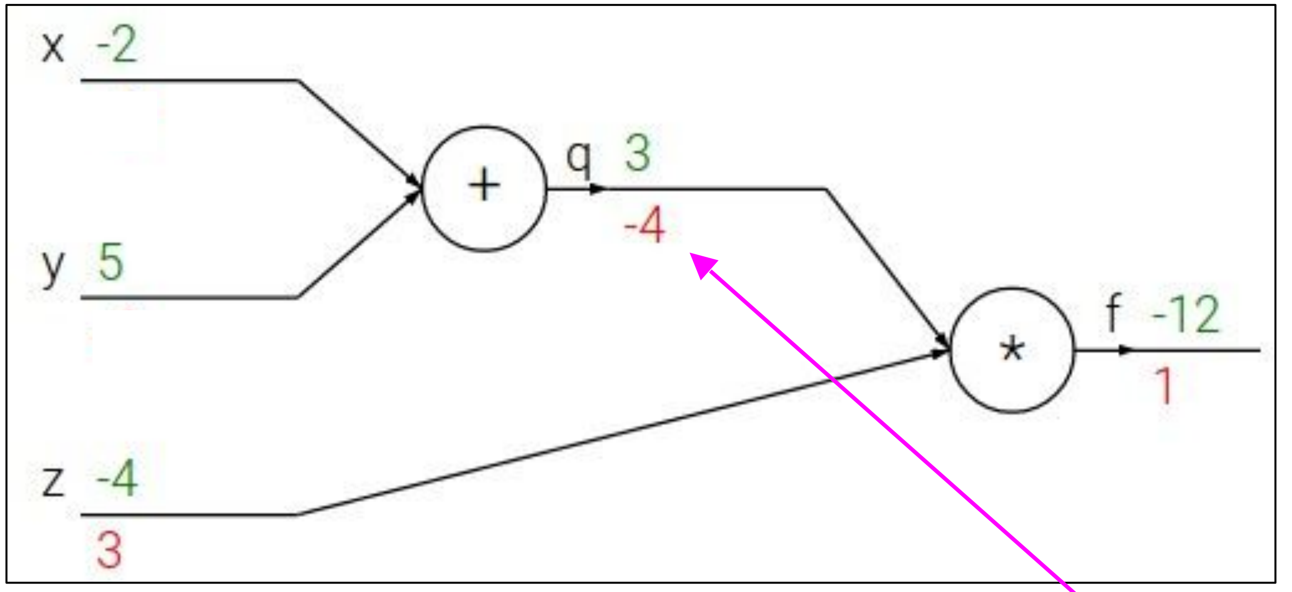

$$\frac{\partial f}{\partial q}$$

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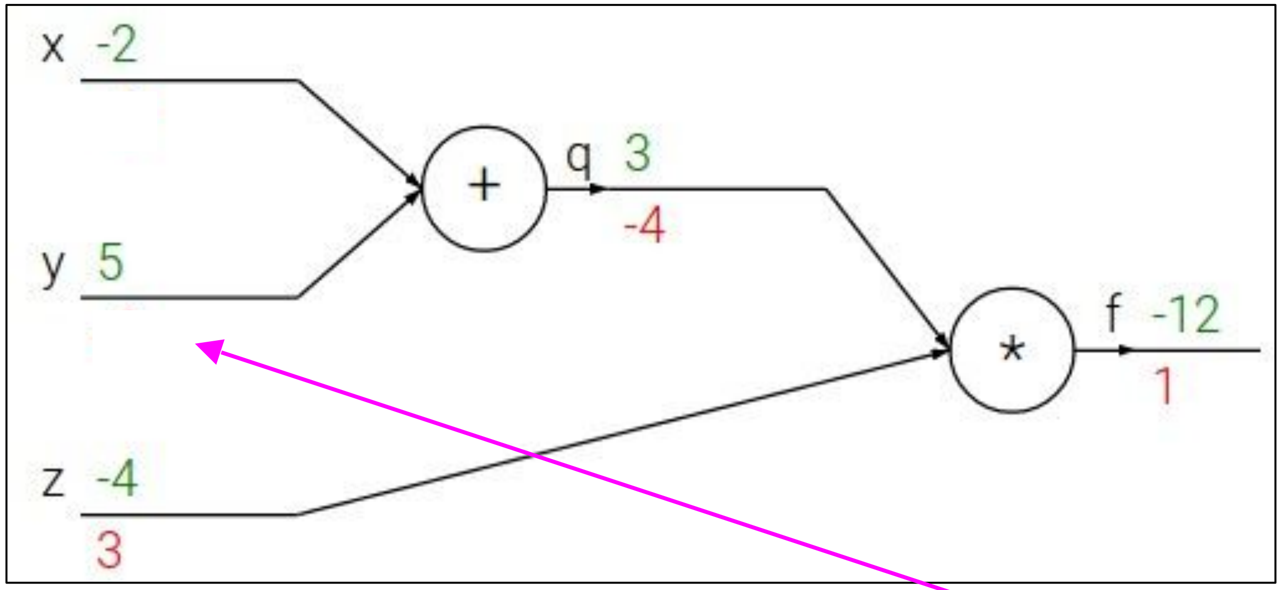

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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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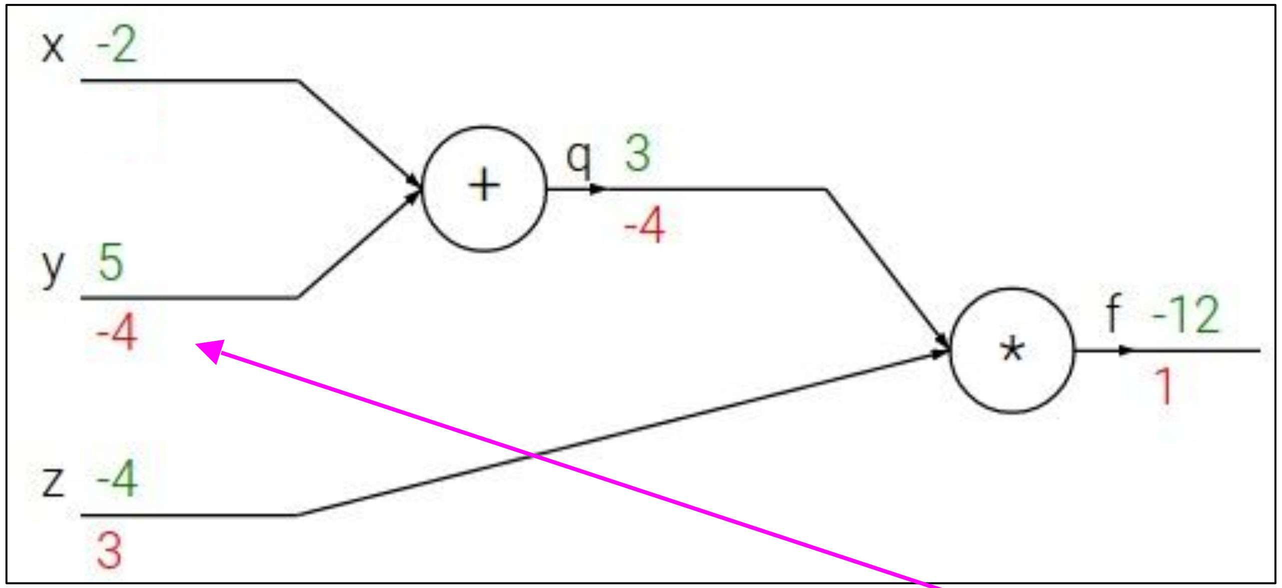

$\frac{\partial f}{\partial y}$

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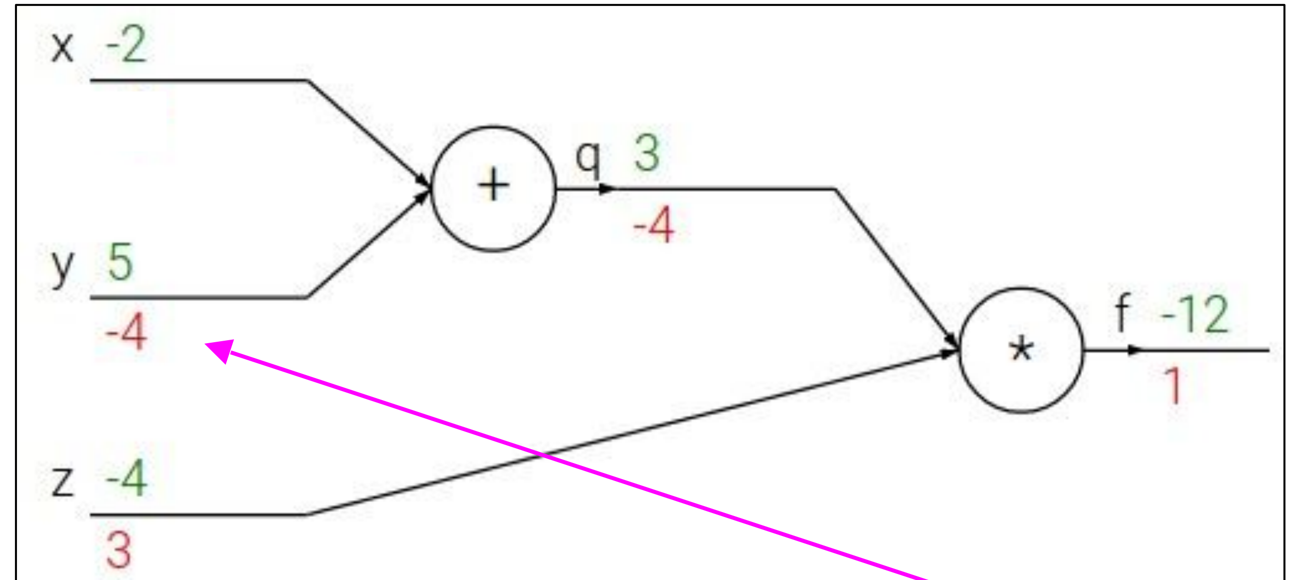

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$$\boxed{\frac{\partial f}{\partial y}}$$

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

Chain rule:

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

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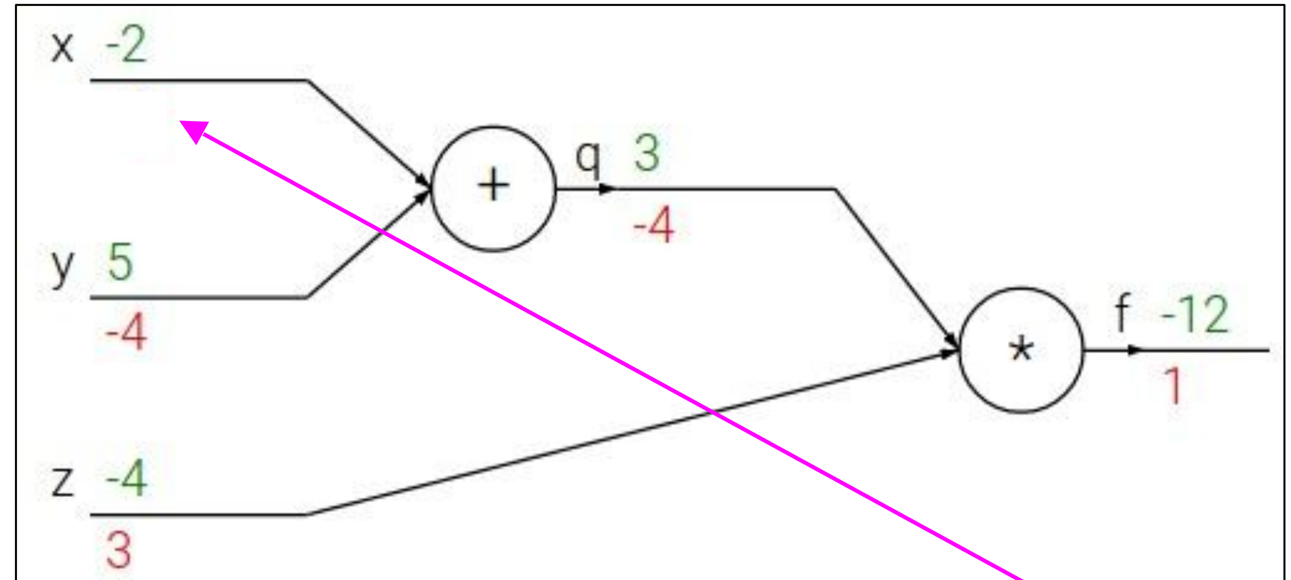
$$f(x, y, z) = (x + y)z$$

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



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

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

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

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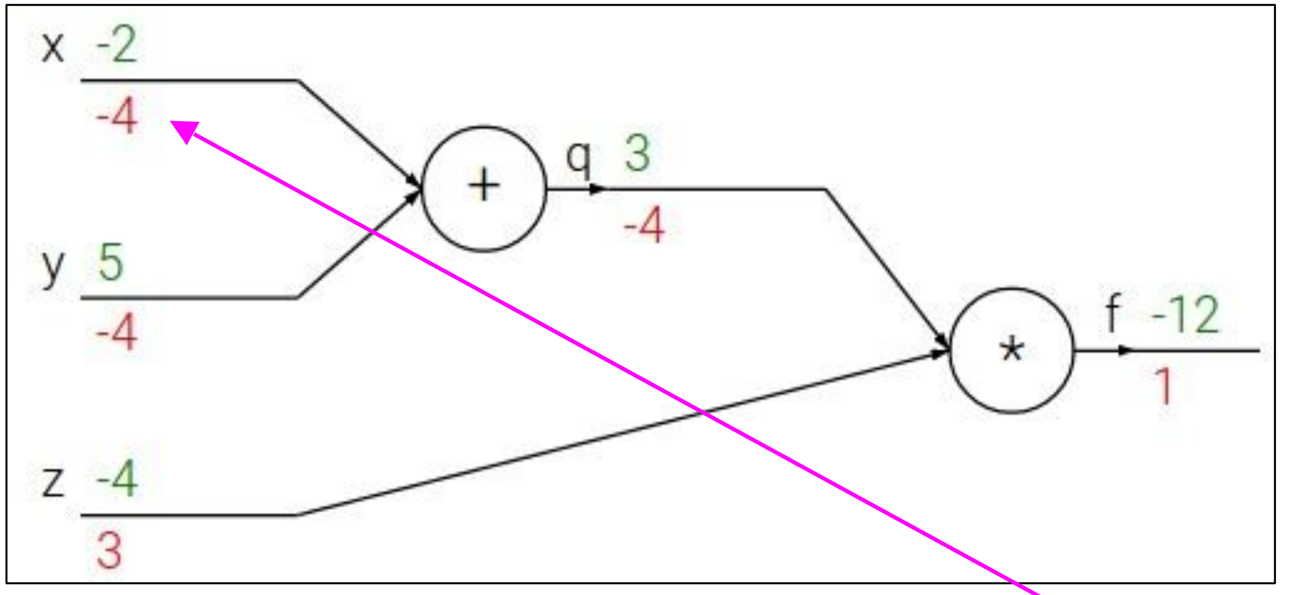

$$\frac{\partial f}{\partial x}$$

Chain rule:

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

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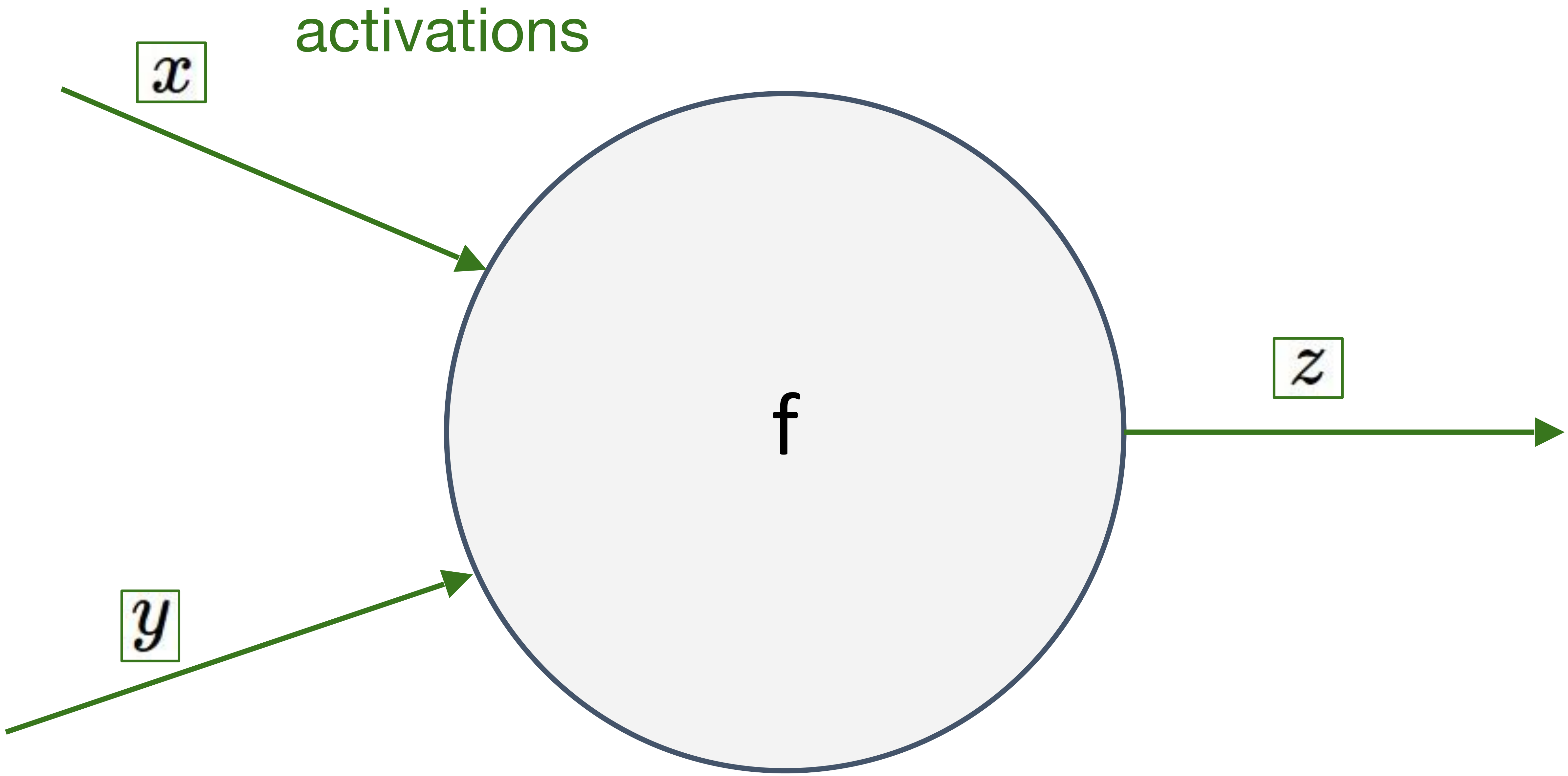
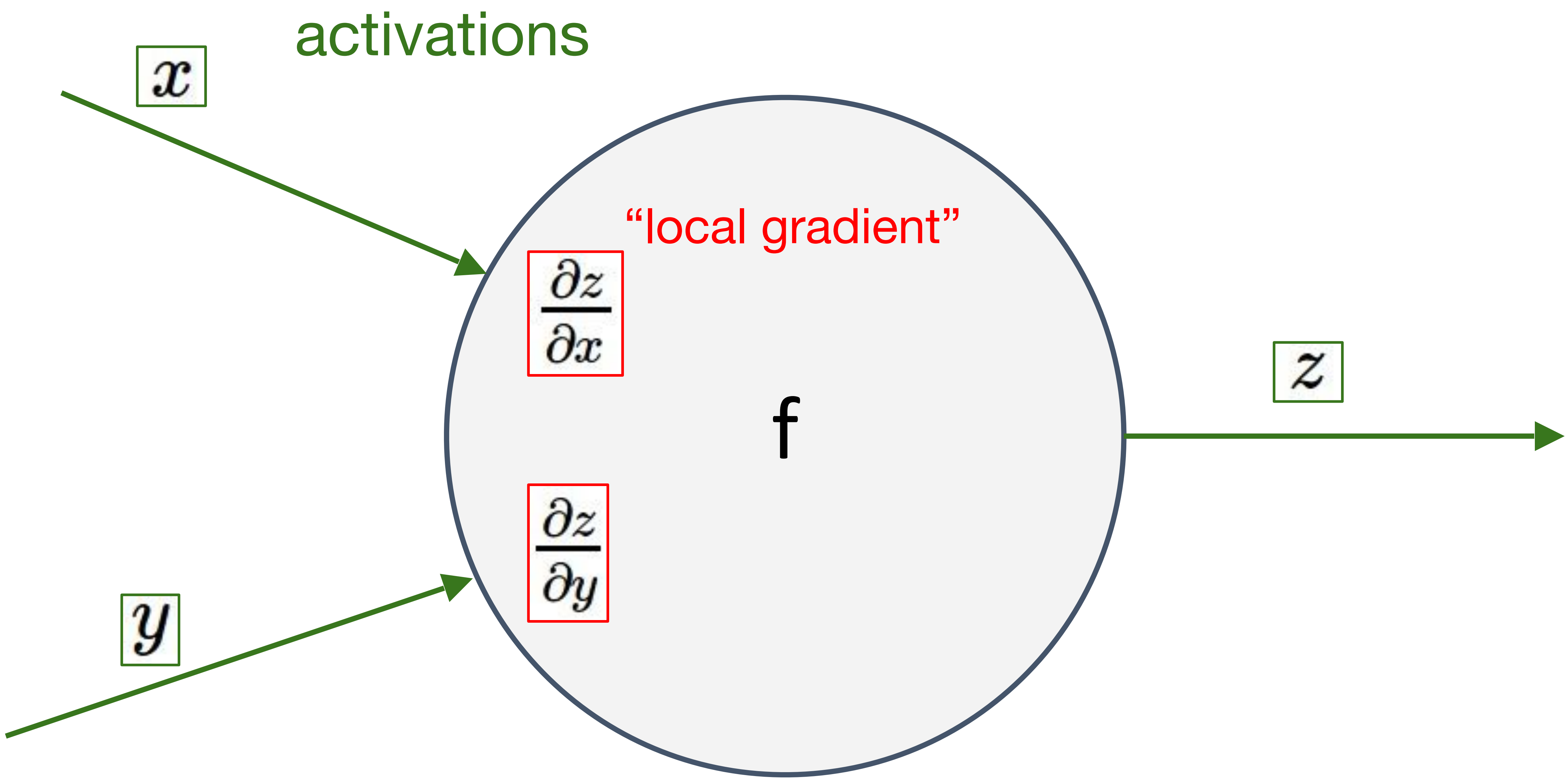

activations
x
y
f
z



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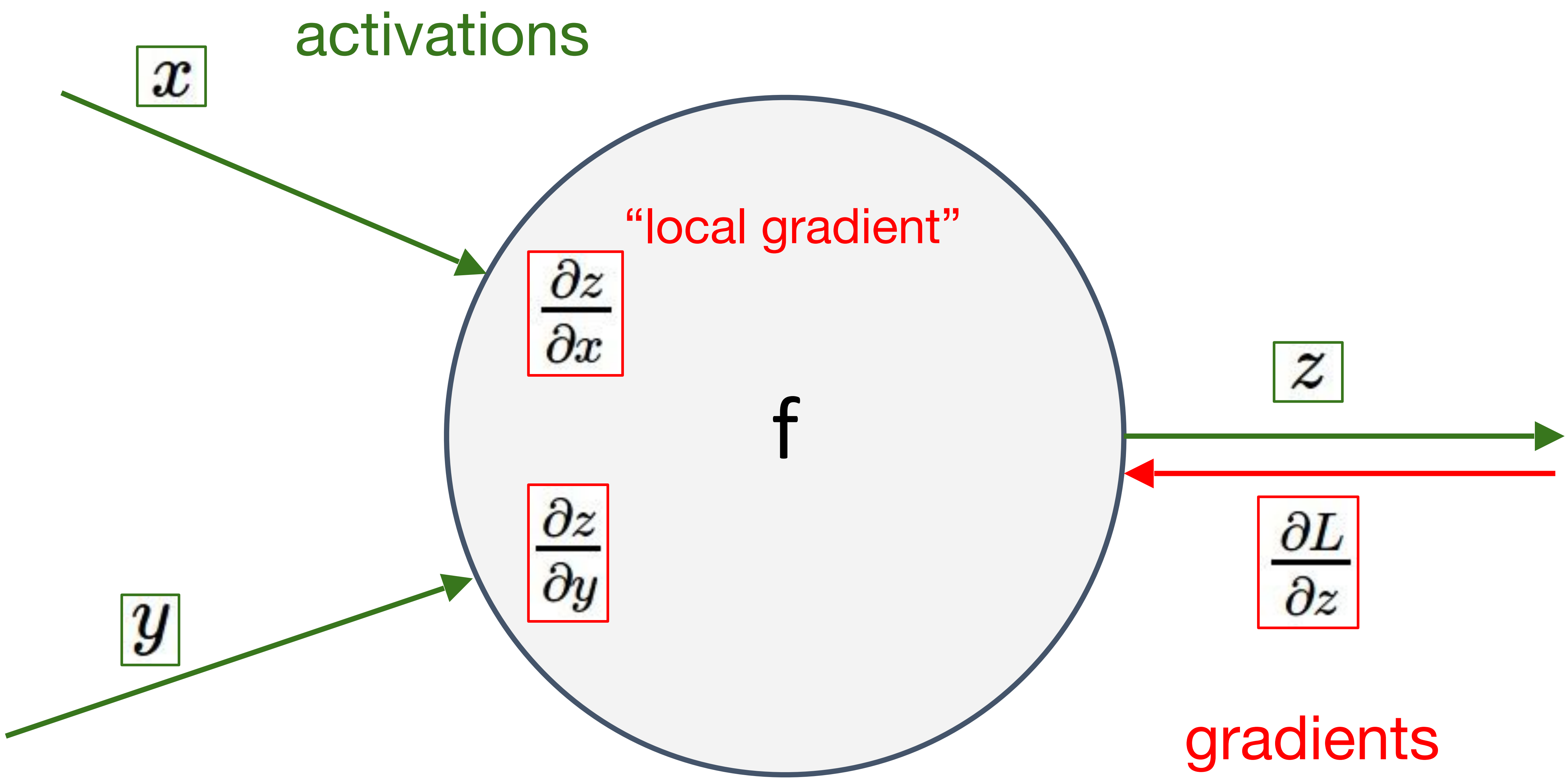
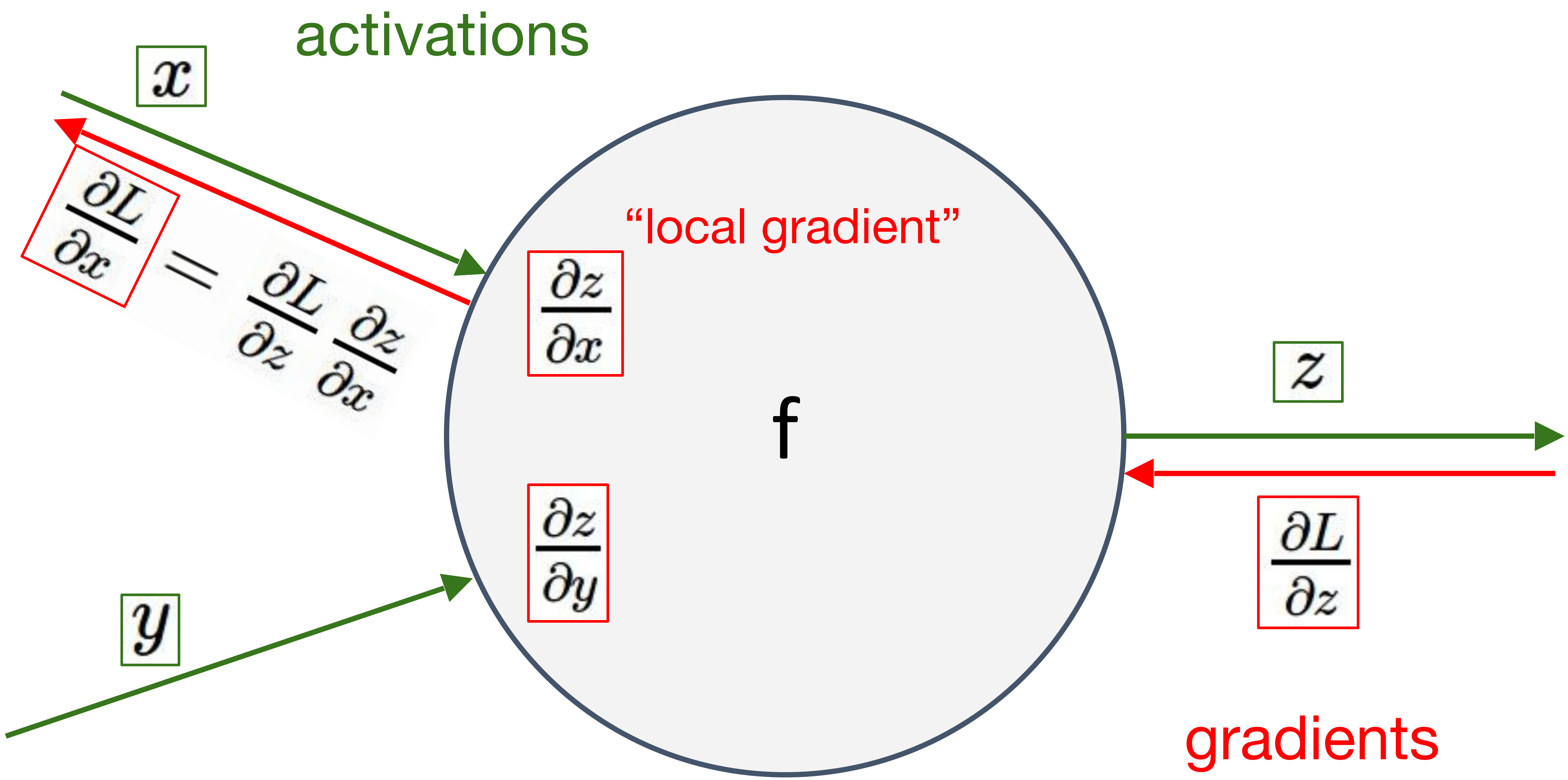

activations
x
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
y
$\frac{\partial L}{\partial z}$
gradients



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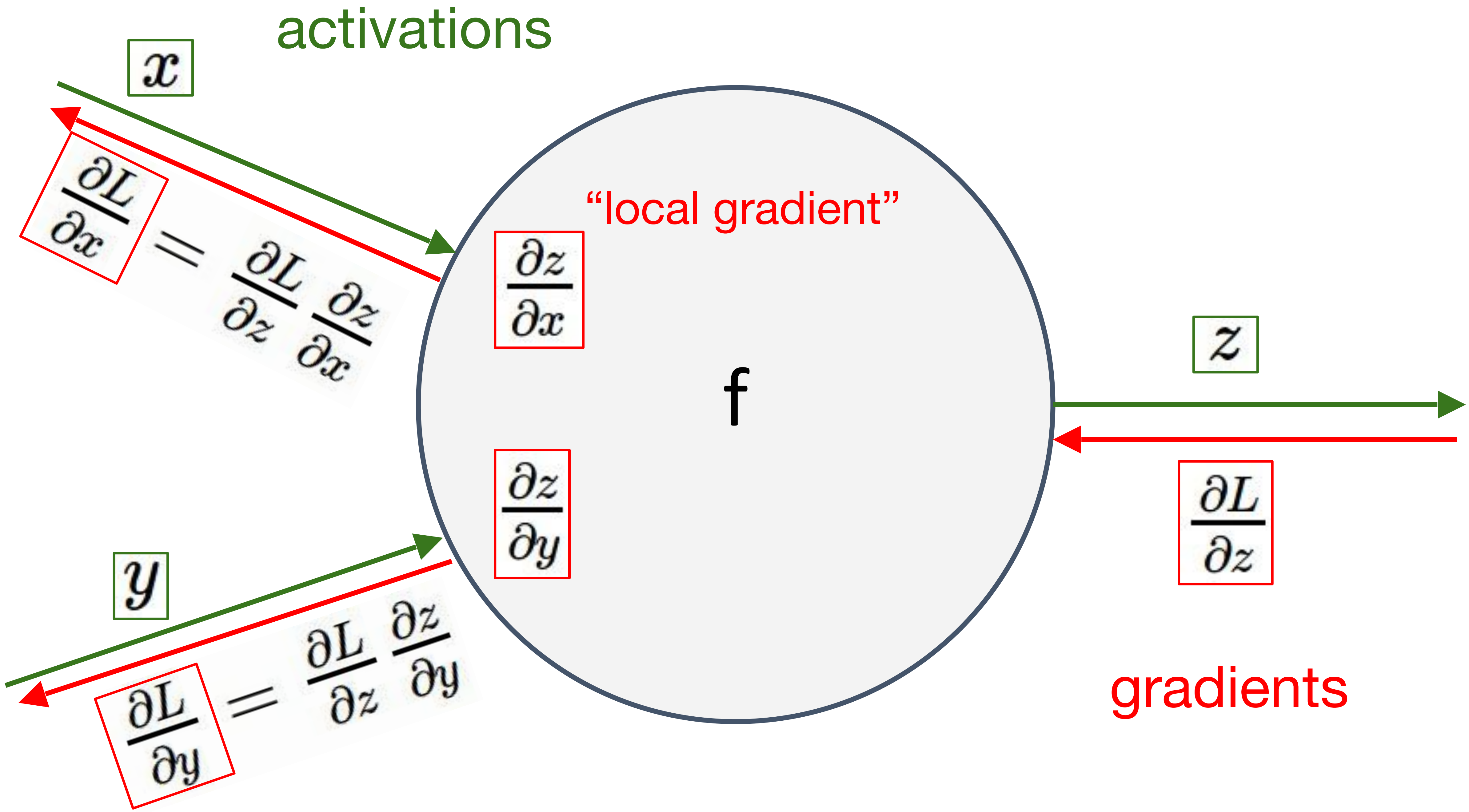

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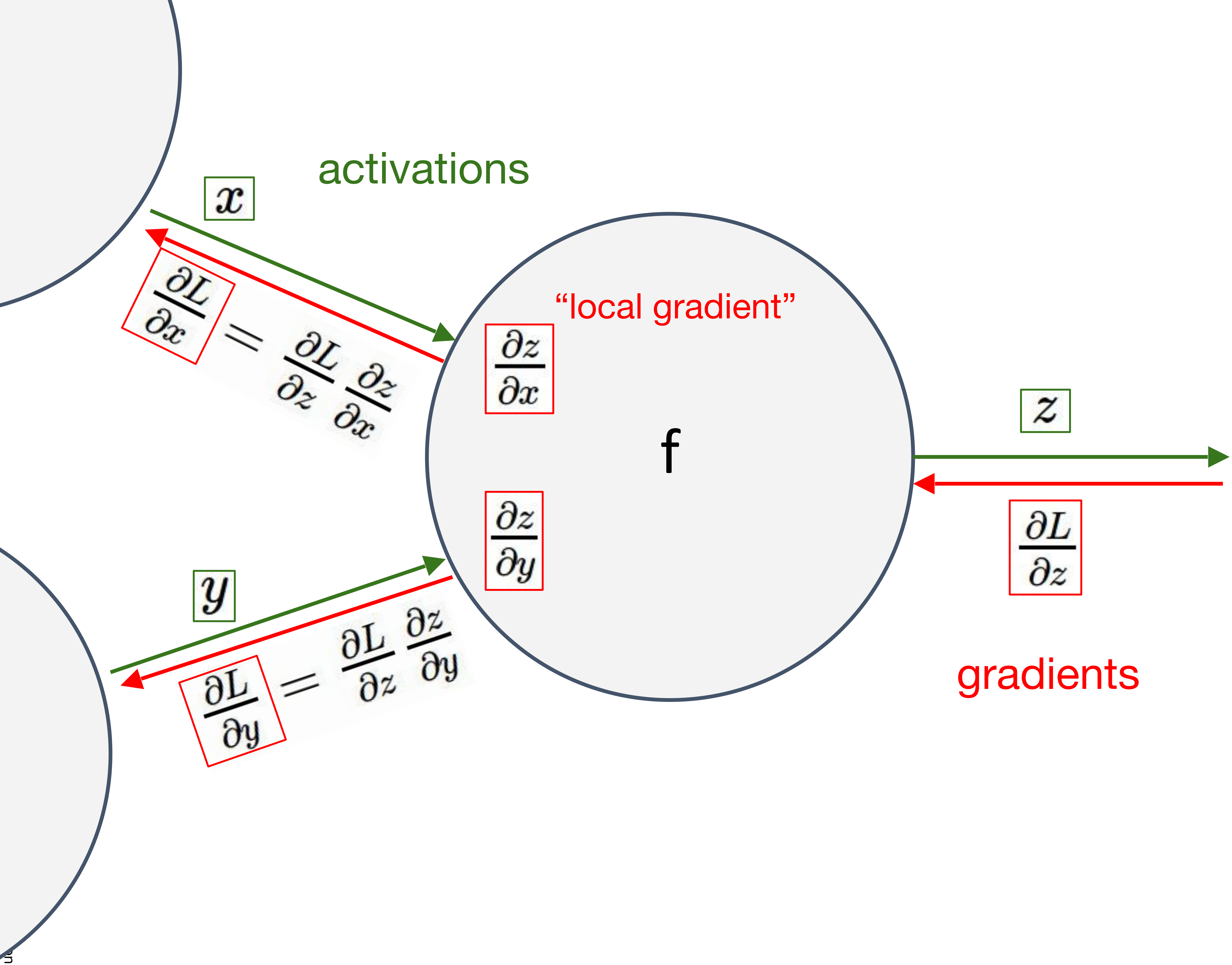
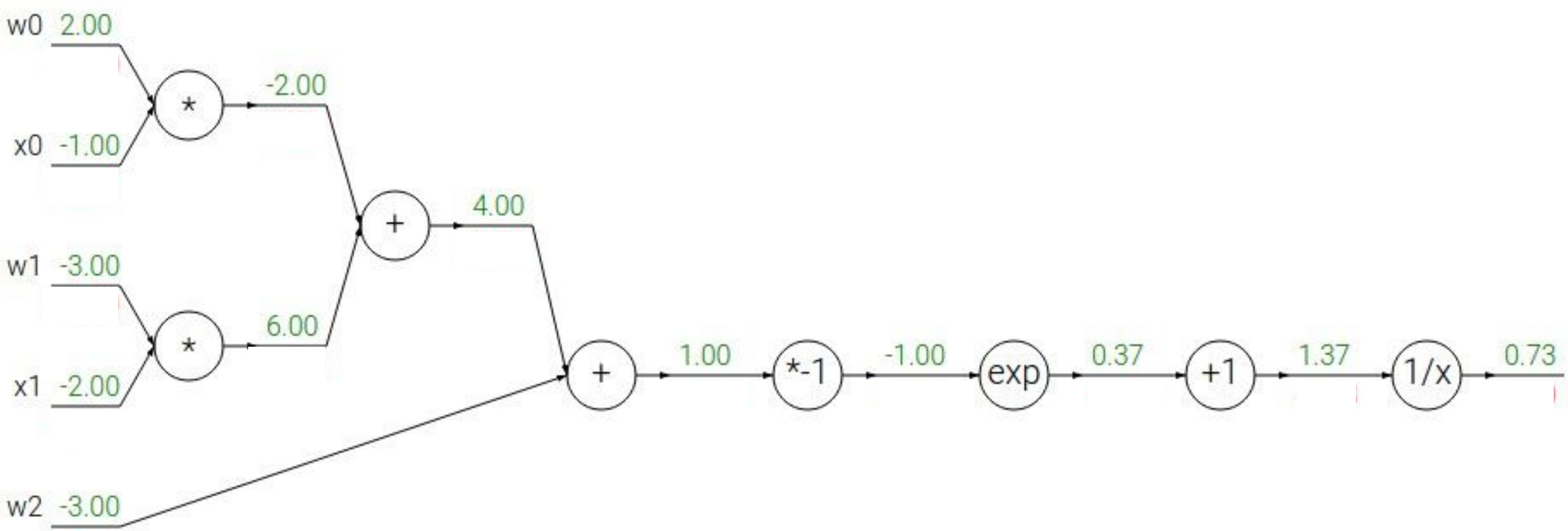

activations
x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
$\frac{\partial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

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



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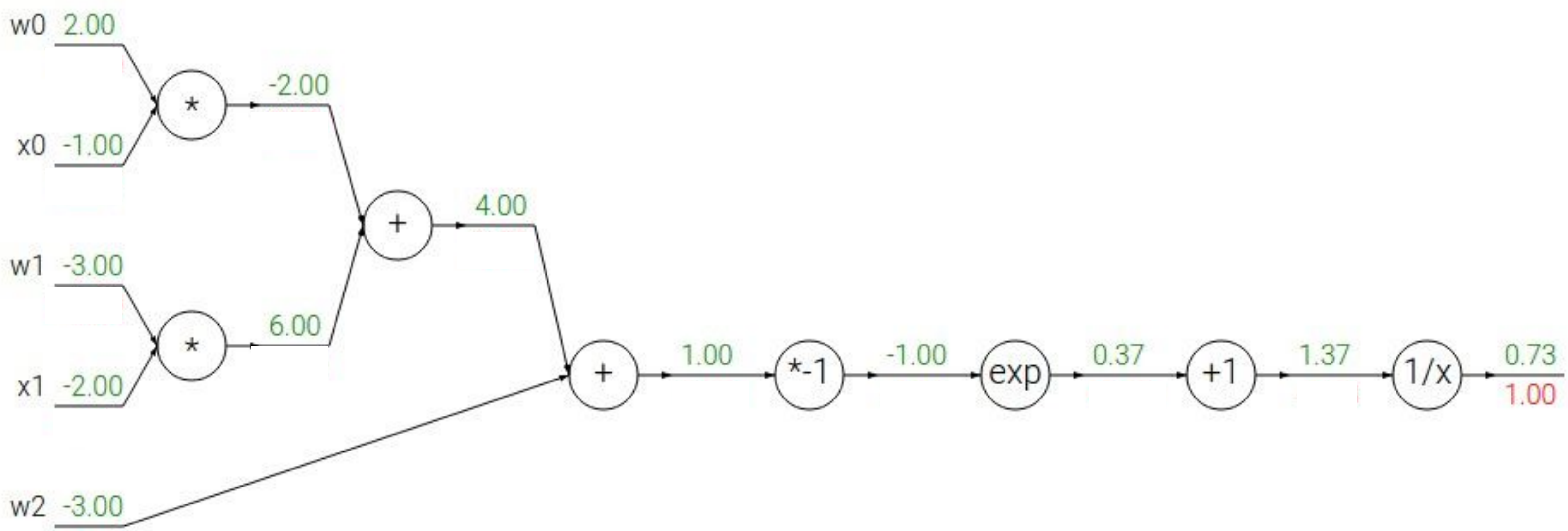

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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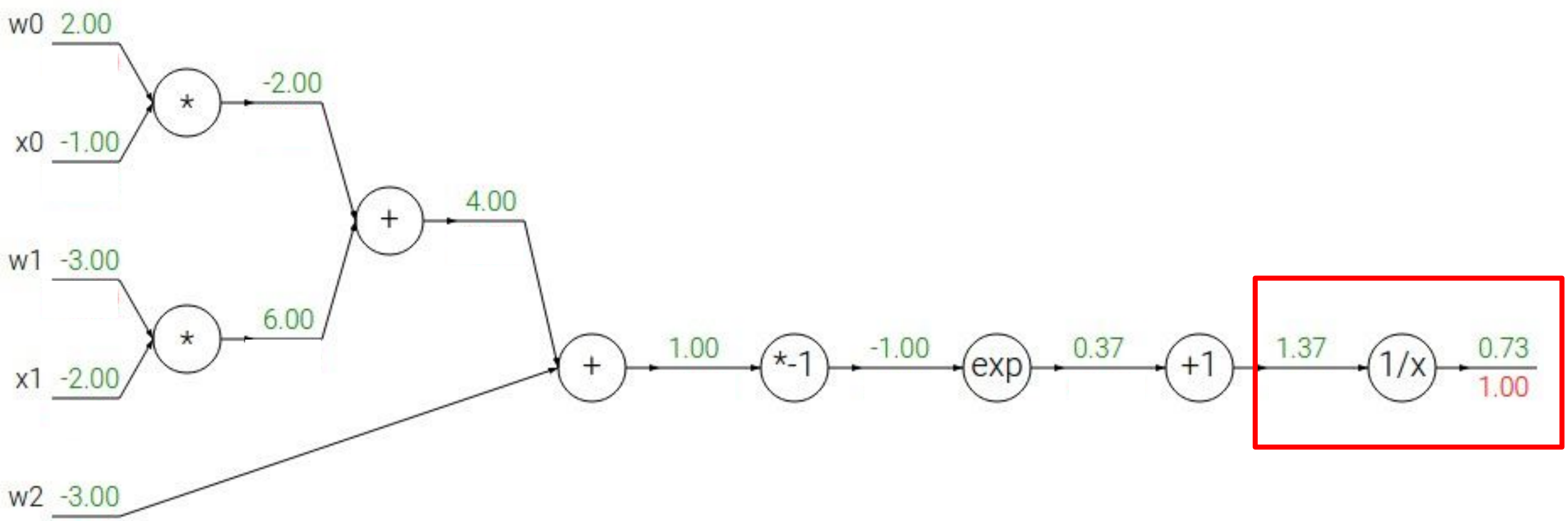

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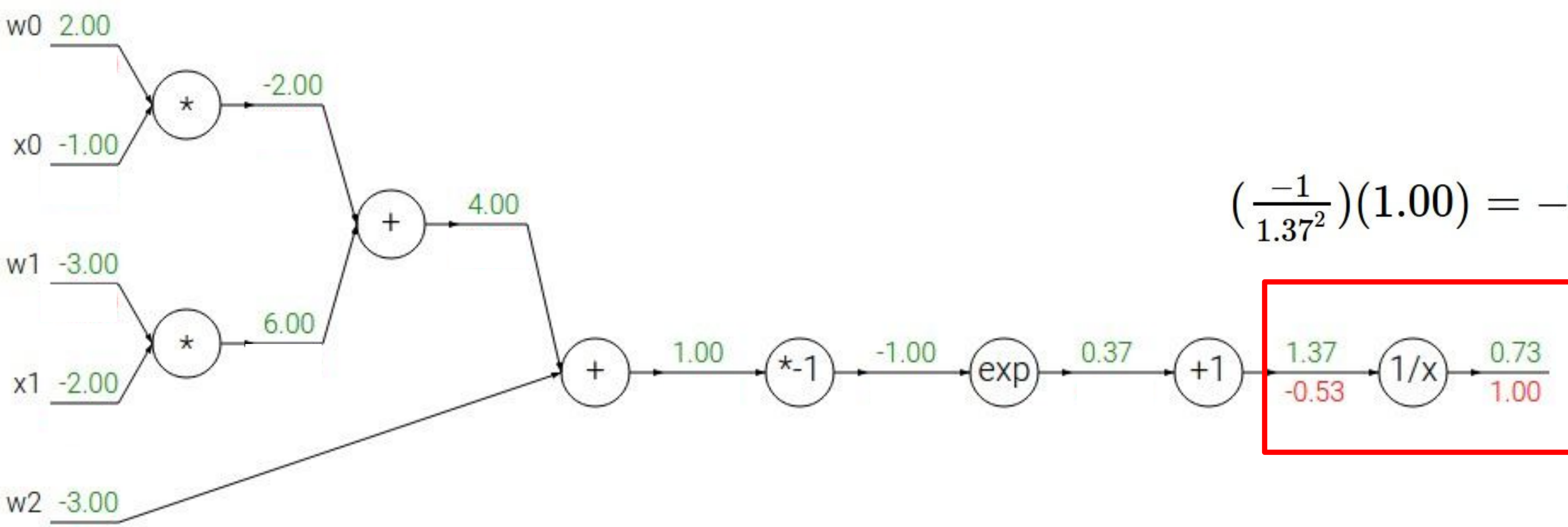

$$\left(\frac{-1}{1.37^2}\right)(1.00) = -0.53$$

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

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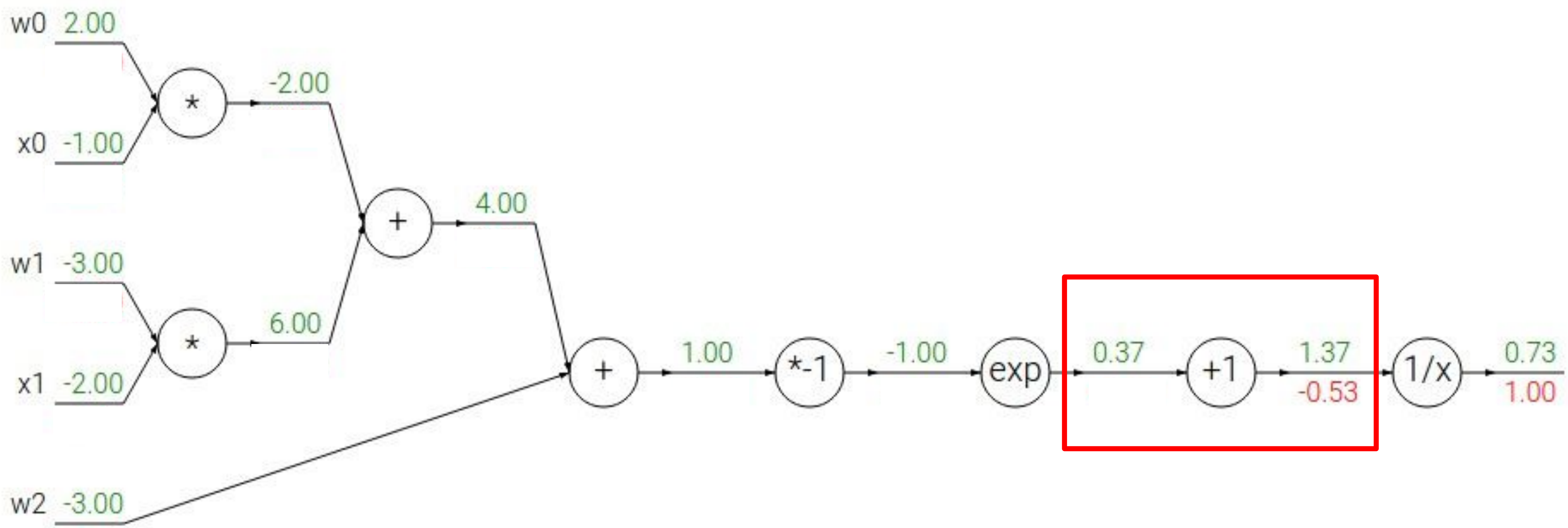

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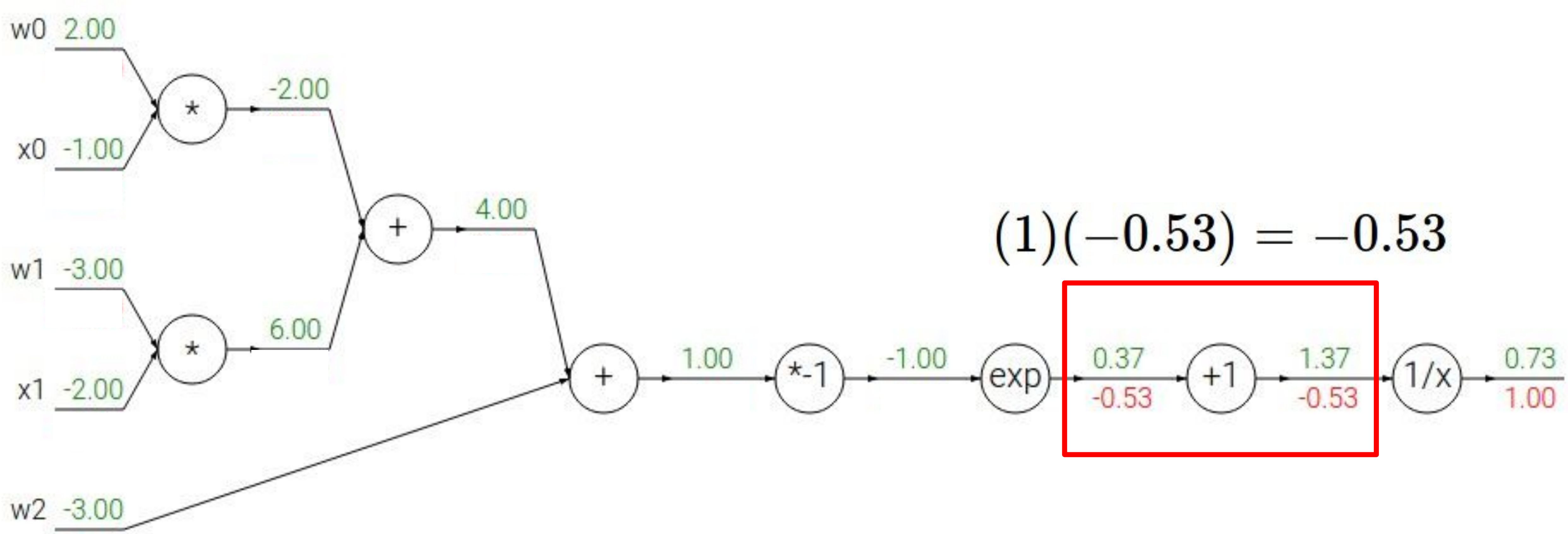

$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$

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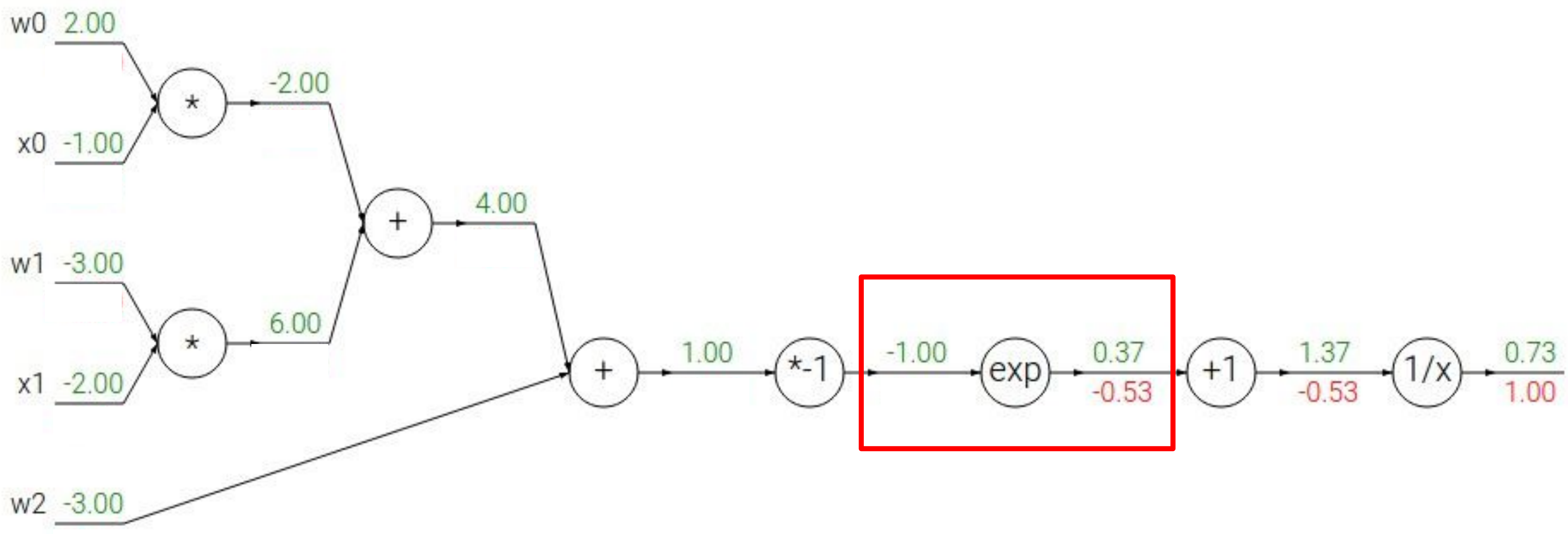

$f(x) = e^x$	$\rightarrow$	$\frac{df}{dx} = e^x$	$f(x) = \frac{1}{x}$	$\rightarrow$	$\frac{df}{dx} = -1/x^2$
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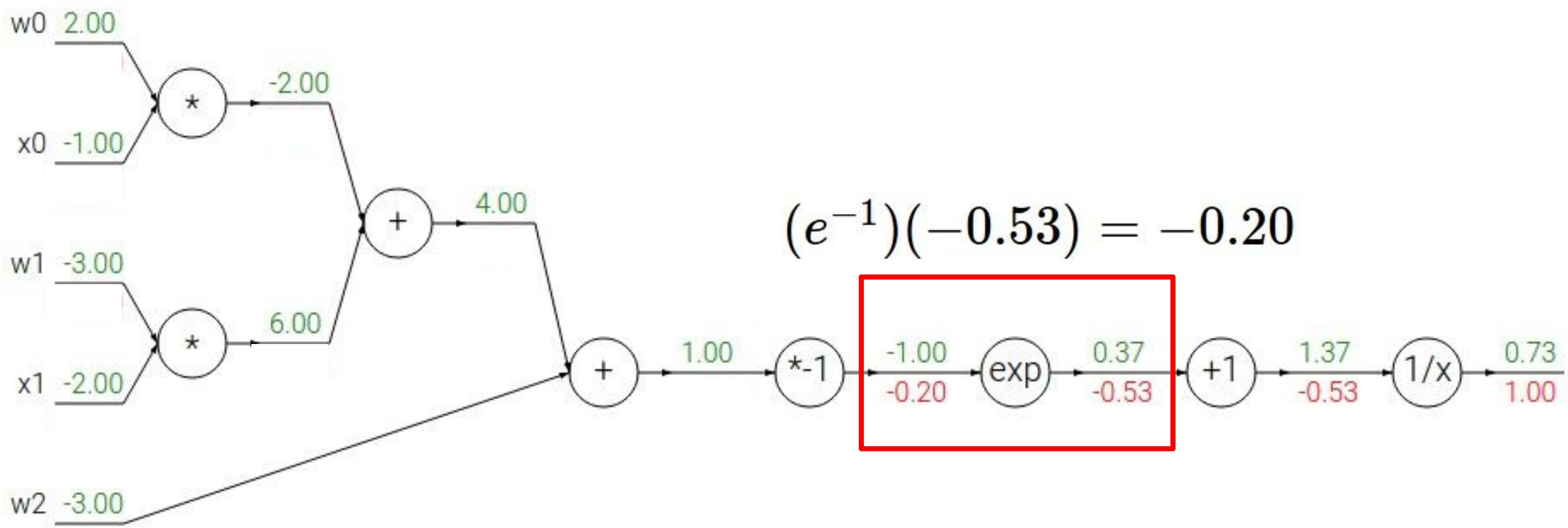
Another example: $f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$

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



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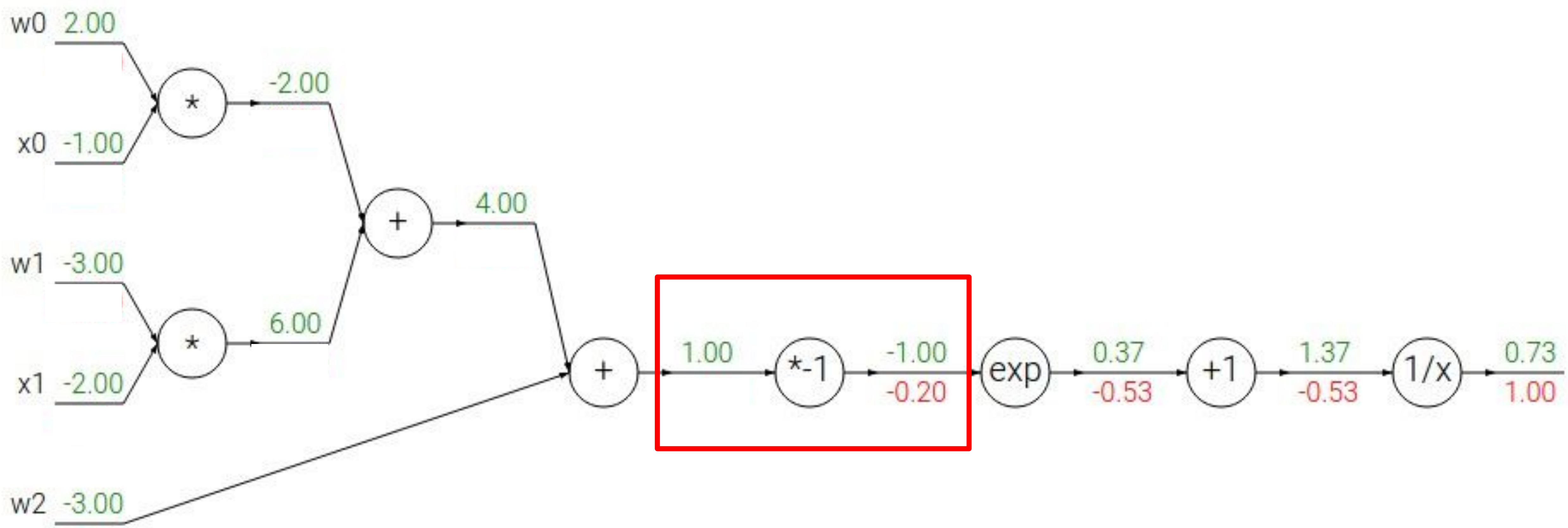

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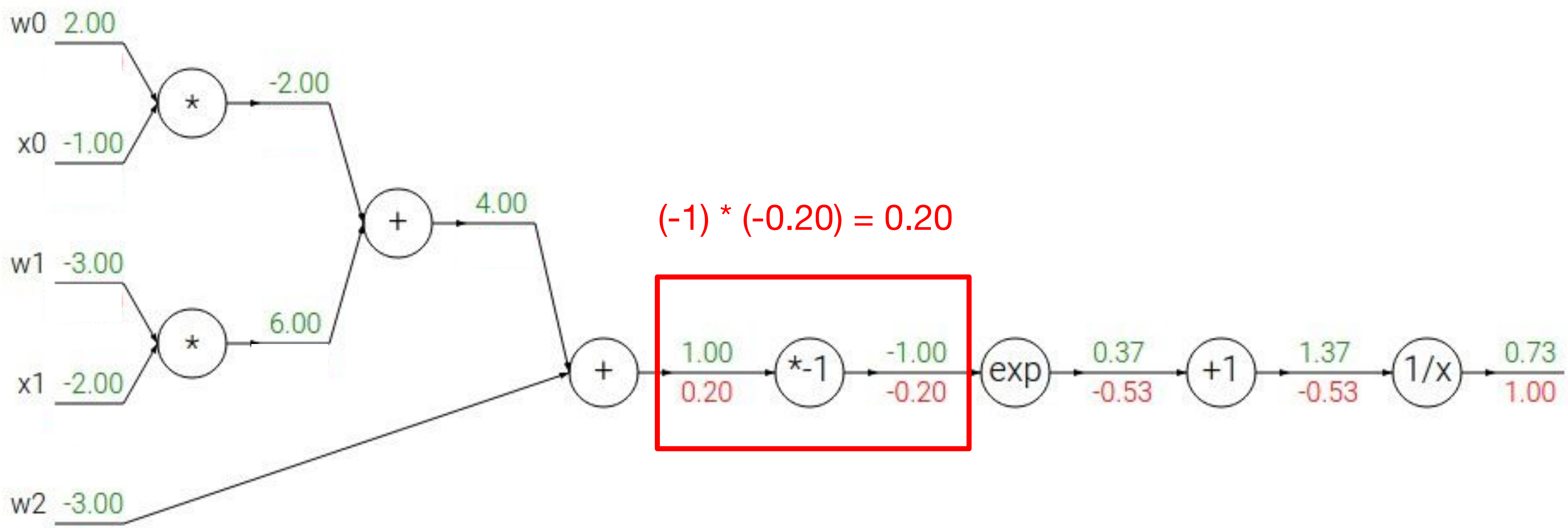

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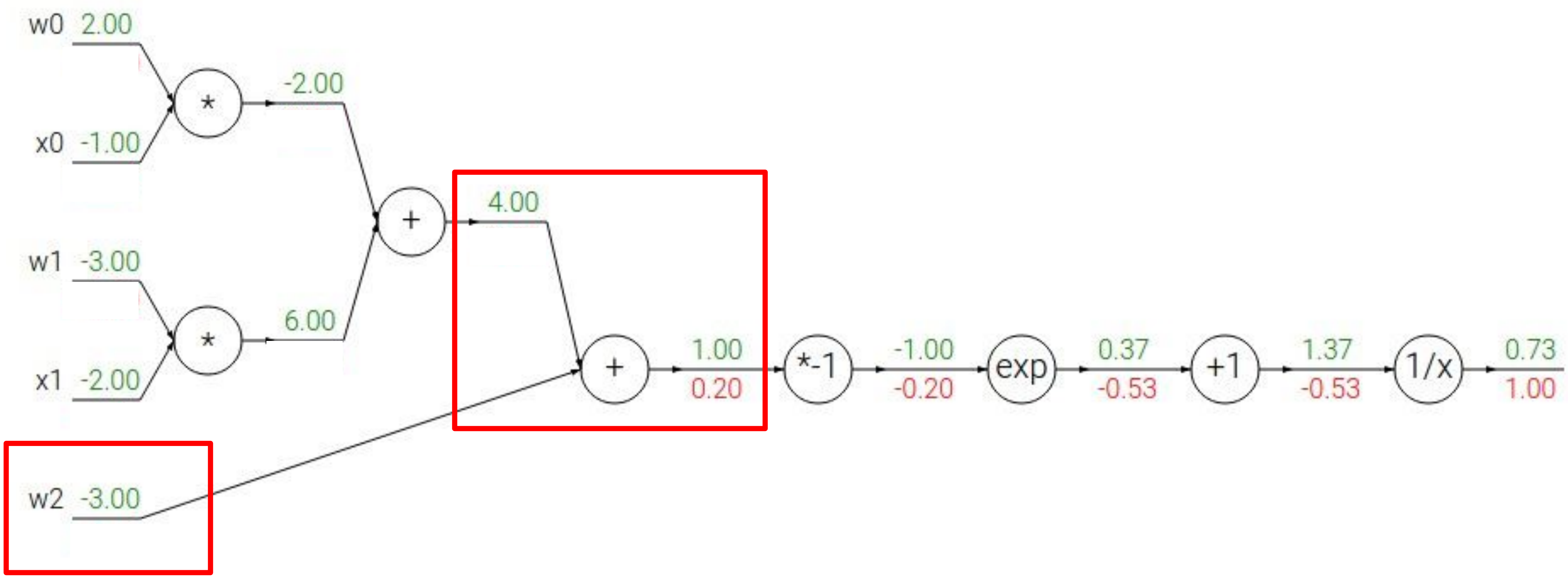

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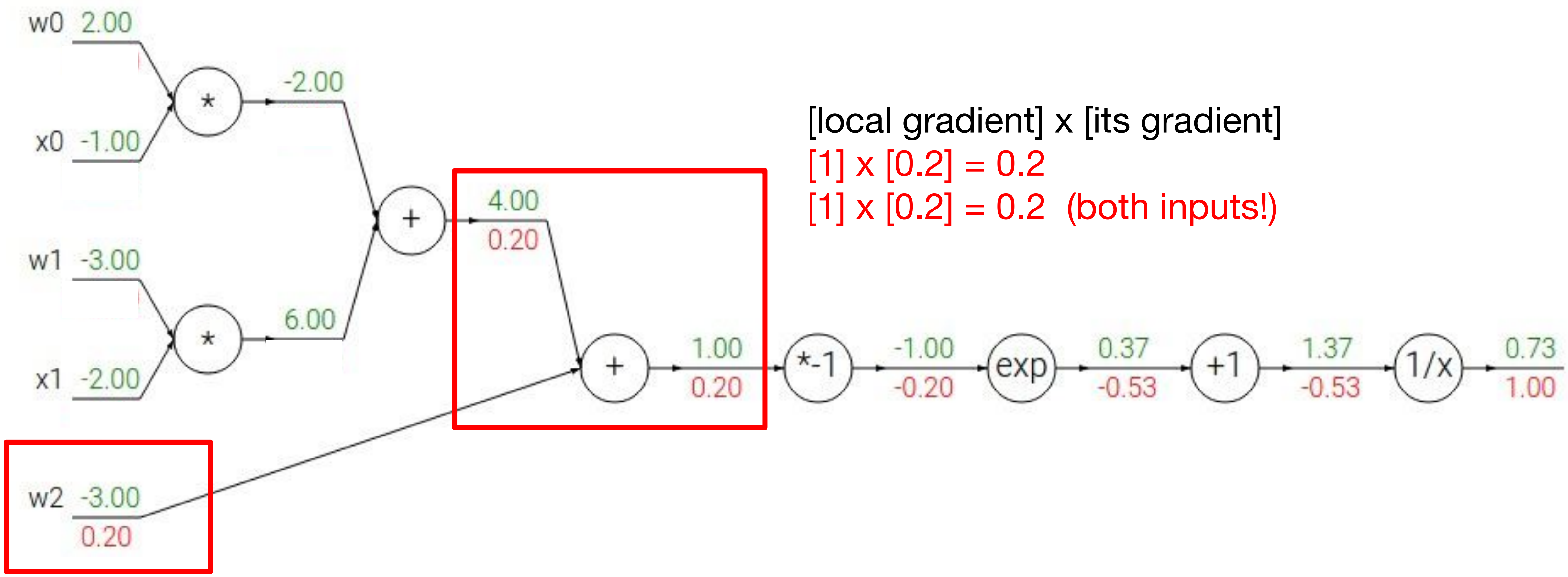

[local gradient] x [its gradient]
[1] x [0.2] = 0.2
[1] x [0.2] = 0.2 (both inputs!)

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

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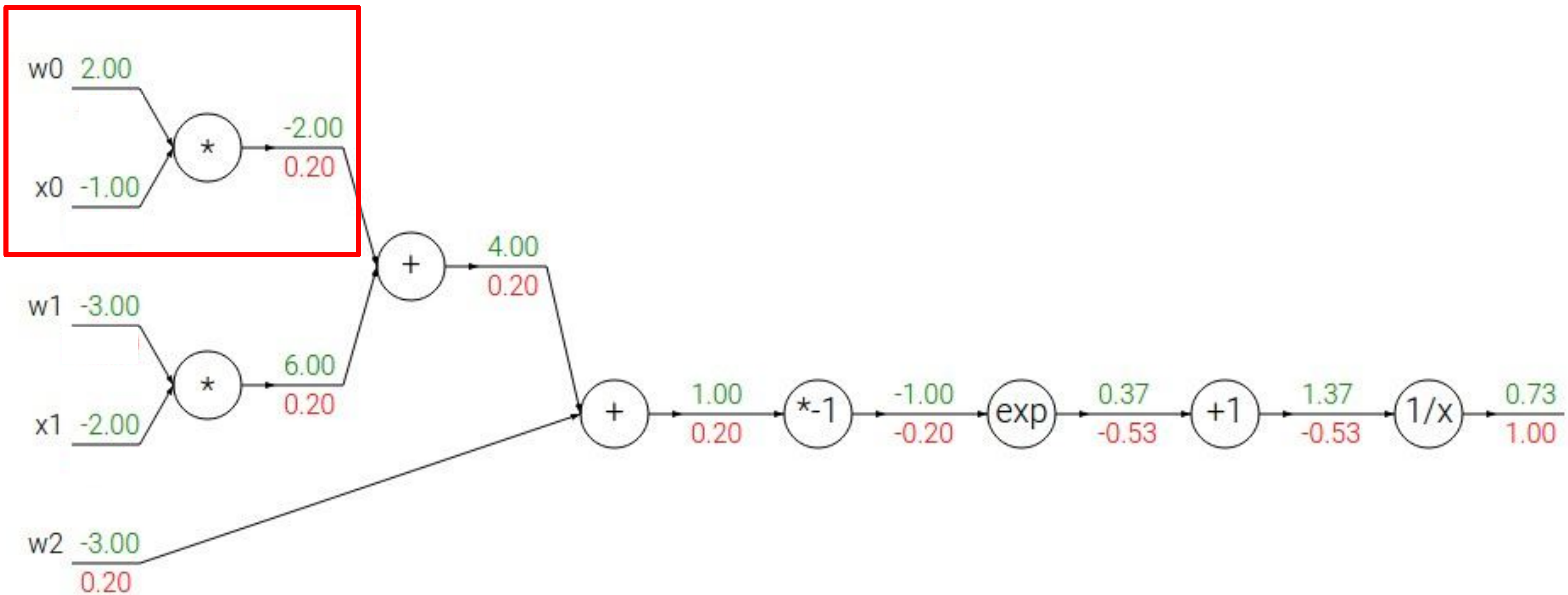

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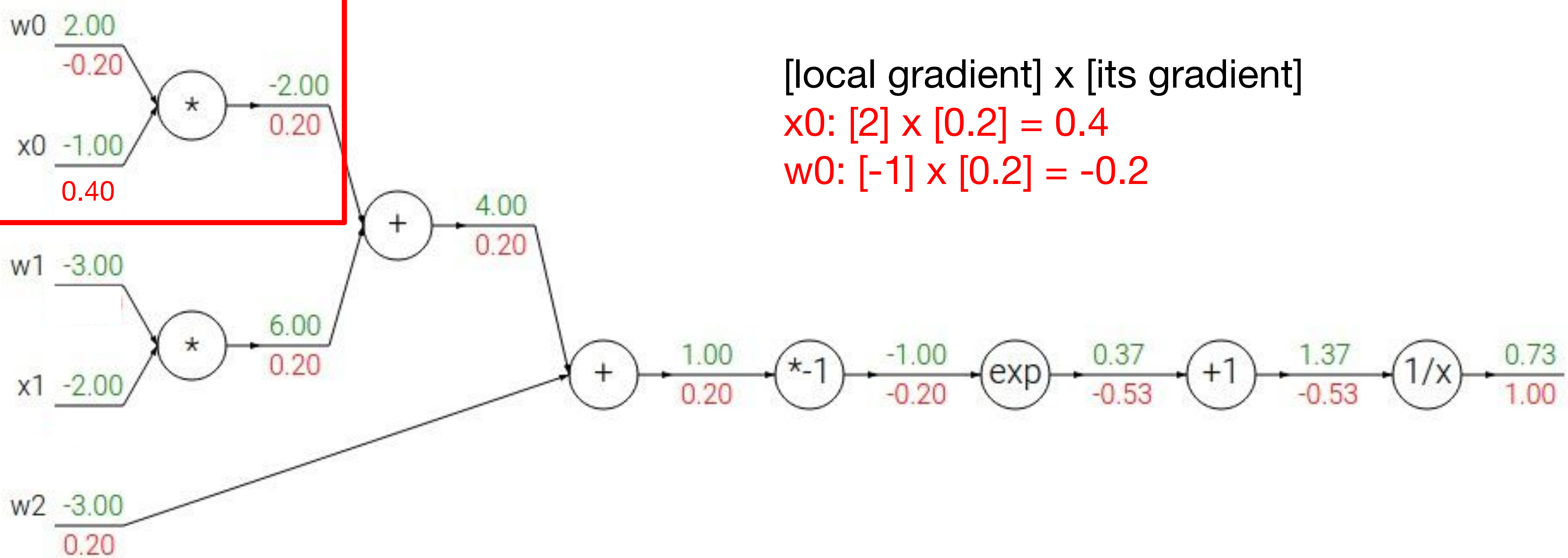

[local gradient] x [its gradient]

x0: [2] x [0.2] = 0.4

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

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

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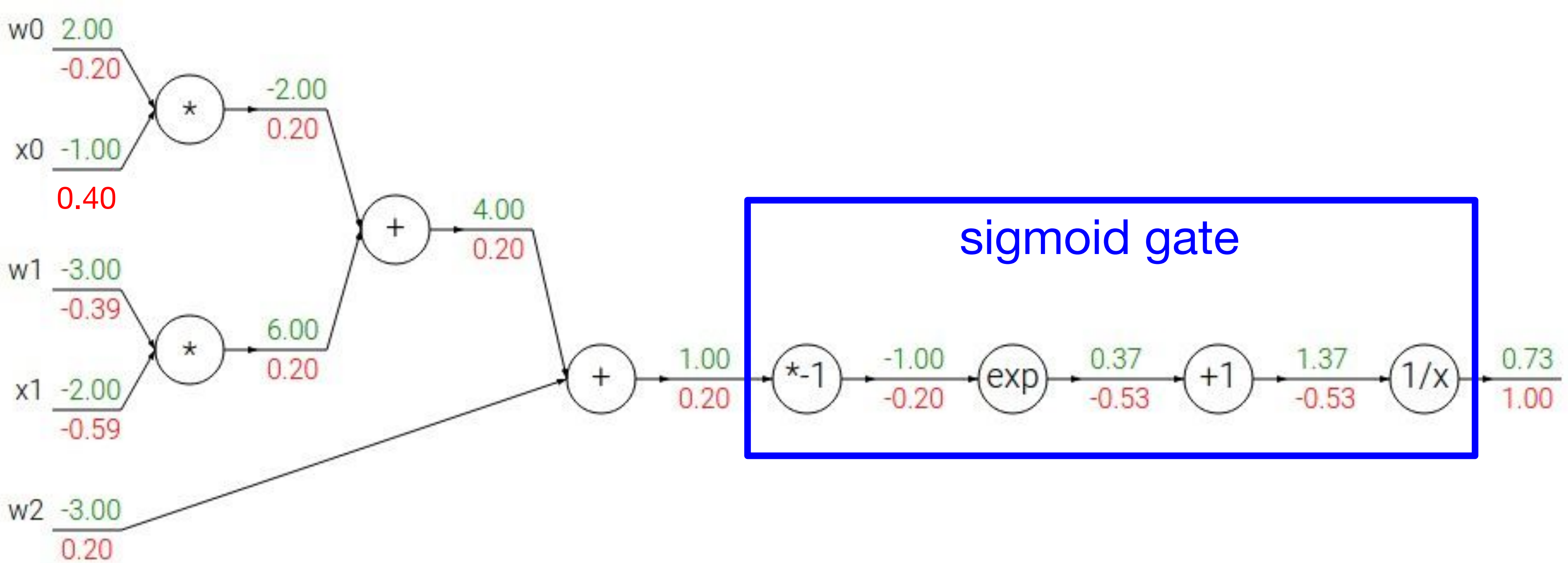
$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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

sigmoid function

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



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

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

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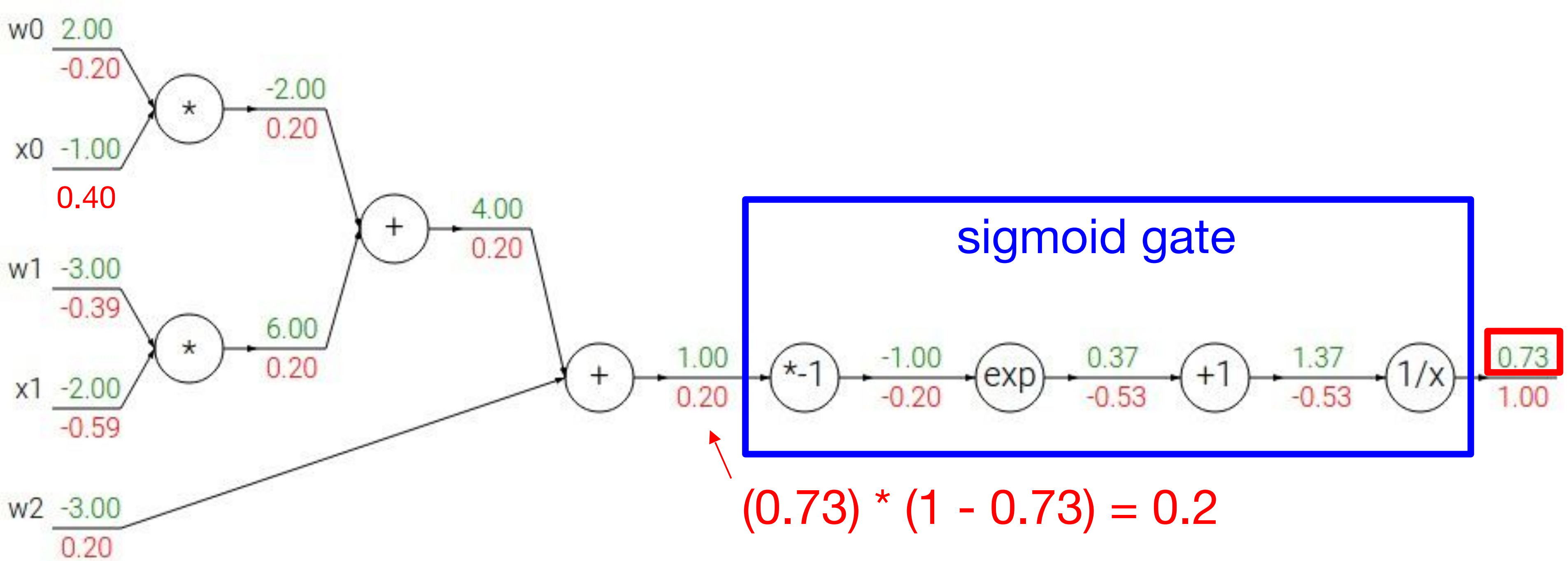

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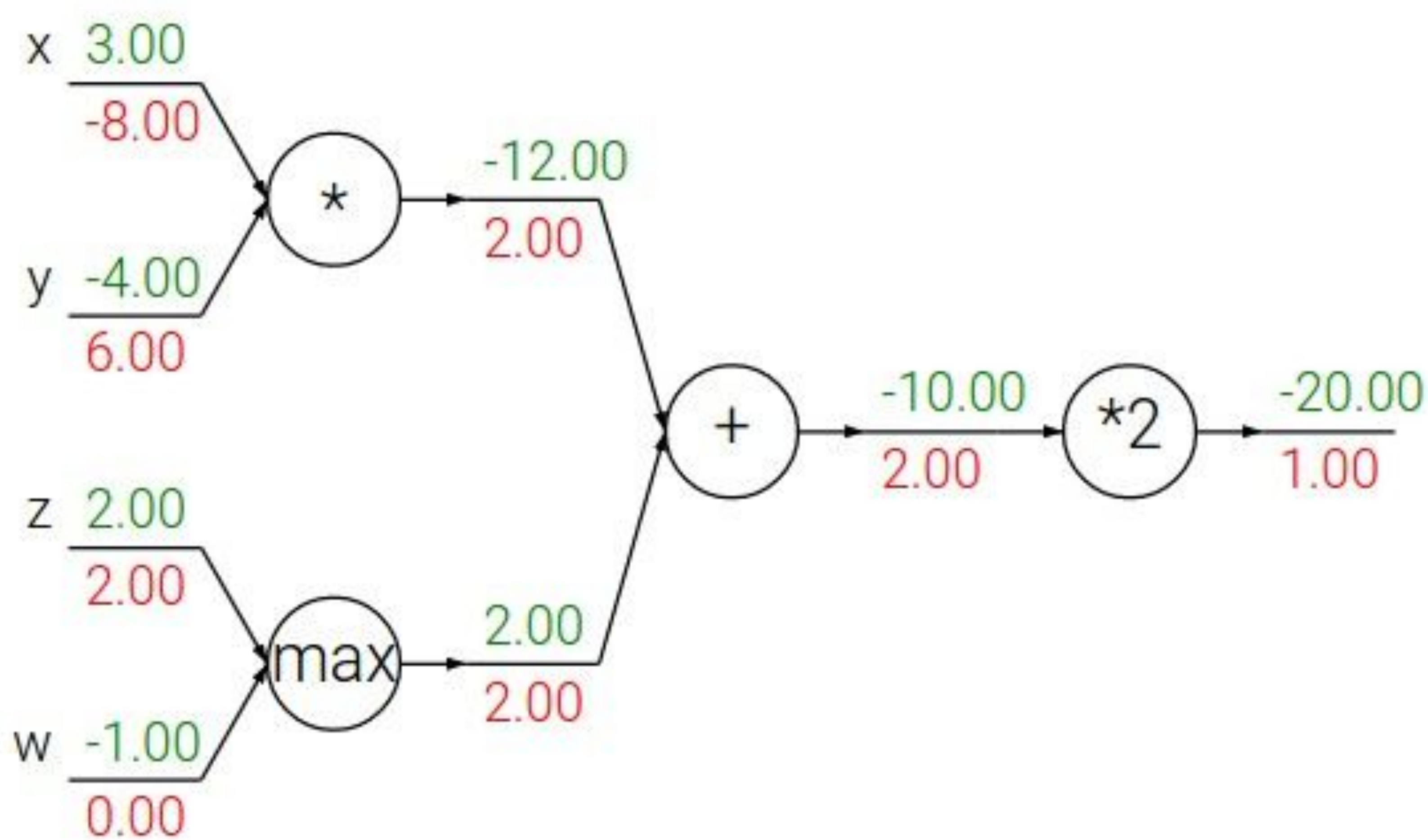
Patterns in backward flow

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



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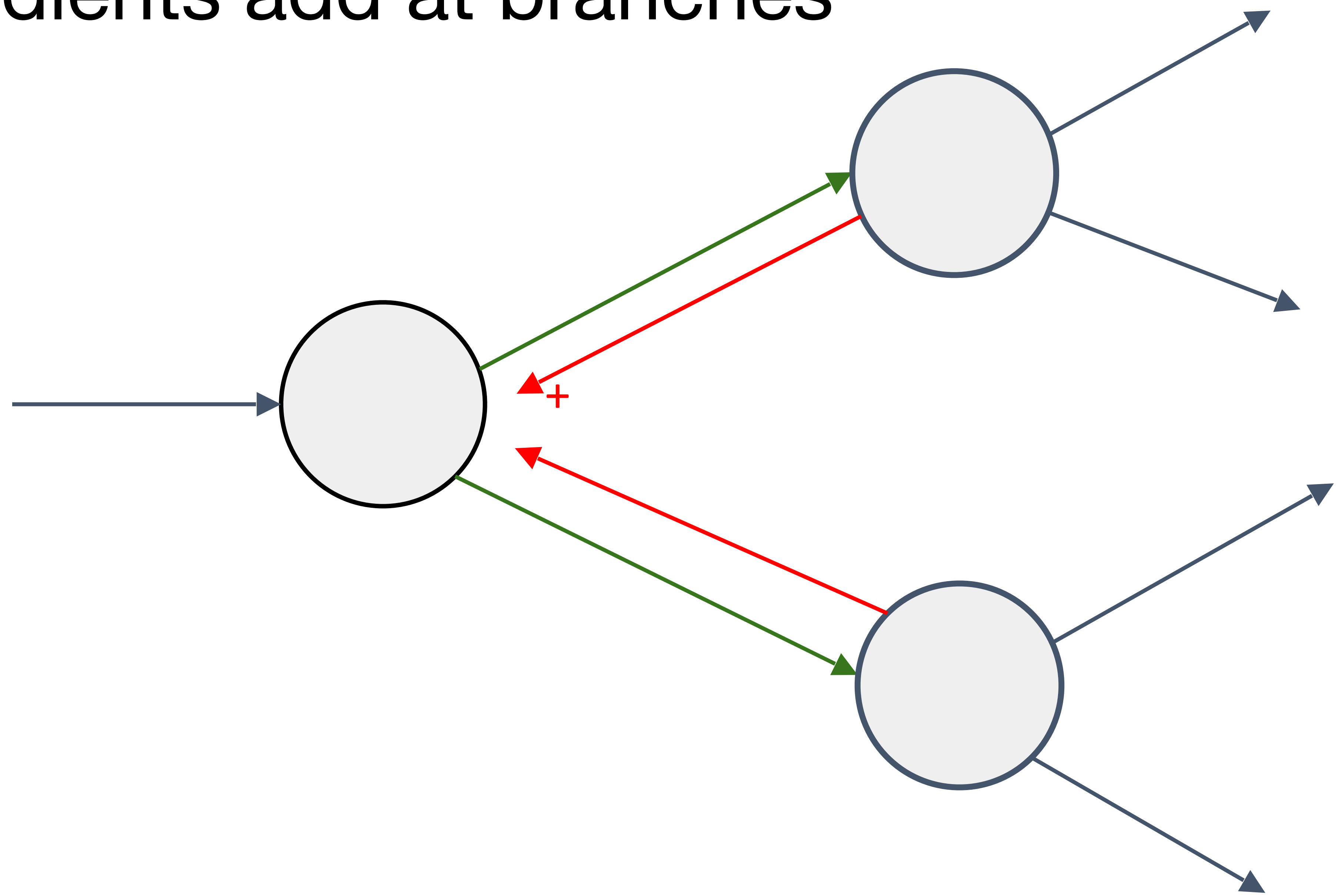
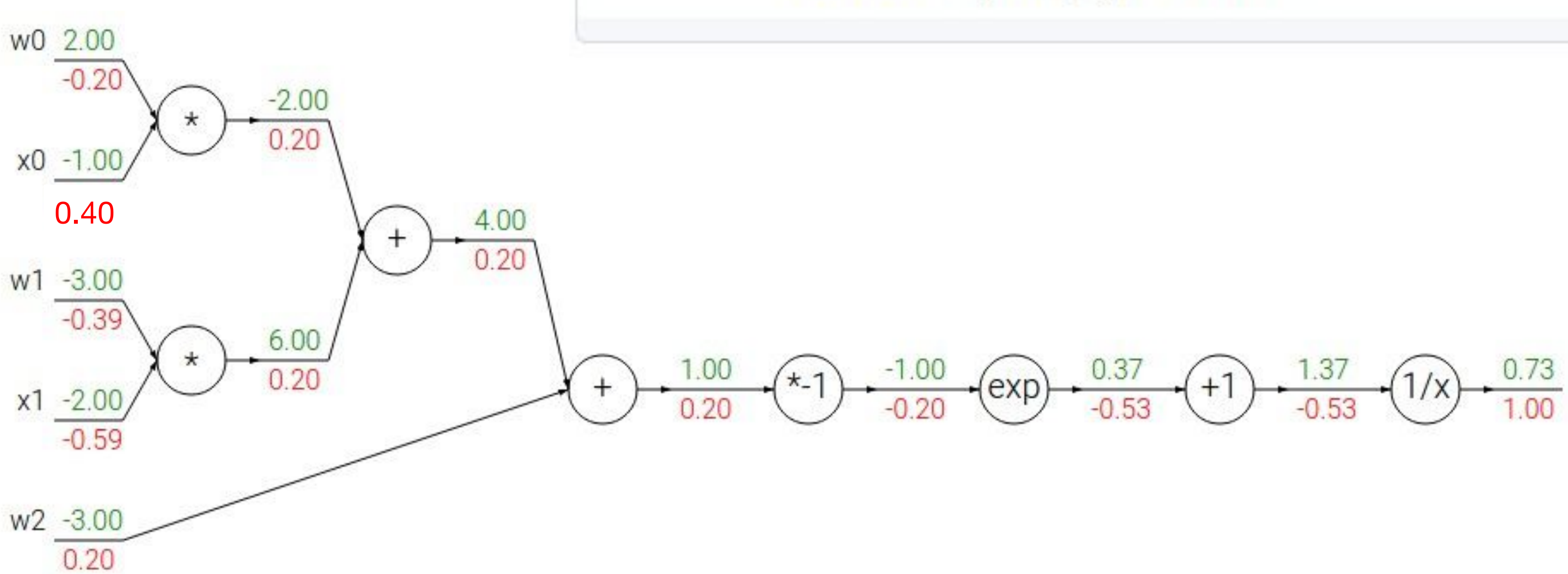
Gradients add at branches



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
```



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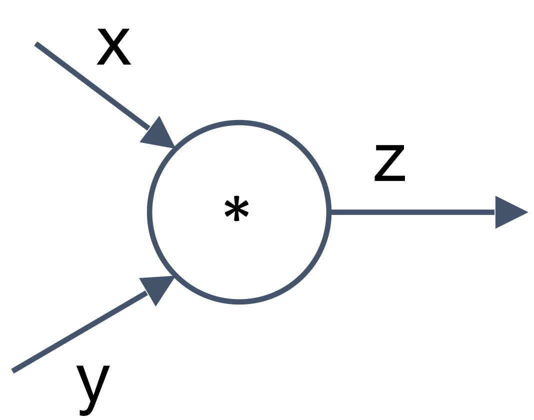
Implementation: forward/backward API



(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]
```

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

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

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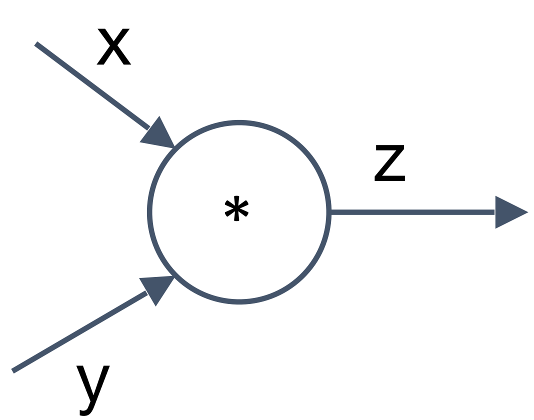
Implementation: forward/backward API



(x,y,z are scalars)

```python
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]
```

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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