# Lecture3

# Neural Networks and Backpropagation

# Neural Networks

# Recall SVM

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

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

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

want $\boxed{\nabla_W L}$

# Now neural networks

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

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

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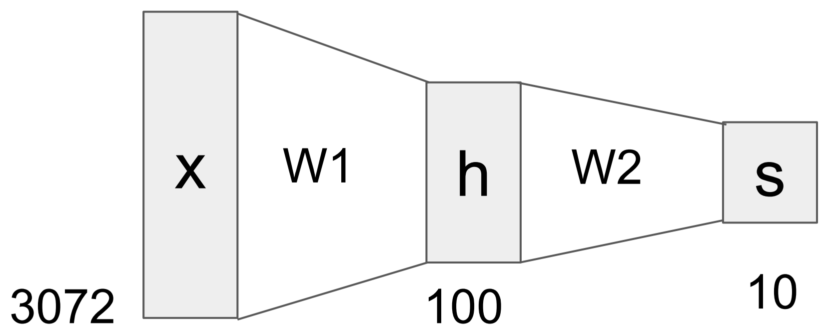


# Now neural networks

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

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

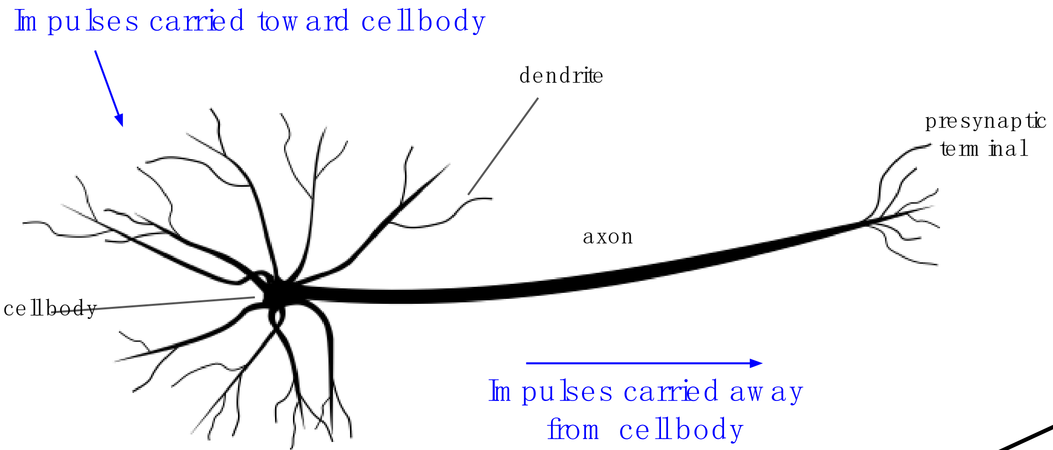
$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

# Now neural networks

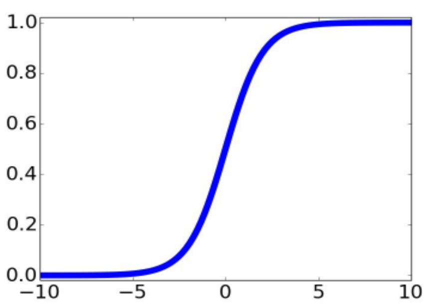
Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
import numpy as np
from numpy.random import randn

N, D_in, H, D_out = 64, 1000, 100, 10
x, y = randn(N, D_in), randn(N, D_out)
w1, w2 = randn(D_in, H), randn(H, D_out)

for t in range(2000):
  h = 1 / (1 + np.exp(-x.dot(w1)))
  y_pred = h.dot(w2)
  loss = np.square(y_pred - y).sum()
  print(t, loss)

  grad_y_pred = 2.0 * (y_pred - y)
  grad_w2 = h.T.dot(grad_y_pred)
  grad_h = grad_y_pred.dot(w2.T)
  grad_w1 = x.T.dot(grad_h * h * (1 - h))

  w1 -= 1e-4 * grad_w1
  w2 -= 1e-4 * grad_w2
```

# Now neural networks

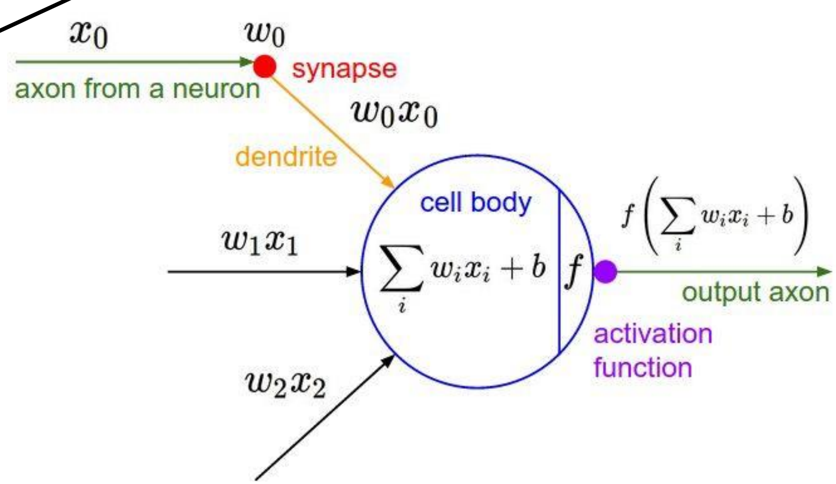




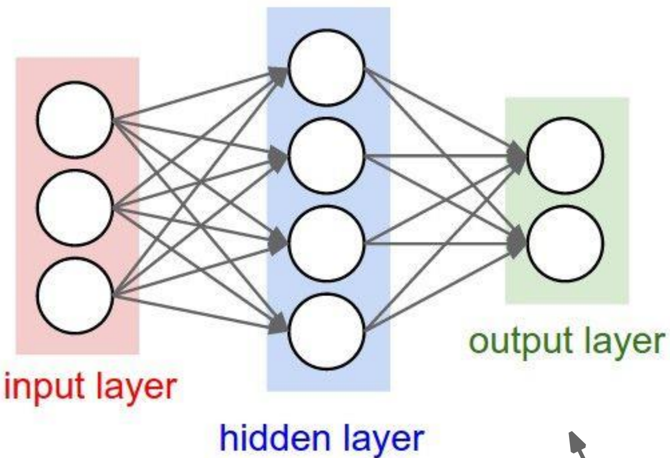



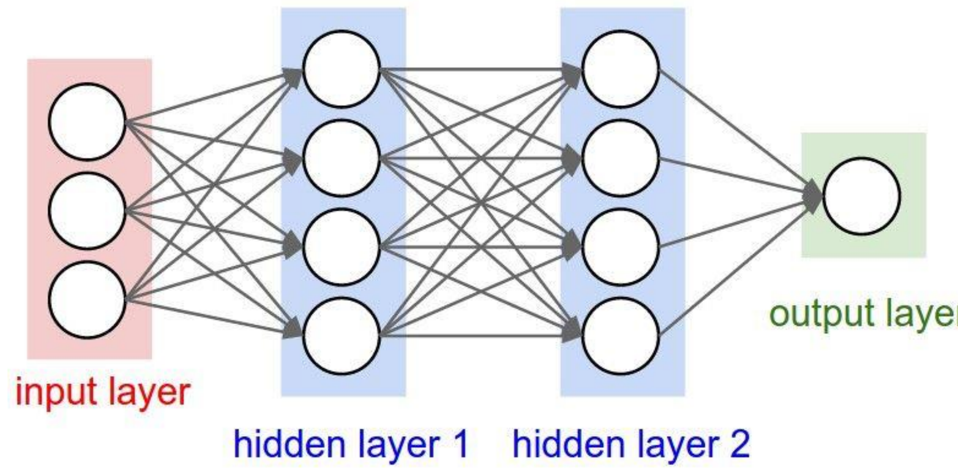

sigmoid activation function

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



# Neural network architectures




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

**"Fully-connected" layers**

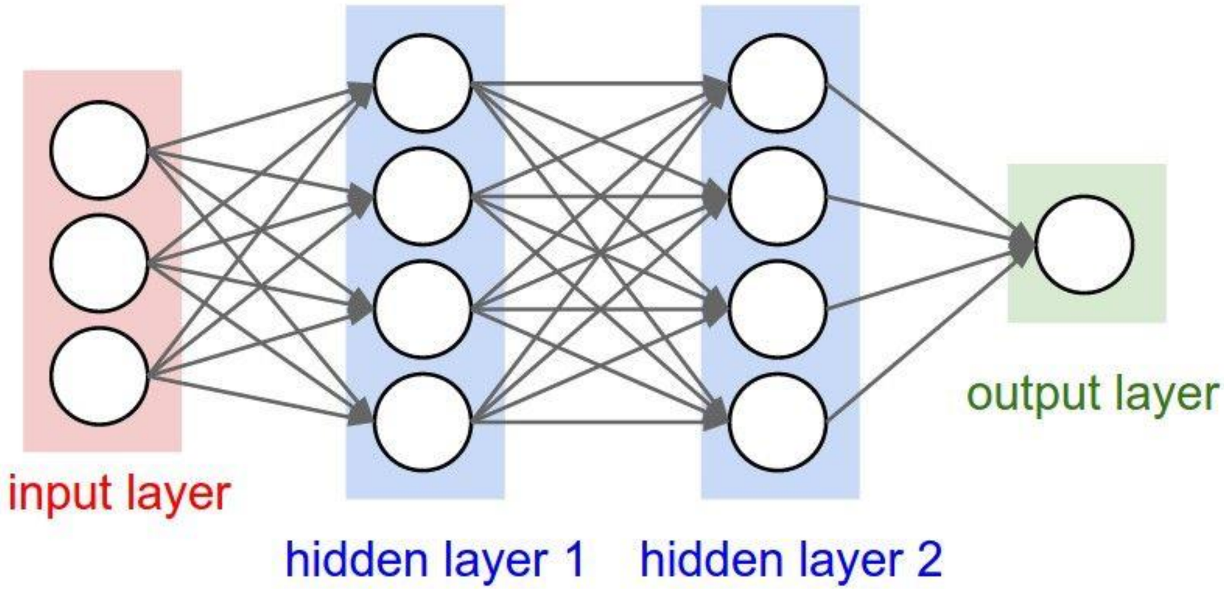
"3-layer Neural Net", or
"2-hidden-layer Neural Net"

# Feed-forward computation

```
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
```

We can efficiently evaluate an entire layer of neurons.

# Feed-forward computation




```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)
```

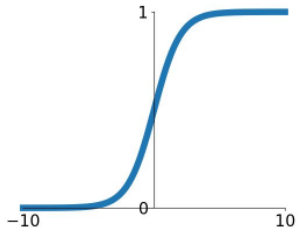
# Activation functions

The gates that decide whether or not messages will be passed through a neuron. Without activations, neural networks are just linear transformations

# Activation functions

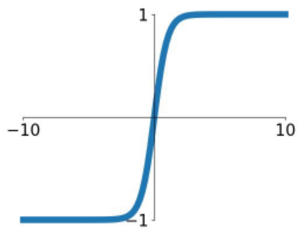
Sigmoid

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



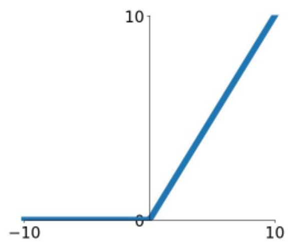

tanh

$\tanh(x)$



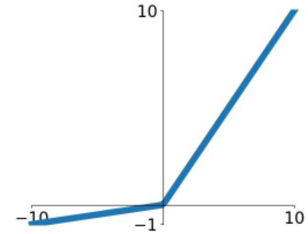

ReLU

$\max(0, x)$




Leaky ReLU

$\max(0.1x, x)$

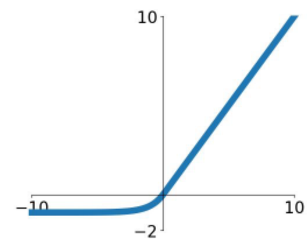



Maxout

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

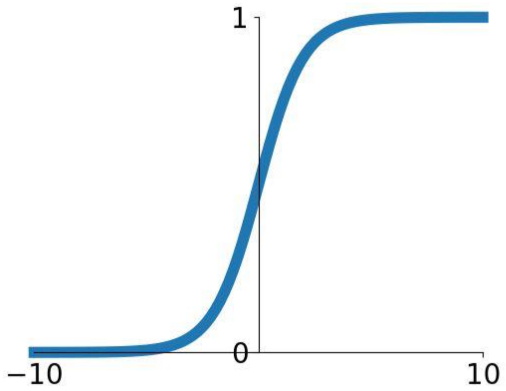
ELU

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



# Sigmoid

## Activation Functions



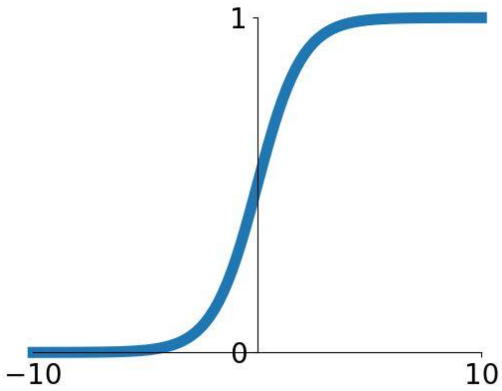

**Sigmoid**

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

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

# Sigmoid

## Activation Functions

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3 problems:

1. Saturated neurons “kill” the gradients

# Sigmoid

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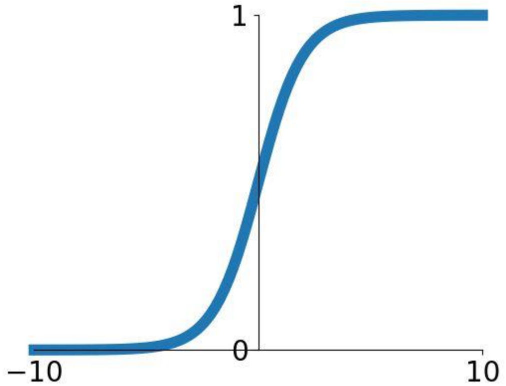


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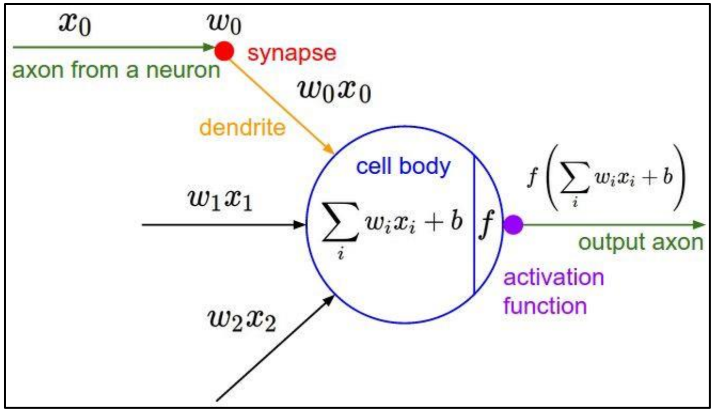
3 problems:

1. Saturated neurons “kill” the gradients
2. Sigmoid outputs are not zero-centered

# Sigmoid

Consider what happens when the input to a neuron (x) is always positive:



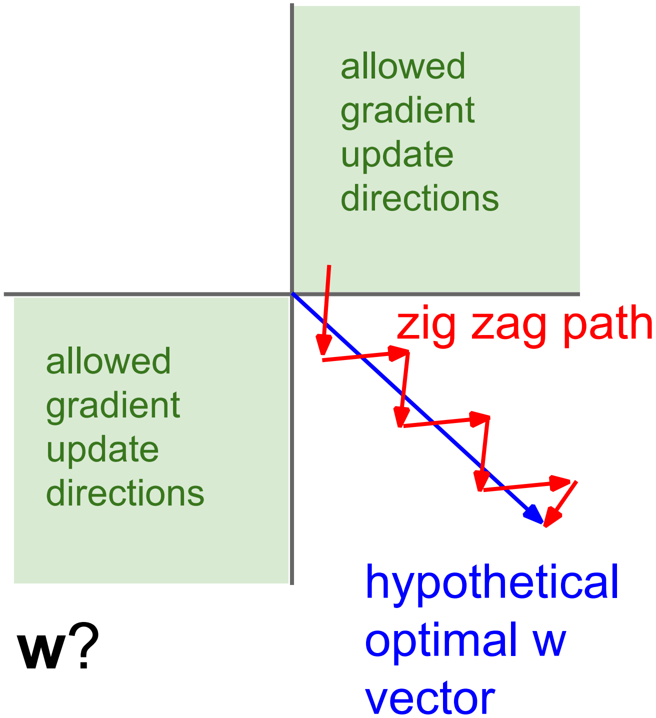

$$f\left(\sum_i w_i x_i + b\right)$$

What can we say about the gradients on **w**?

# Sigmoid

Consider what happens when the input to a neuron is always positive...

$$f\left(\sum_i w_i x_i + b\right)$$




What can we say about the gradients on **w**?

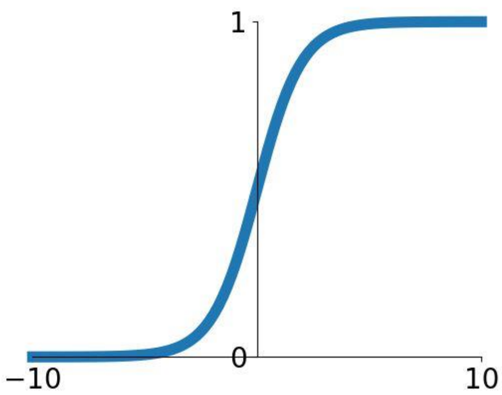
Always all positive or all negative :(

(this is also why you want zero-mean data!)

dL/dw = dL/dp * dp/dw = dL/dp * x',
where p = w'x + b
Note x is the output of the previous activation function

# Sigmoid

## Activation Functions

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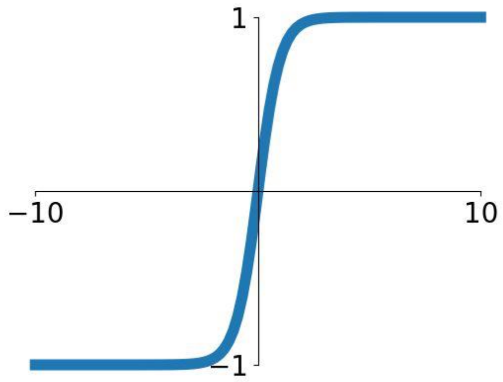
3 problems:

1. Saturated neurons “kill” the gradients
2. Sigmoid outputs are not zero-centered
3. exp() is a bit compute expensive

# Tanh

## Activation Functions




**tanh(x)**

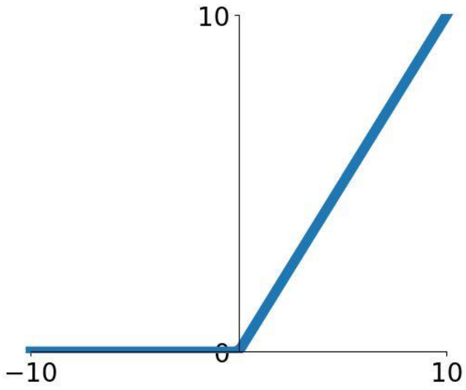
- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

Used to be very popular in sequence modeling (e.g., LSTM/GRU)

[LeCun et al., 1991]

# ReLU

## Activation Functions




**ReLU**
(Rectified Linear Unit)

- Computes **f(x) = max(0,x)**

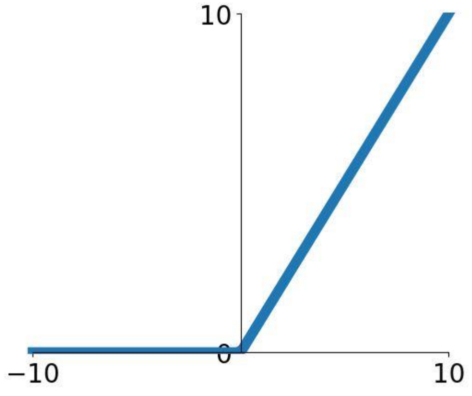
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)
- Actually more biologically plausible than sigmoid

[Nair & Hinton, 2010]

[Krizhevsky et al., 2012]

# ReLU

## Activation Functions

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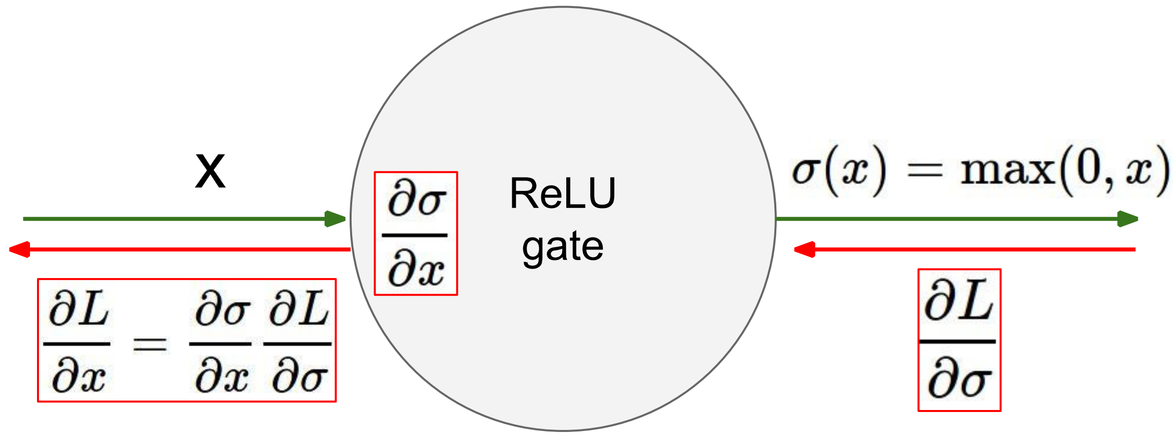
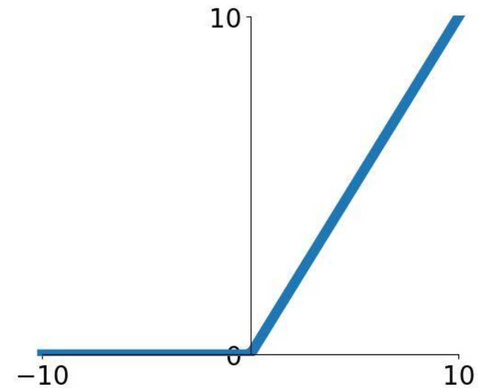
Two weakness:

1. Non-smooth point at x=0 (why ELU and GELU is proposed)
2. Saturate for x<0 (why LReLU and maxout is proposed)

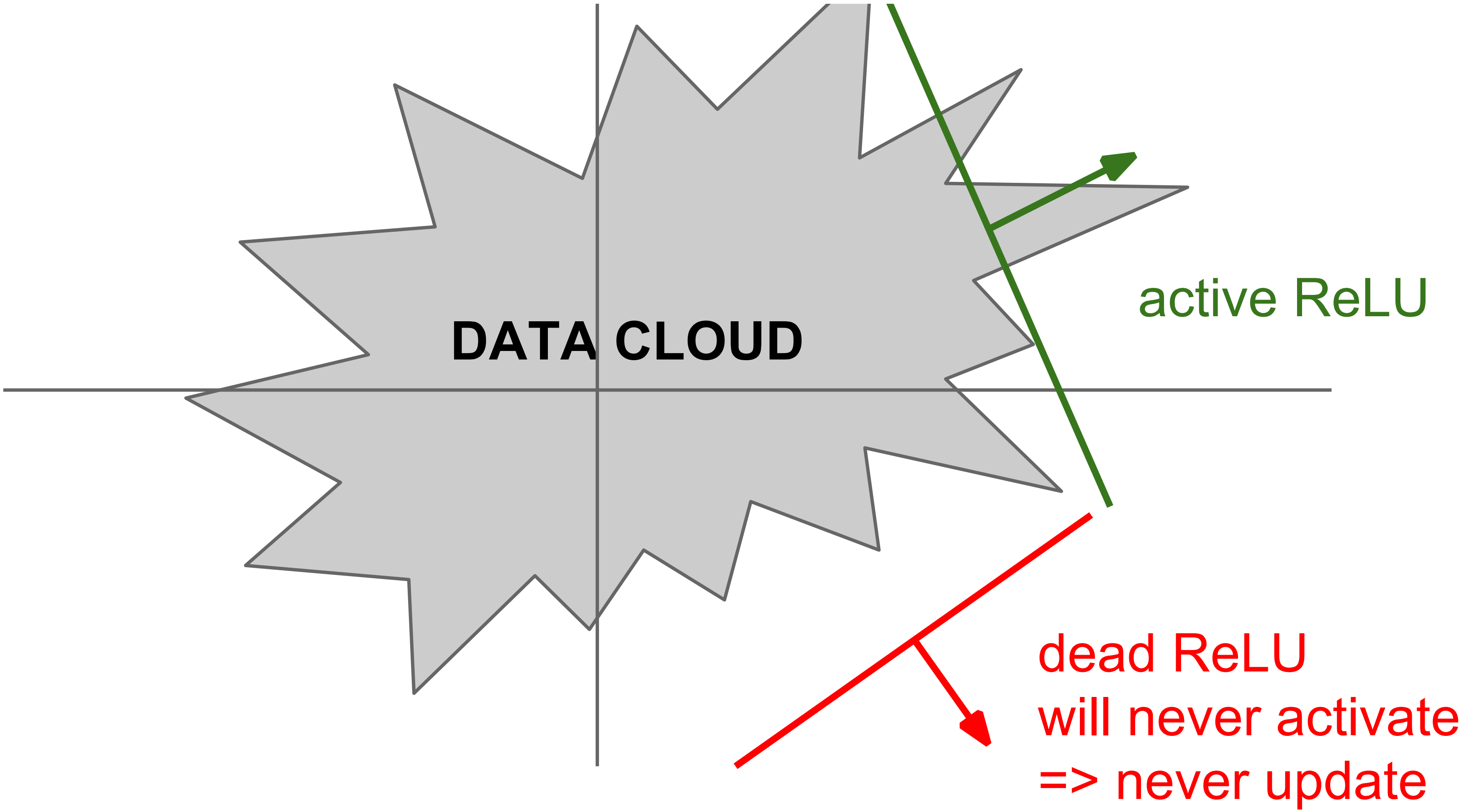
# ReLU



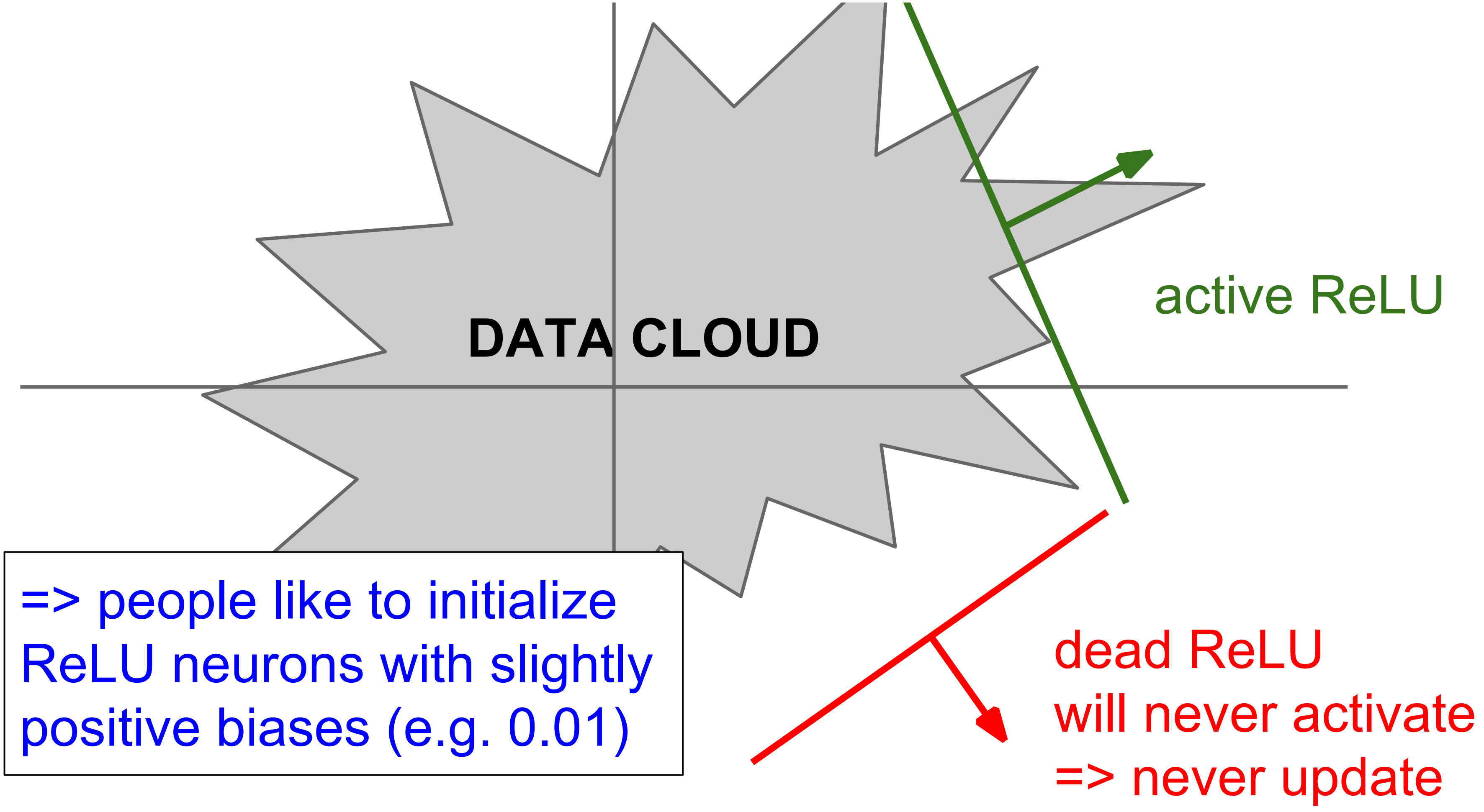

What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

# ReLU



DATA CLOUD
active ReLU
dead ReLU
will never activate
=> never update

# ReLU

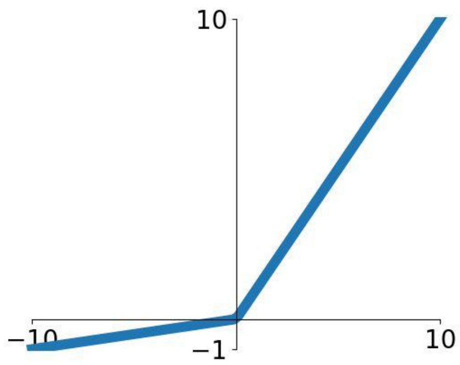



=> people like to initialize ReLU neurons with slightly positive biases (e.g. 0.01)

# Leaky ReLU

## Activation Functions

[Mass et al., 2013]
[He et al., 2015]




- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not “die”.**

**Leaky ReLU**

$$f(x) = \max(0.01x, x)$$

# Maxout "Neuron"

**Maxout "Neuron"**

[Goodfellow et al., 2013]

- Does not have the basic form of dot product -> nonlinearity
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

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

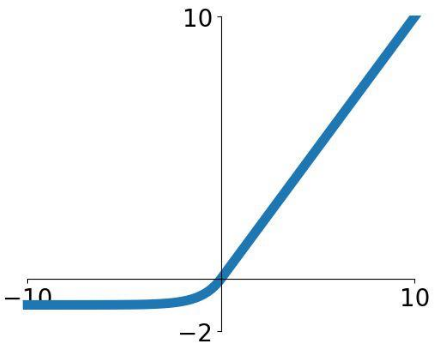
Problem: doubles the number of parameters/neuron :(

# Exponential Linear Units (ELU)

## Activation Functions

[Clevert et al., 2015]

**Exponential Linear Units (ELU)**



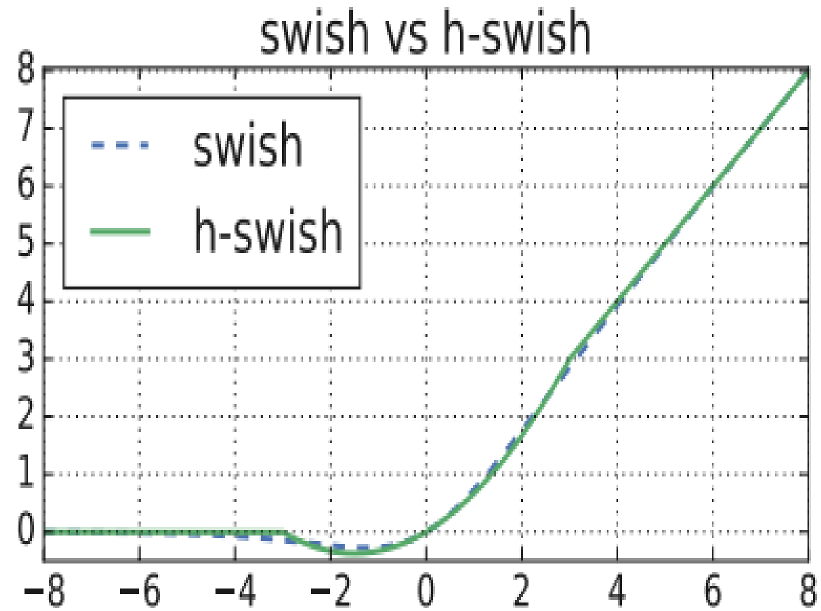

- All benefits of ReLU
- Closer to zero mean outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise

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

- Computation requires exp()

# Swish and H-Swish

- Swith is a smooth version of RELU: It is slightly better in performance as compared to ReLU since its graph is quite similar to ReLU. However, because it does not change abruptly at a point as ReLU does at x = 0, this makes it easier to converge while training.
- Swith is slow: the drawback of Swish is that it is computationally expensive. To solve that we come to the next version of Swish.
- Hswish (Hard swish) is faster: The best part of Hswish is that it is almost similar to swish but it is less expensive computationally since it replaces sigmoid (exponential function) with a ReLU (linear type).




Swish: $$f(x) = x * sigmoid(x) \\ = x * (1 + e^{-x})^{-1}$$

$$\text{h-swish}[x] = x\frac{\text{ReLU6}(x+3)}{6}$$

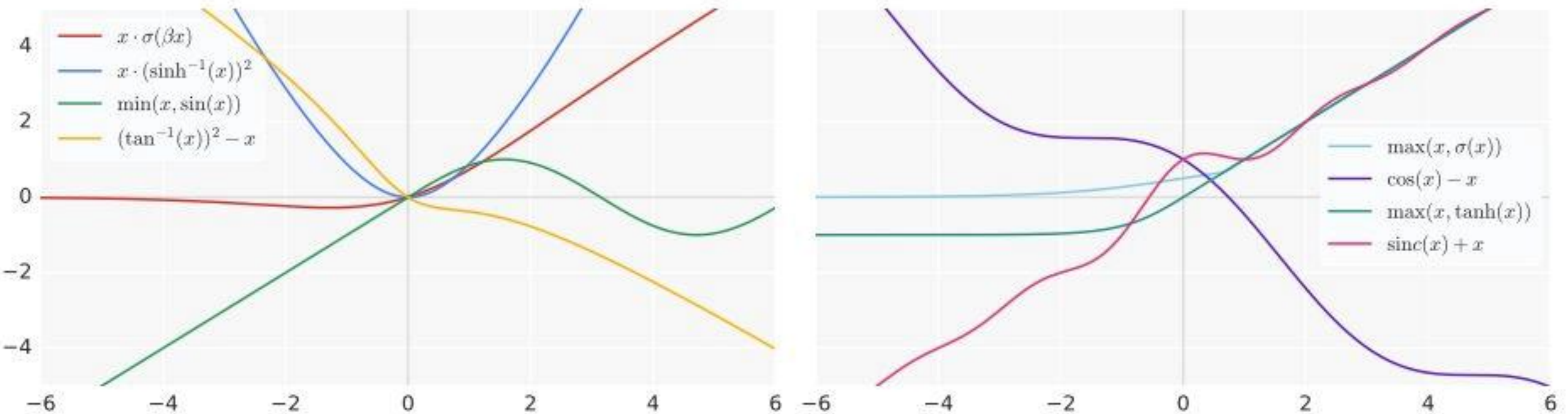
[P. Ramachandran, et al. 2017]

# Swish and H-Swish

- Swish is automatically searched!

- **Unary functions**: $x$, $-x$, $|x|$, $x^2$, $x^3$, $\sqrt{x}$, $\beta x$, $x+\beta$, $\log(|x|+\epsilon)$, $\exp(x)$ $\sin(x)$, $\cos(x)$, $\sinh(x)$, $\cosh(x)$, $\tanh(x)$, $\sinh^{-1}(x)$, $\tan^{-1}(x)$, $\mathrm{sinc}(x)$, $\max(x,0)$, $\min(x,0)$, $\sigma(x)$, $\log(1+\exp(x))$, $\exp(-x^2)$, $\mathrm{erf}(x)$, $\beta$

- **Binary functions**: $x_1+x_2$, $x_1 \cdot x_2$, $x_1-x_2$, $\frac{x_1}{x_2+\epsilon}$, $\max(x_1,x_2)$, $\min(x_1,x_2)$, $\sigma(x_1)\cdot x_2$, $\exp(-\beta(x_1-x_2)^2)$, $\exp(-\beta|x_1-x_2|)$, $\beta x_1+(1-\beta)x_2$




The corresponding paper “SEARCHING FOR ACTIVATION FUNCTIONS” by P. Ramachandran, B. Zoph, Quoc V. Le is rejected by ICLR18, as reviewers and anonymous ones counter that PRelus should be doing quite well too.
But now it has 900+ citations.

# Activation functions in practice

- Use ReLU. Be careful with your learning rates
- Try out Leaky ReLU / Maxout / ELU
- Try out tanh but don’t expect much
- Don’t use sigmoid

- Replacing ReLU by swish improves performance, at a cost of slower speed
- GELU is widely adopted in NLP (BERT, GPT)

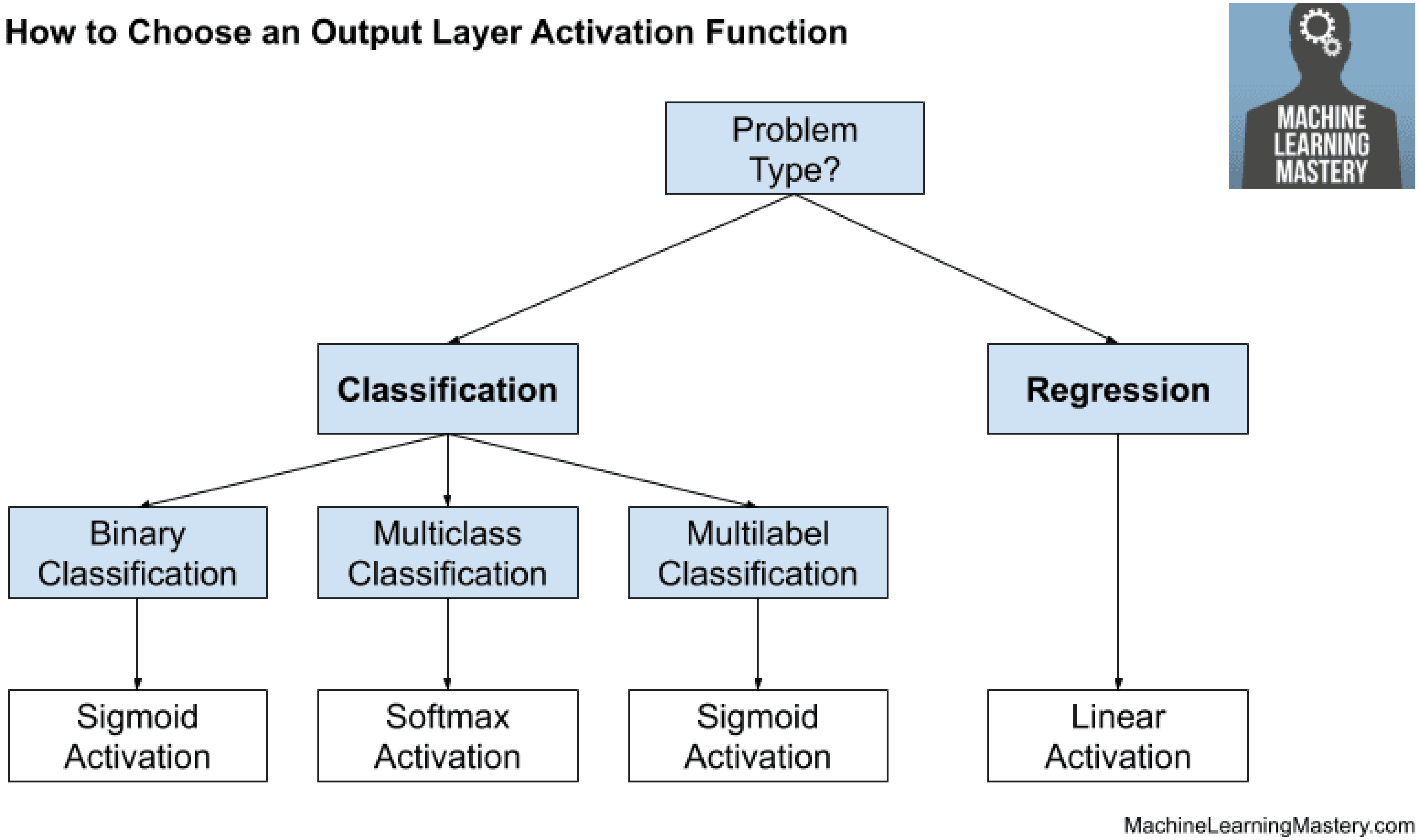
> “Although various hand-designed alternatives to ReLU have been proposed, none have managed to replace it due to inconsistent gains.”
>
> In “Searching for Activation Functions”, 2017

Dead neuron will not exist after using batch normalization

# What features a good activation should have

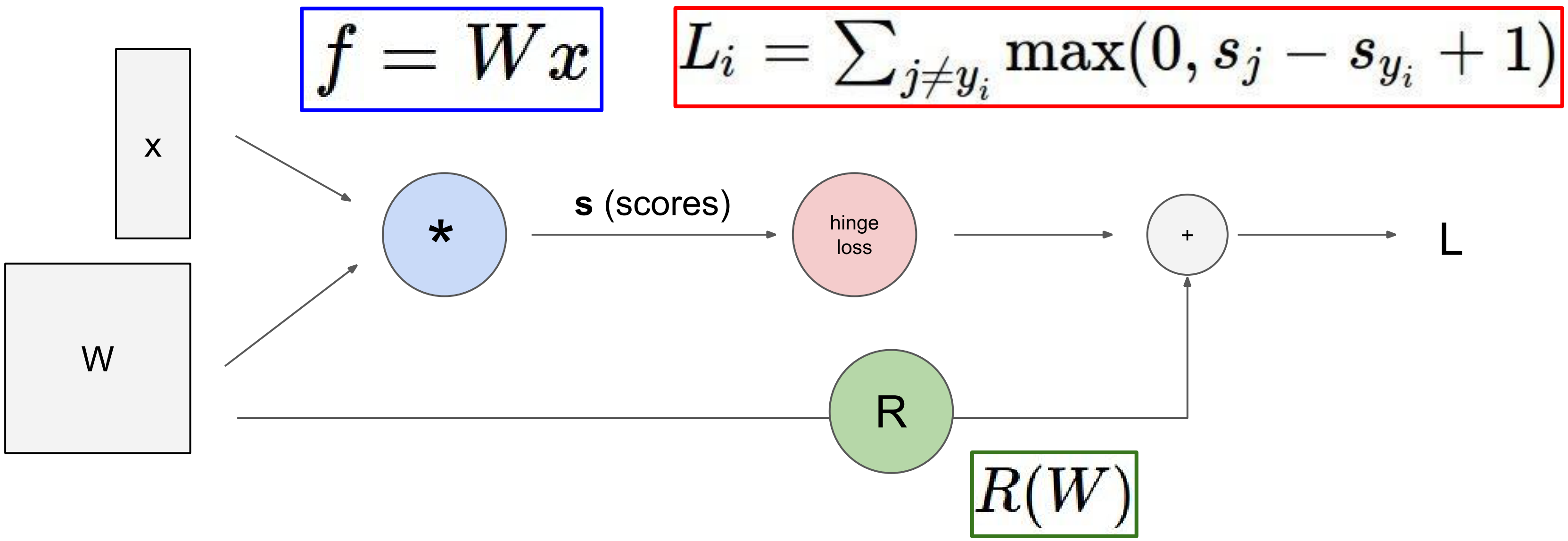
1. Non-linear
2. Differentiable at almost everywhere
3. Simple computation
4. Non-saturation

# How to Choose an Output Layer Activation Function



# Back propagation

# Computation of SVM



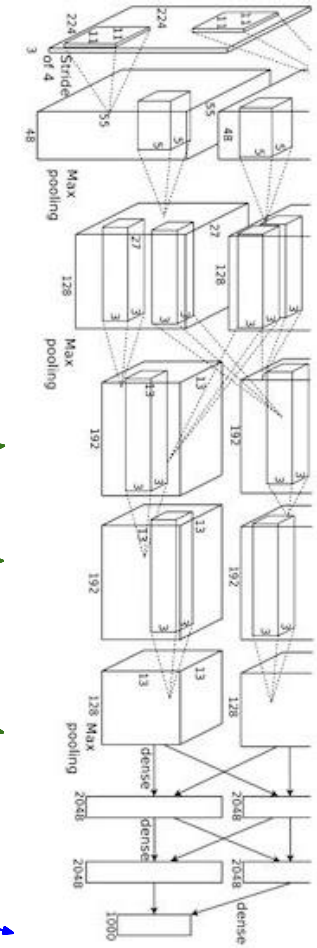
# Computation of DNN

Convolutional network
(AlexNet)

input image

weights

loss



# Computation of DNN

## Neural Turing Machine

input image

loss

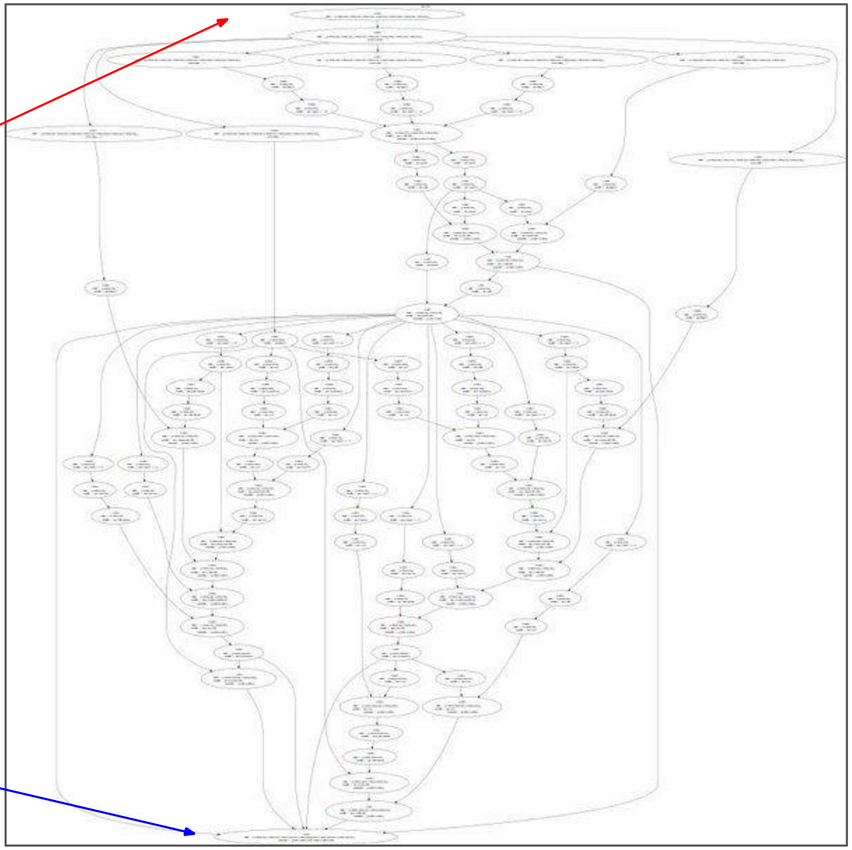
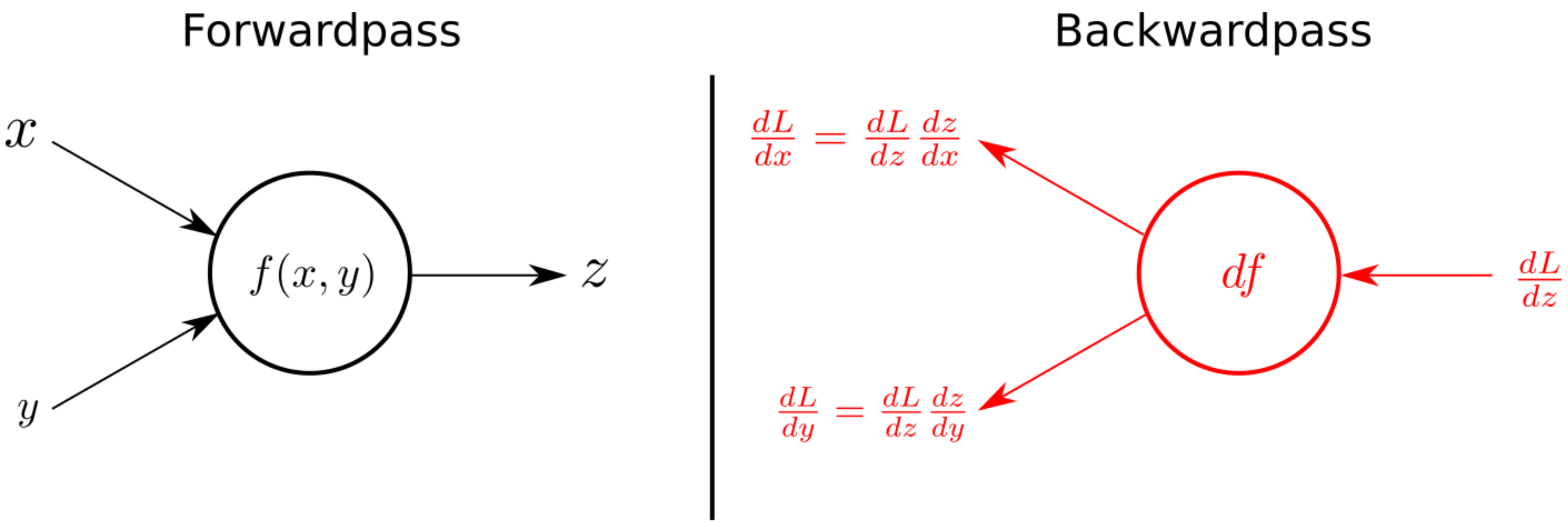


Figure reproduced with permission from a [Twitter post]() by Andrej Karpathy.

# Forwardpass and Backwardpass

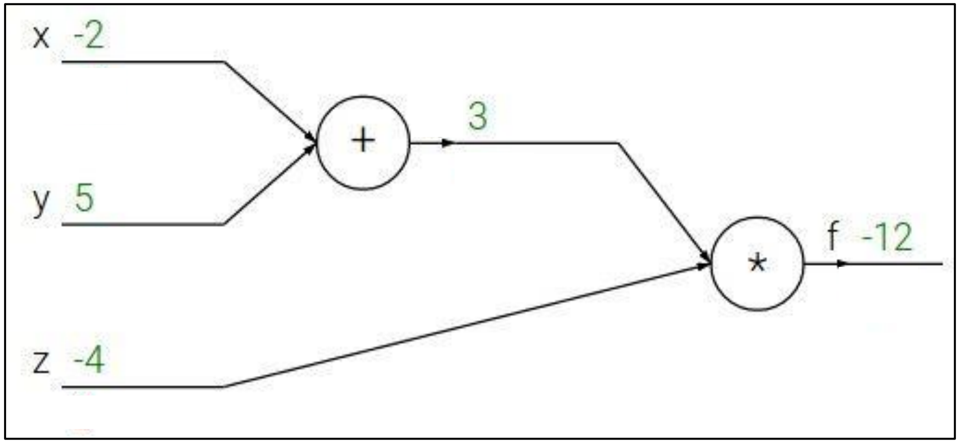


# Backpropagation: a simple example

Backpropagation: a simple example

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

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



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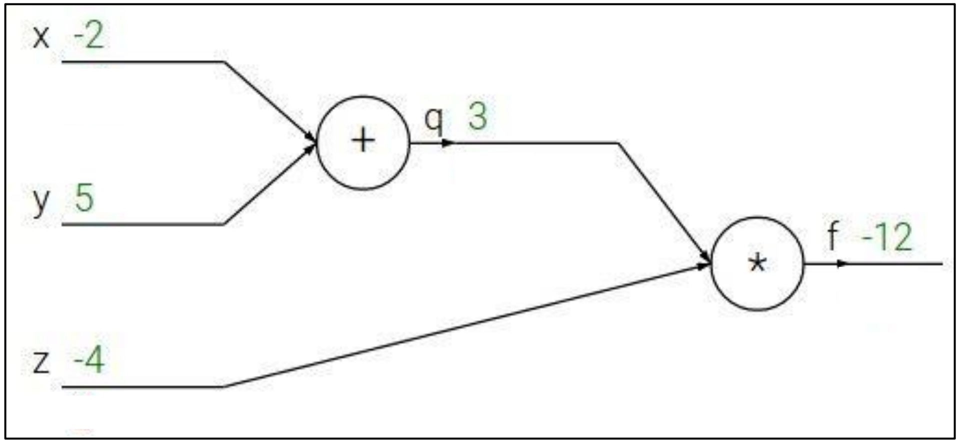
$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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

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



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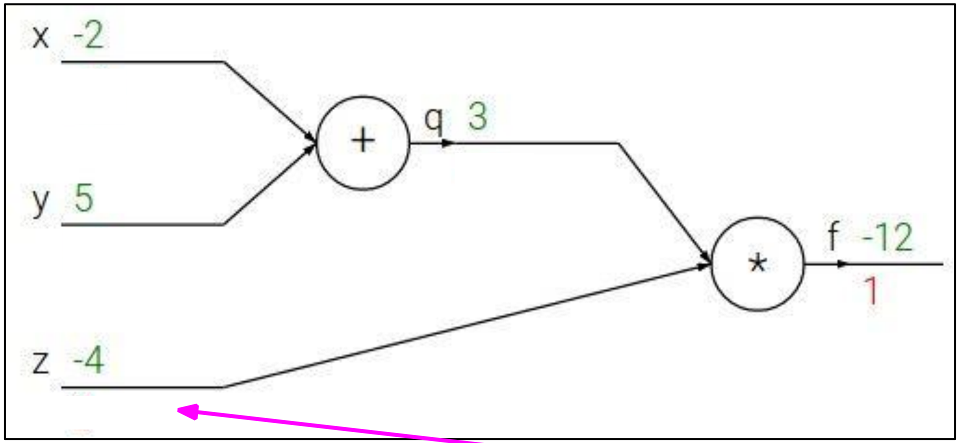


$$\frac{\partial f}{\partial z}$$

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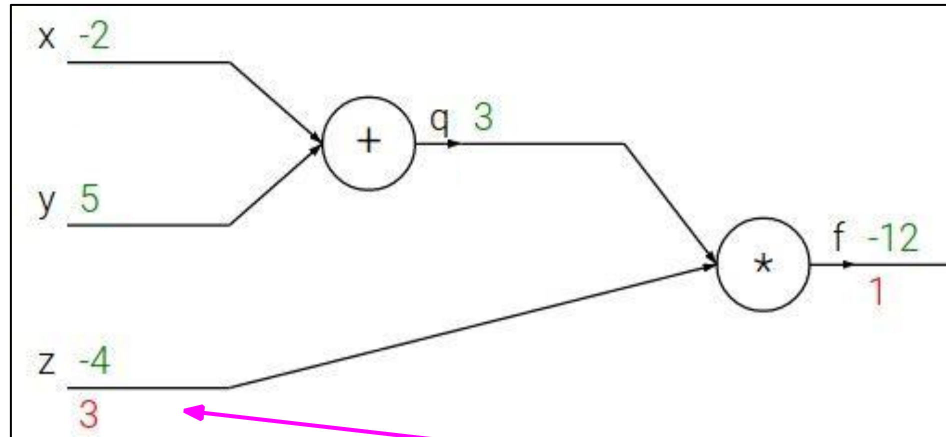


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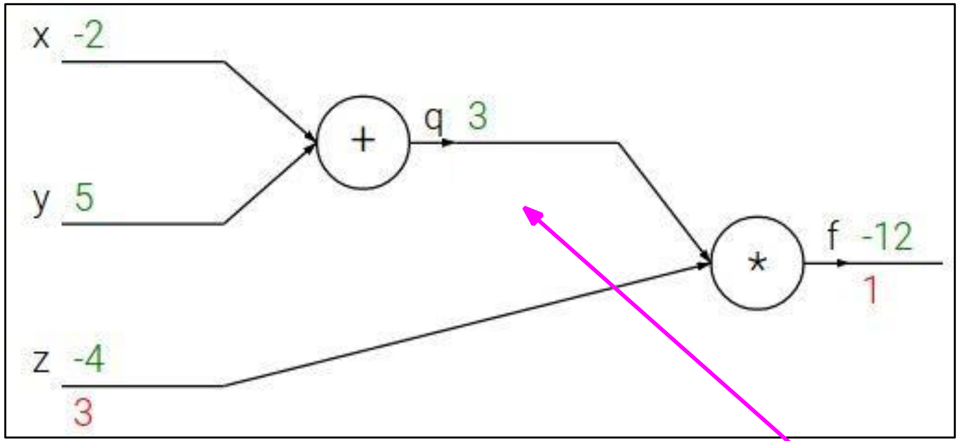


$$\frac{\partial f}{\partial q}$$

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Backpropagation: a simple example

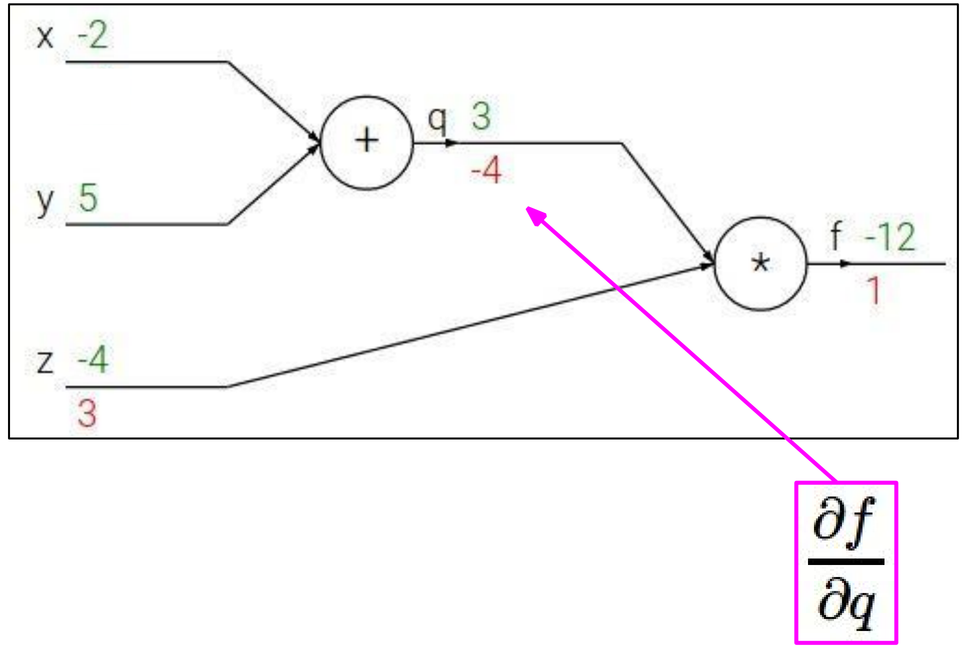
$$f(x, y, z) = (x + y)z$$

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

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

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

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



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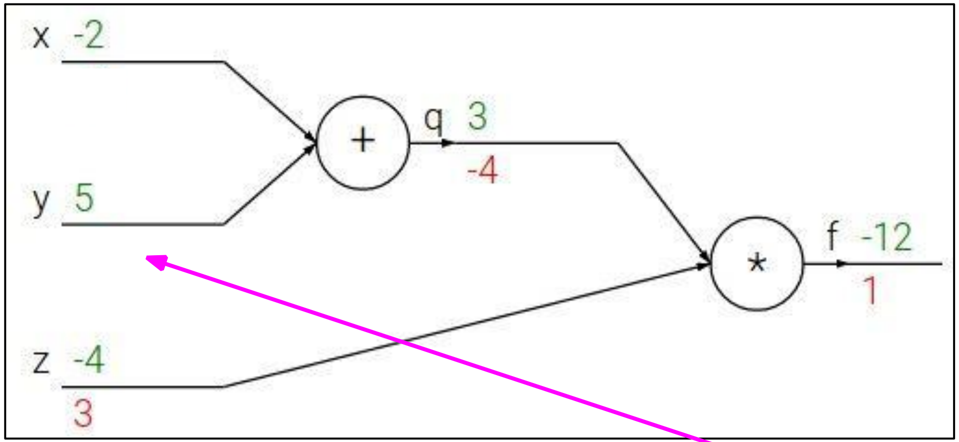


$$\frac{\partial f}{\partial y}$$

# Backpropagation: a simple example

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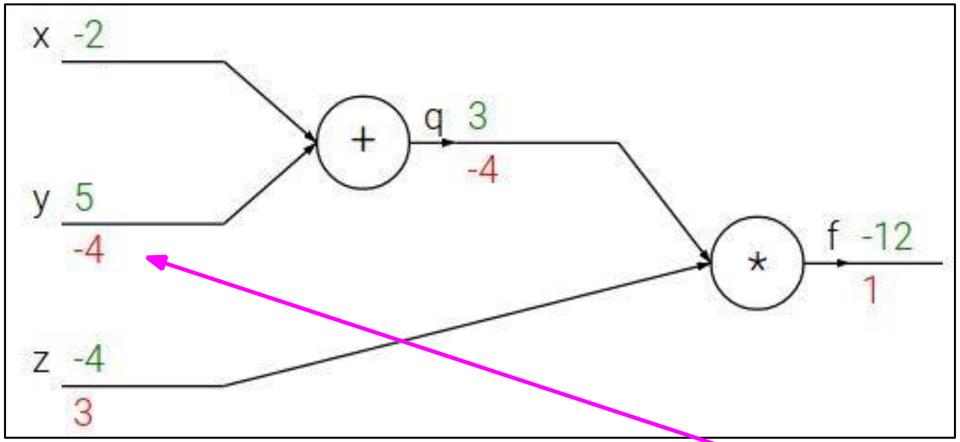


$$\boxed{\frac{\partial f}{\partial y}}$$

Chain rule:

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

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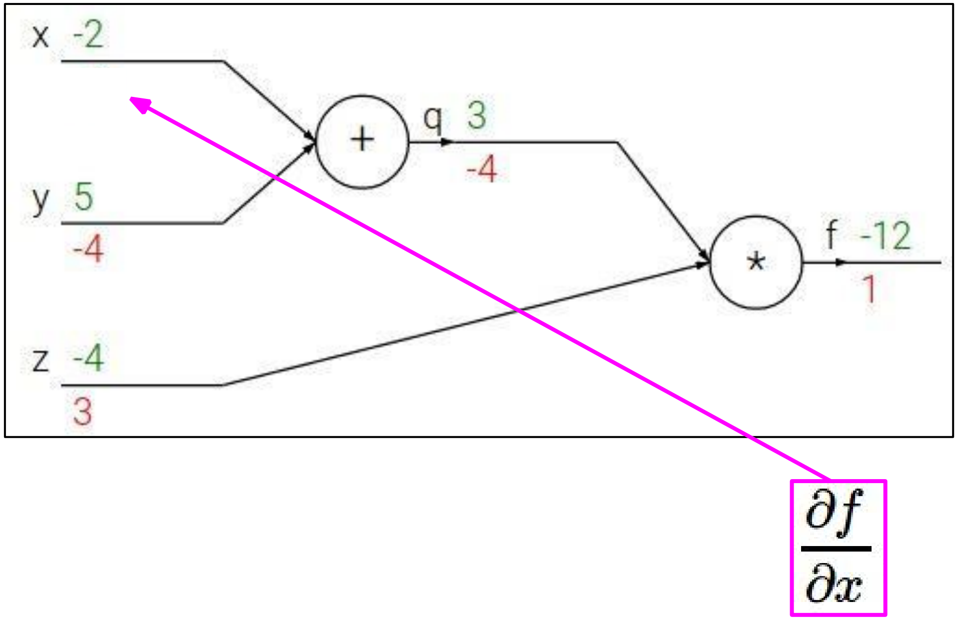

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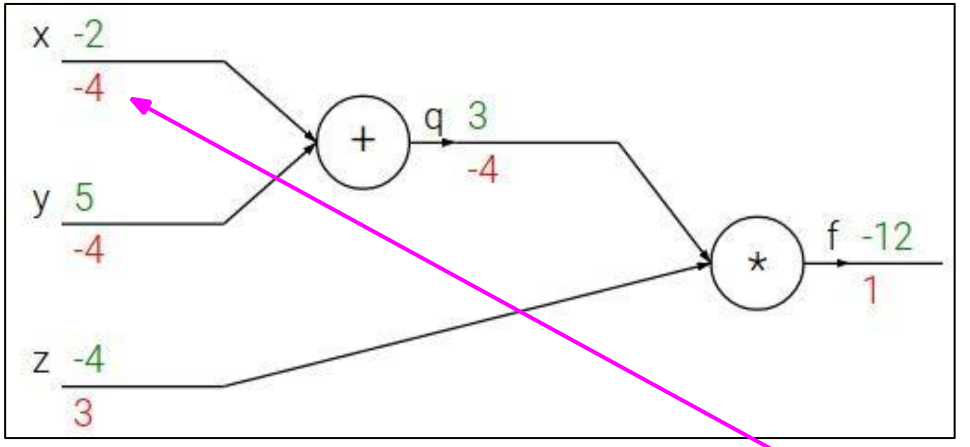


$$\frac{\partial f}{\partial x}$$

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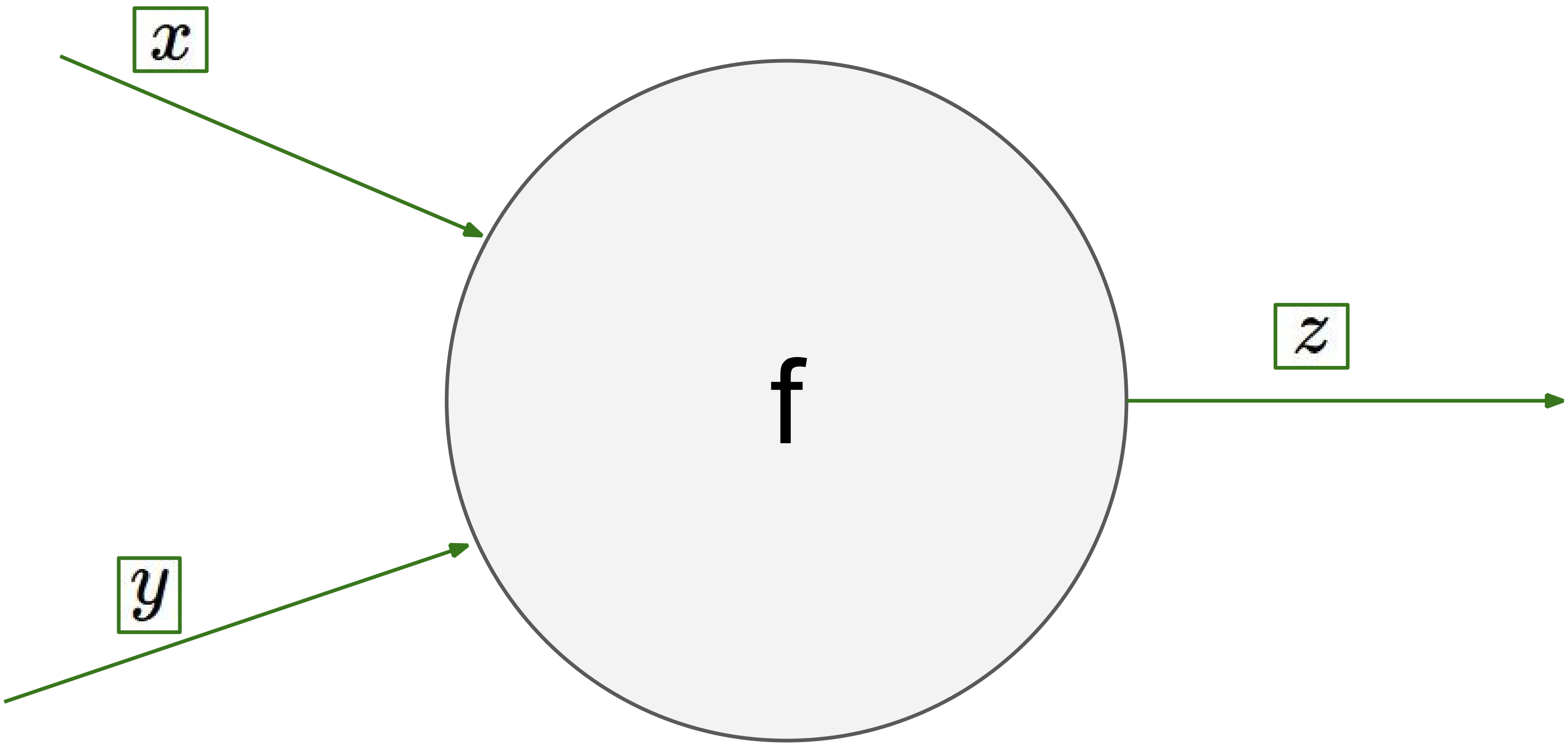

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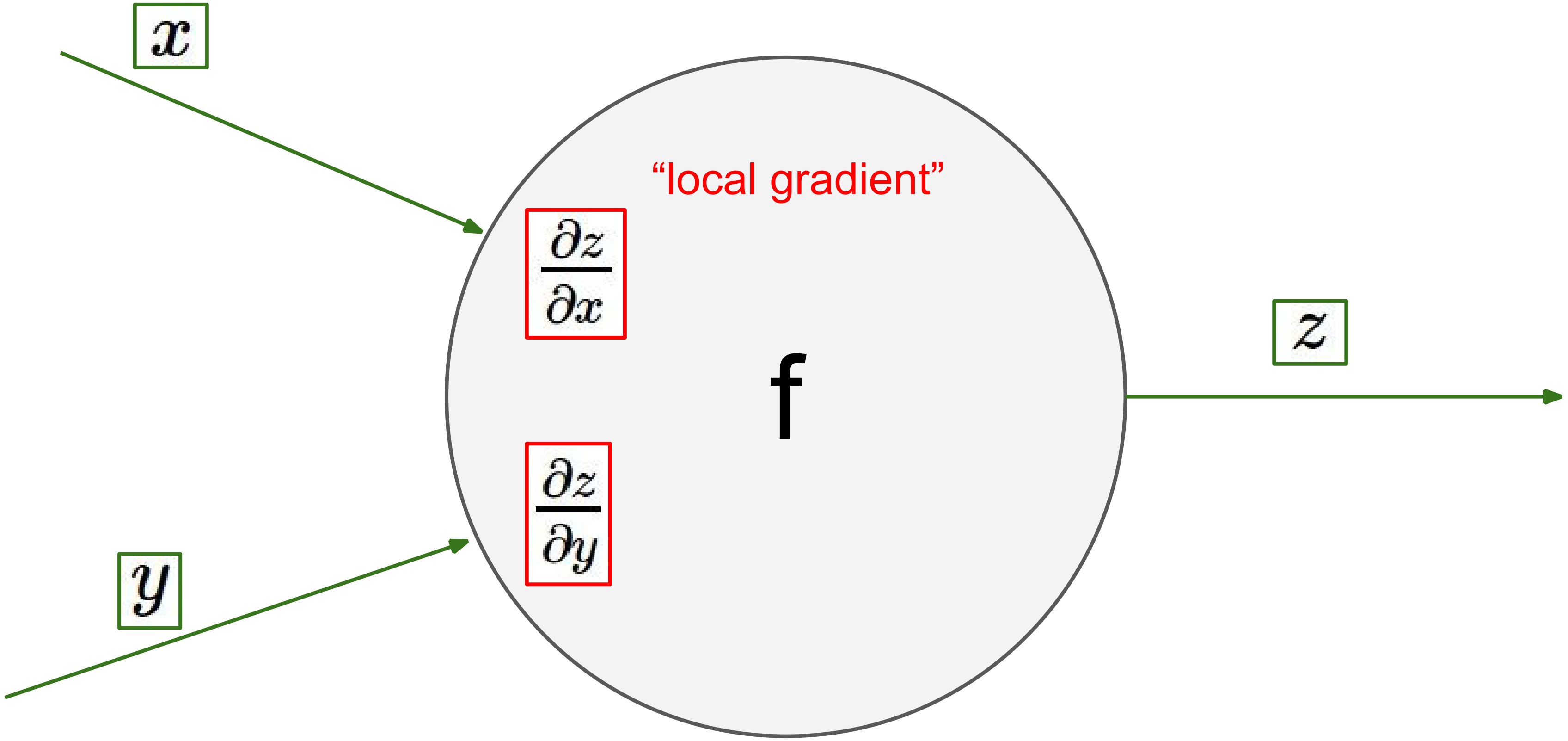

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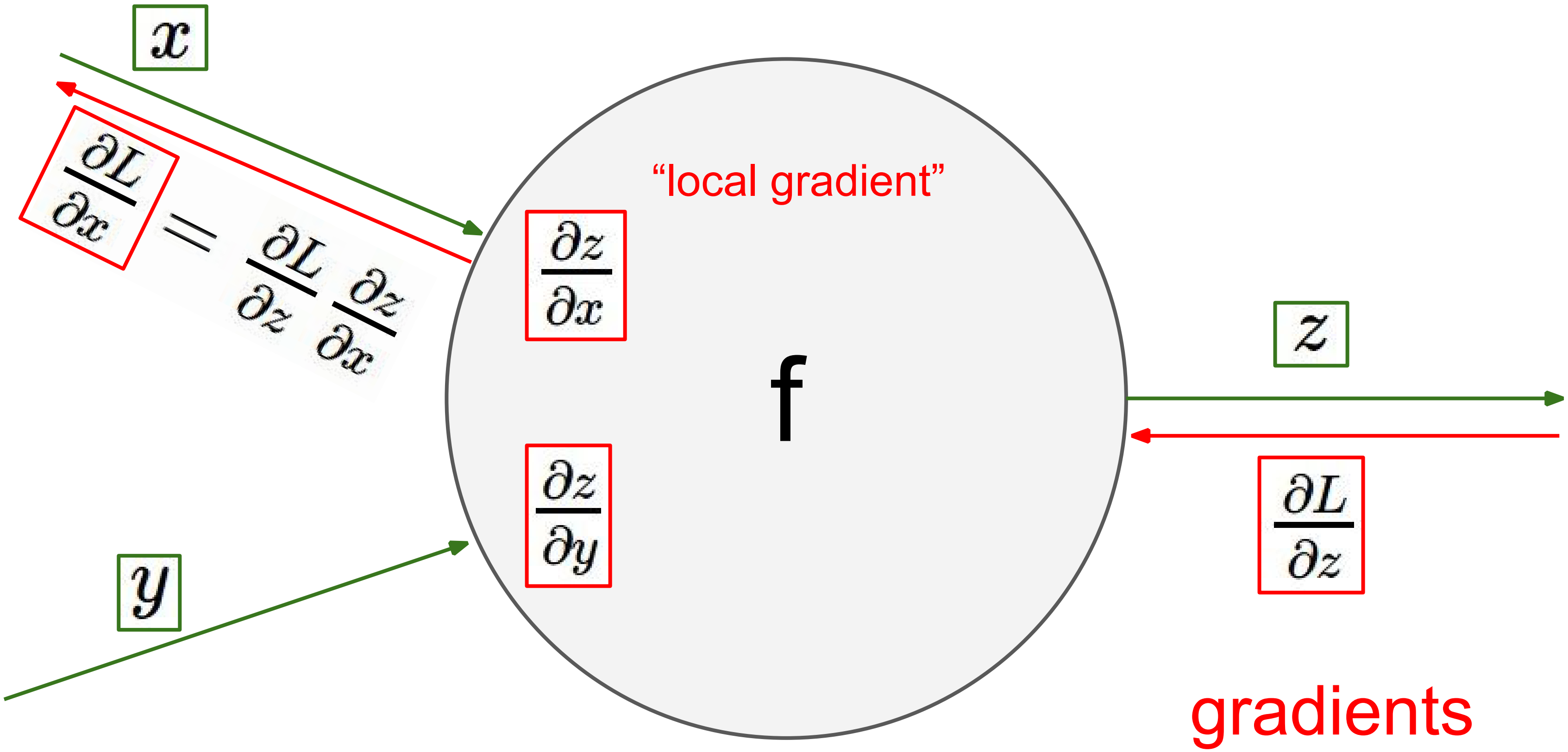

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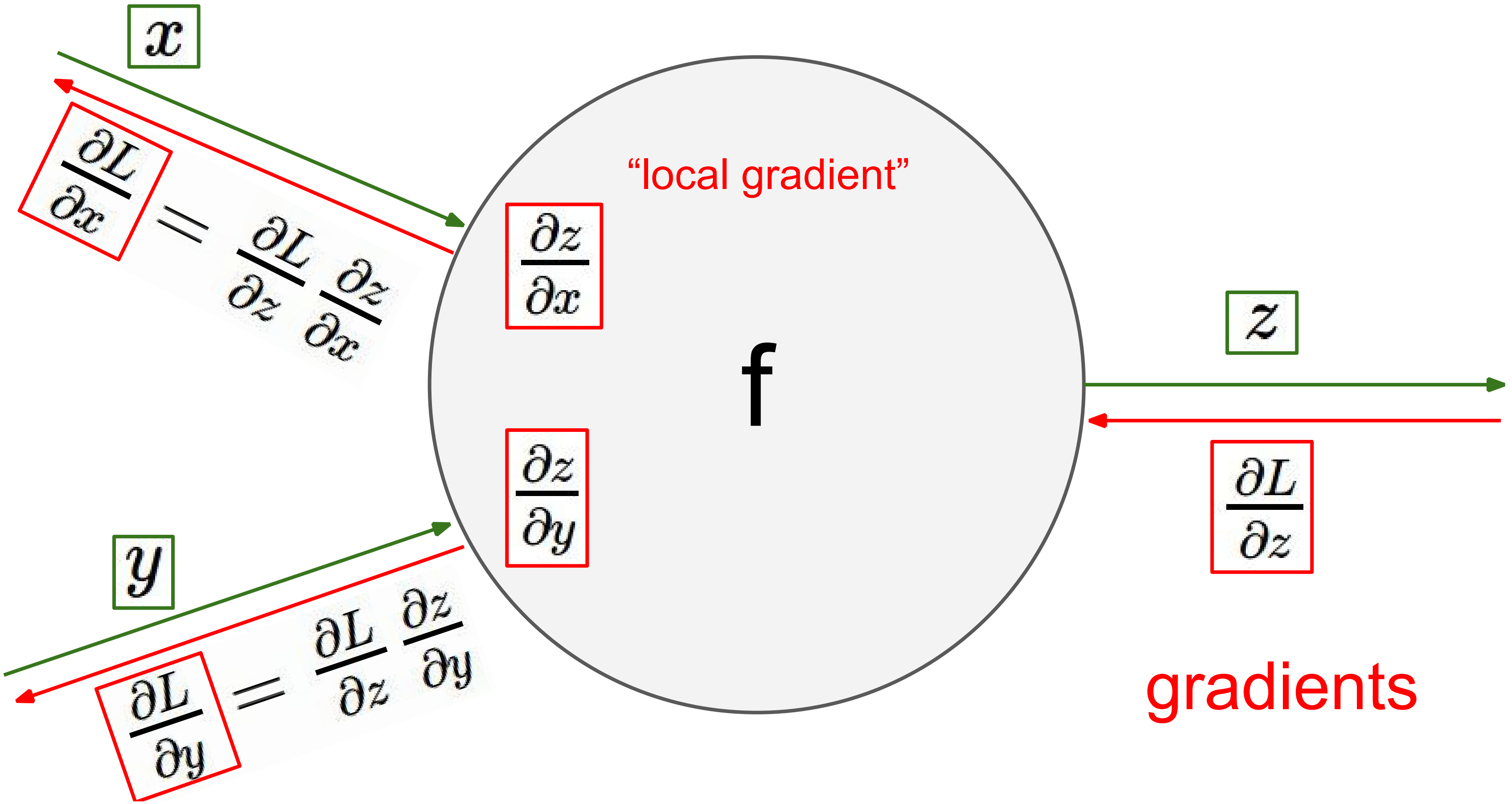

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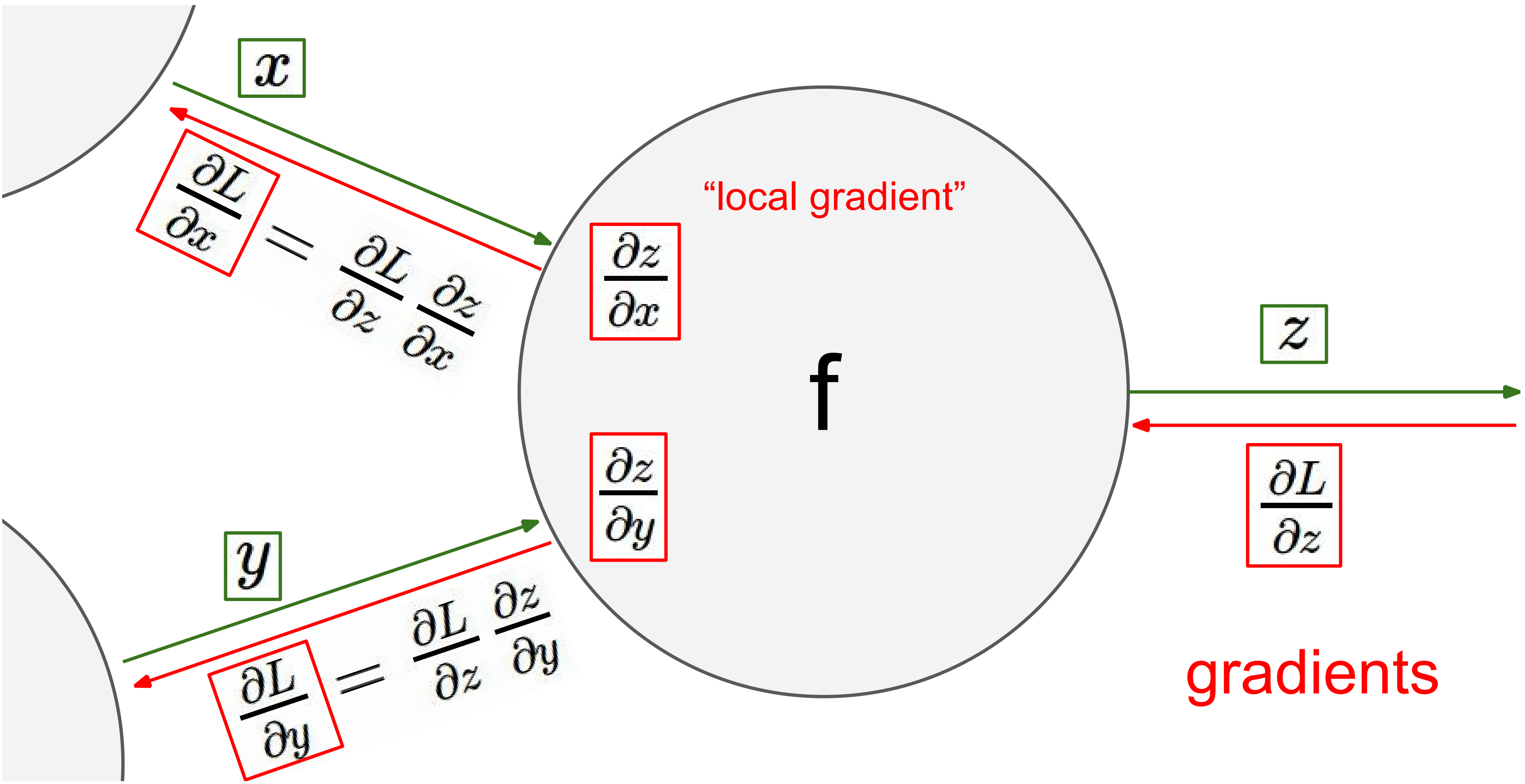
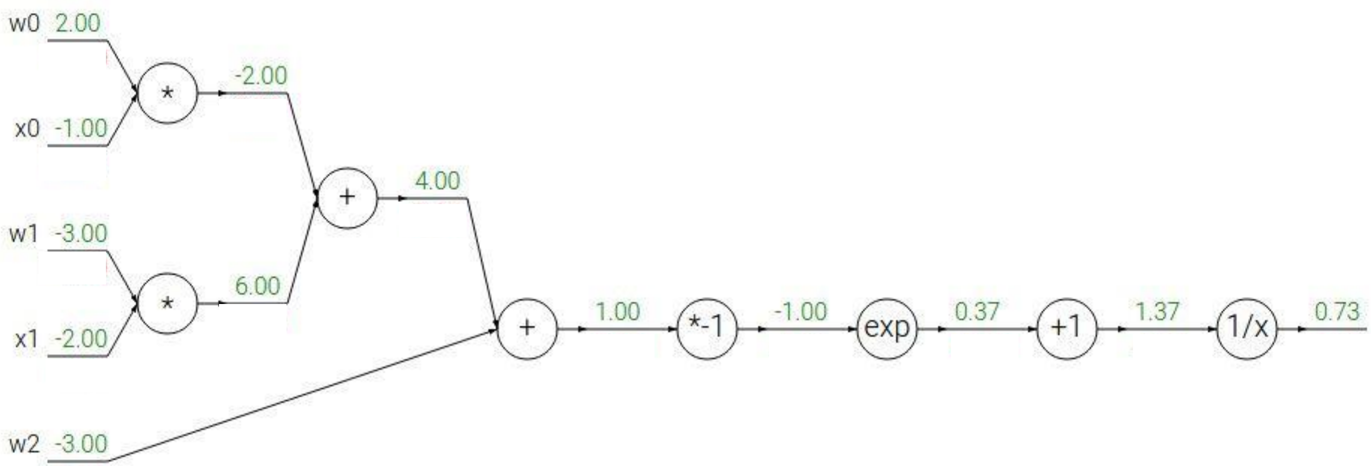


# Backpropagation: another example

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



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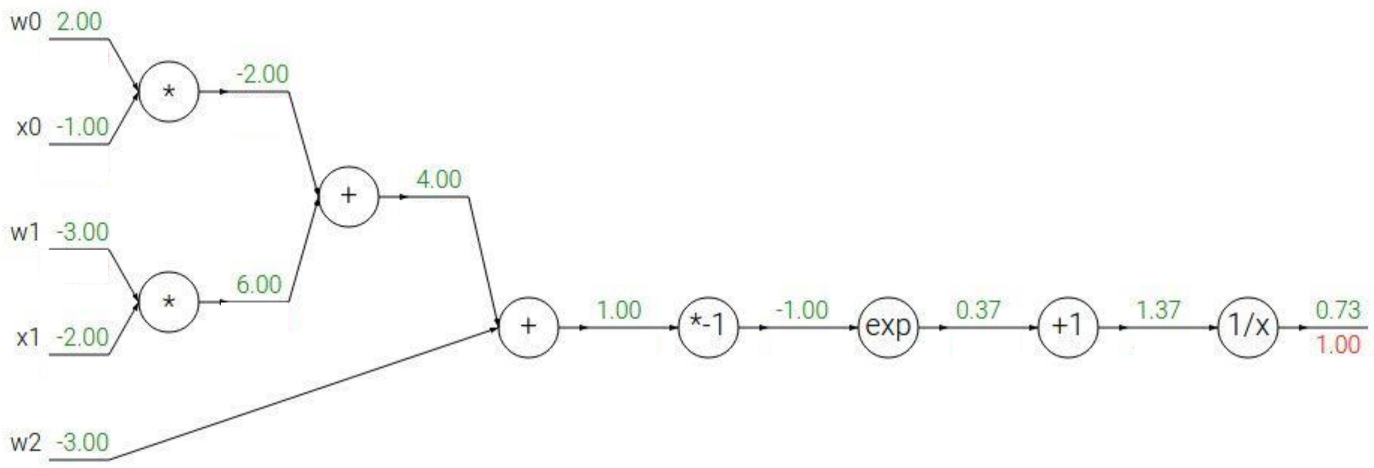


$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$

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

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

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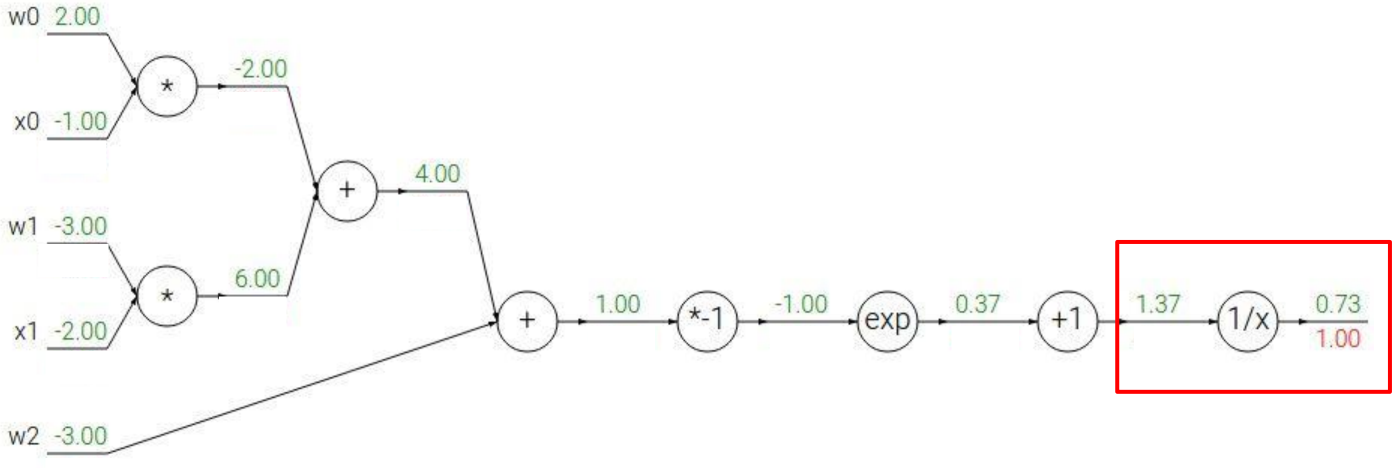


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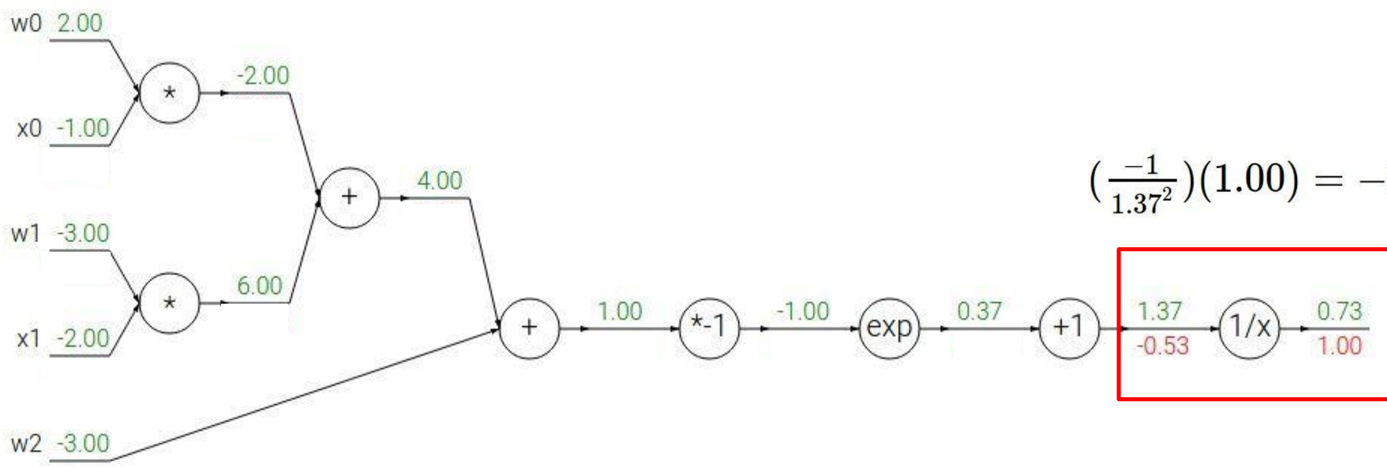


$$\left(\frac{-1}{1.37^2}\right)(1.00) = -0.53$$

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

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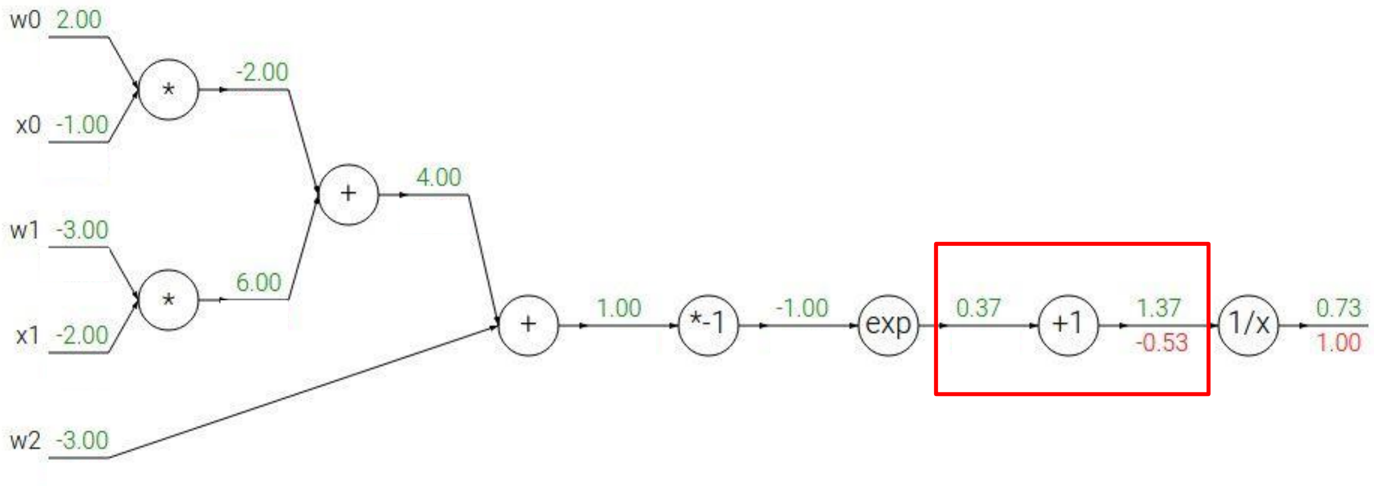


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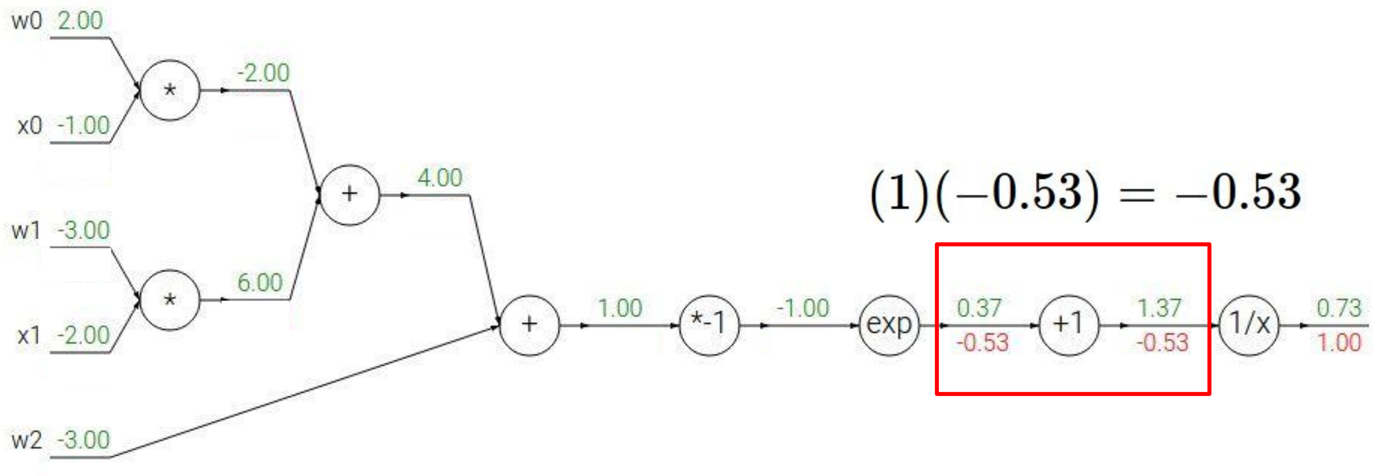
# Backpropagation: another example

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

$$(1)(-0.53) = -0.53$$




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

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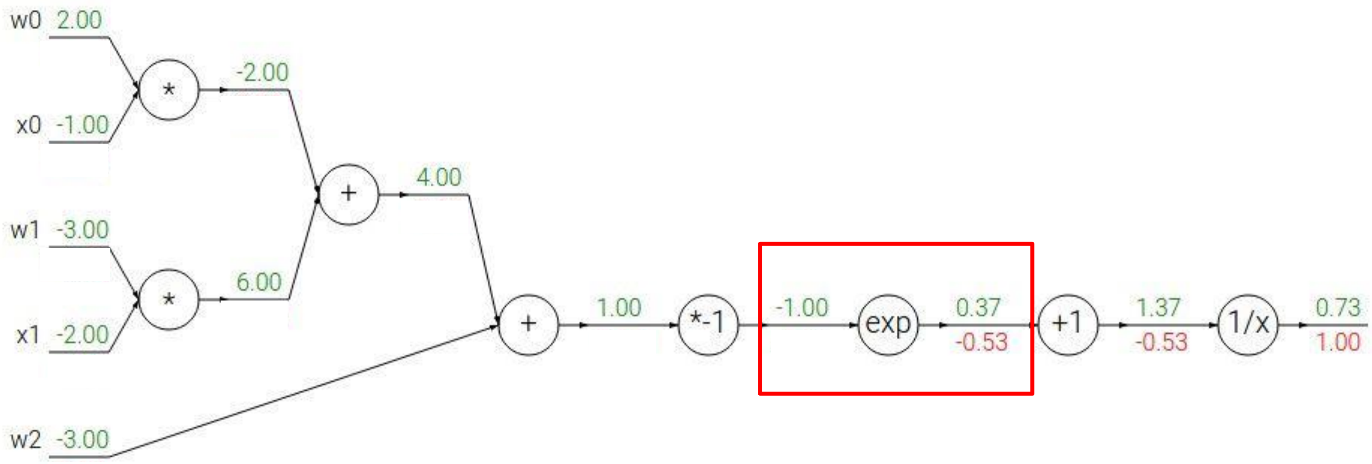


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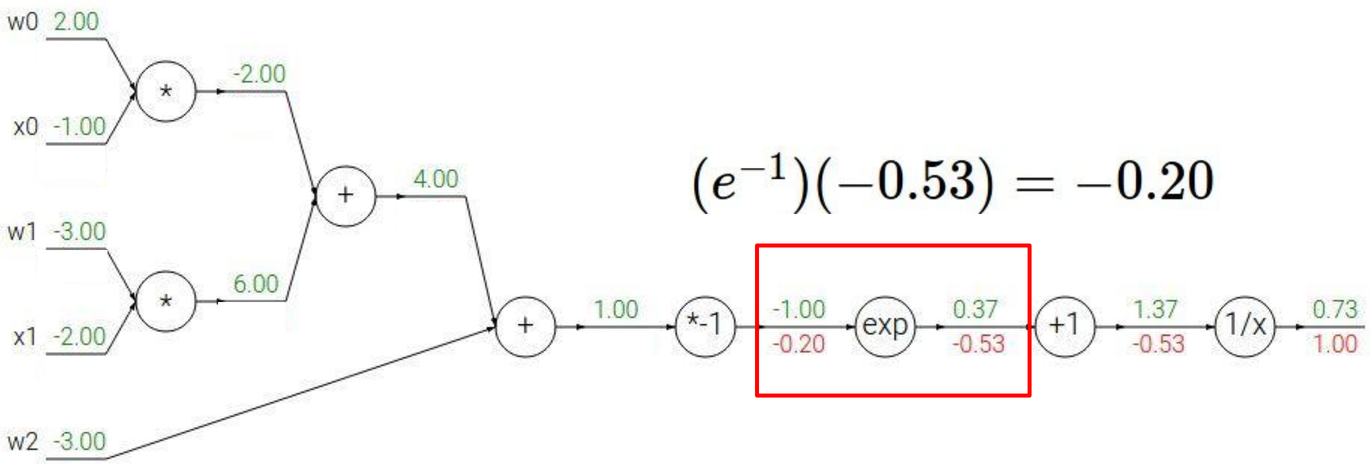


$$(e^{-1})(-0.53) = -0.20$$

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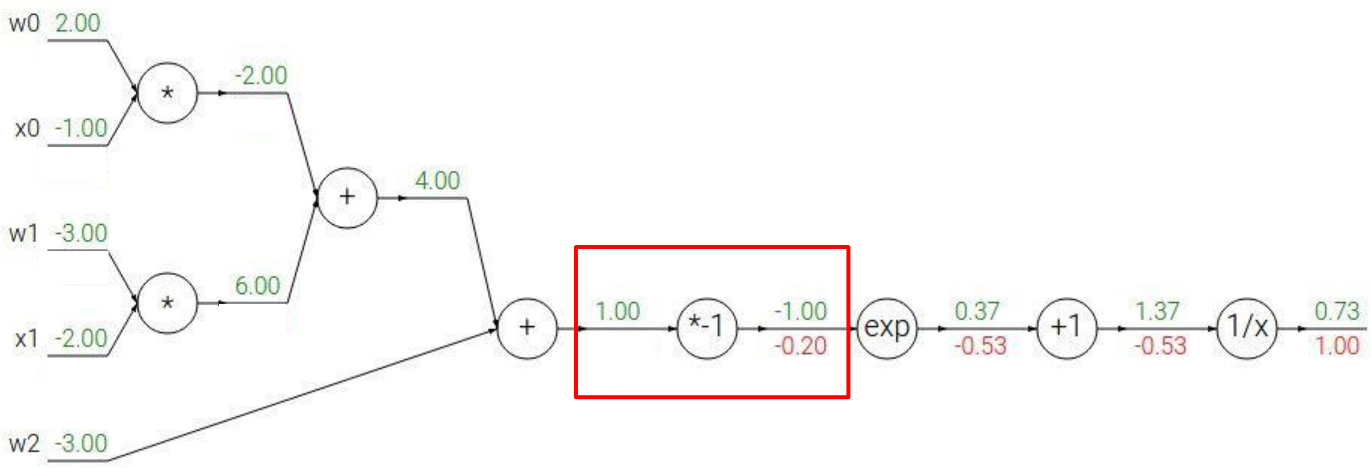


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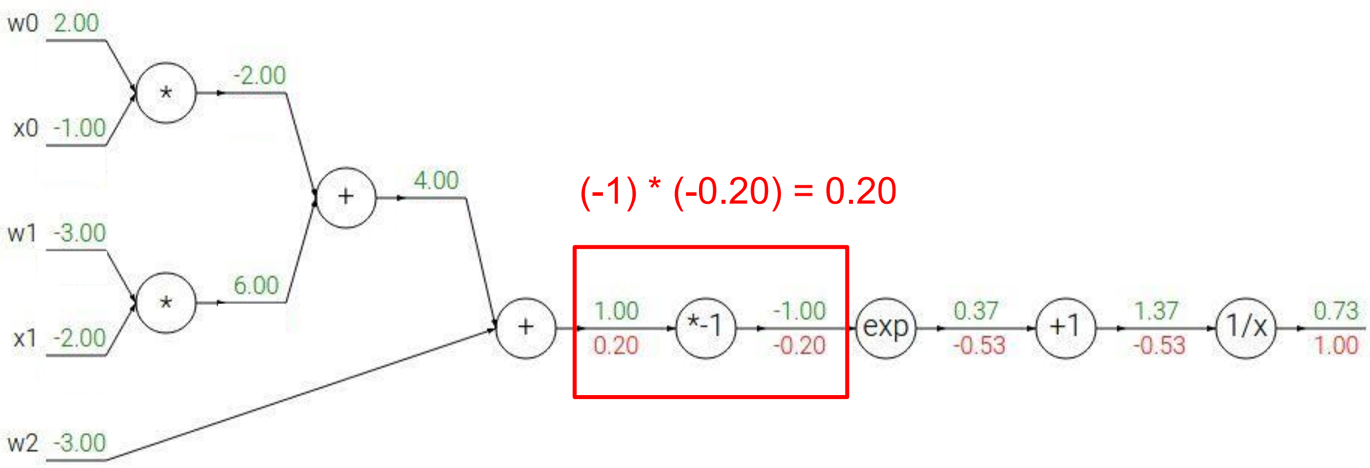


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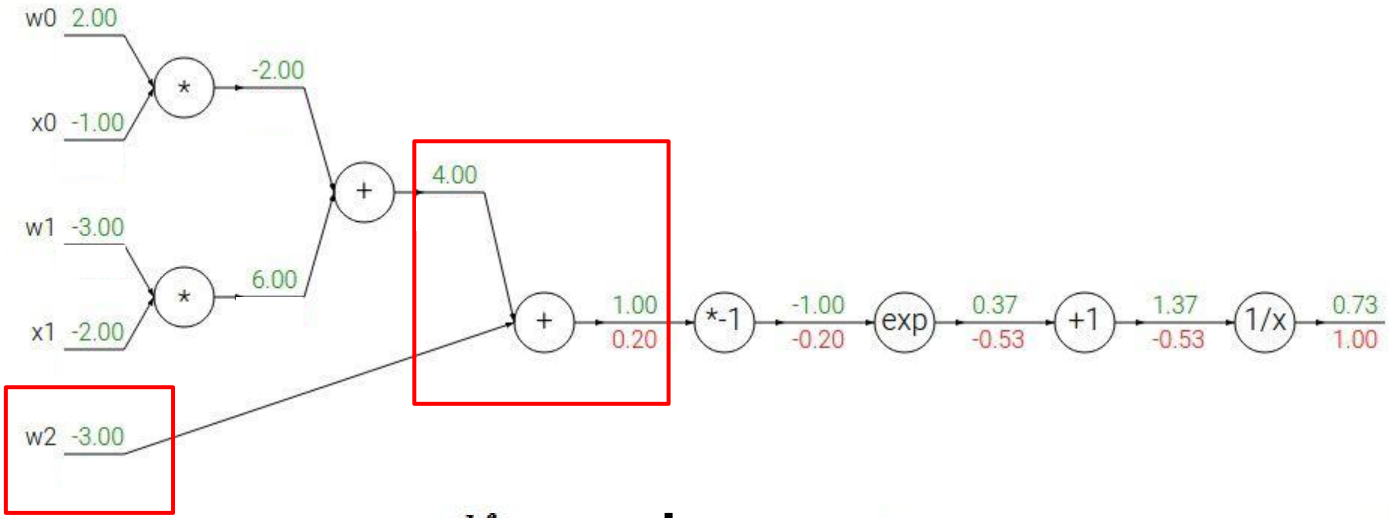


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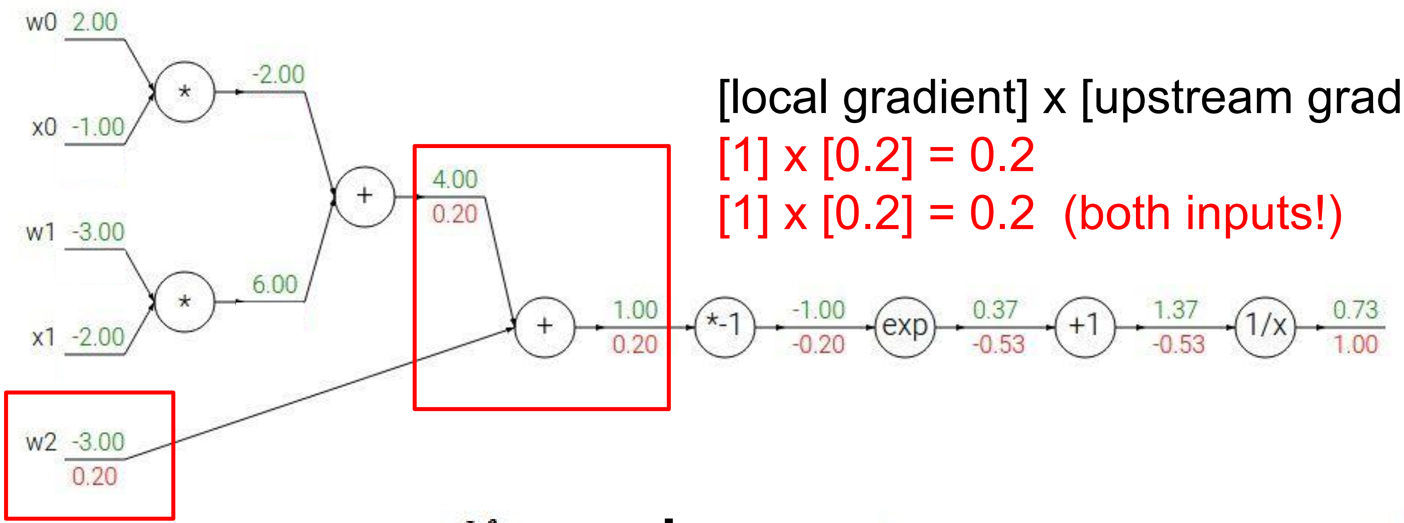


[local gradient] x [upstream gradient]

[1] x [0.2] = 0.2

[1] x [0.2] = 0.2 (both inputs!)

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

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

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

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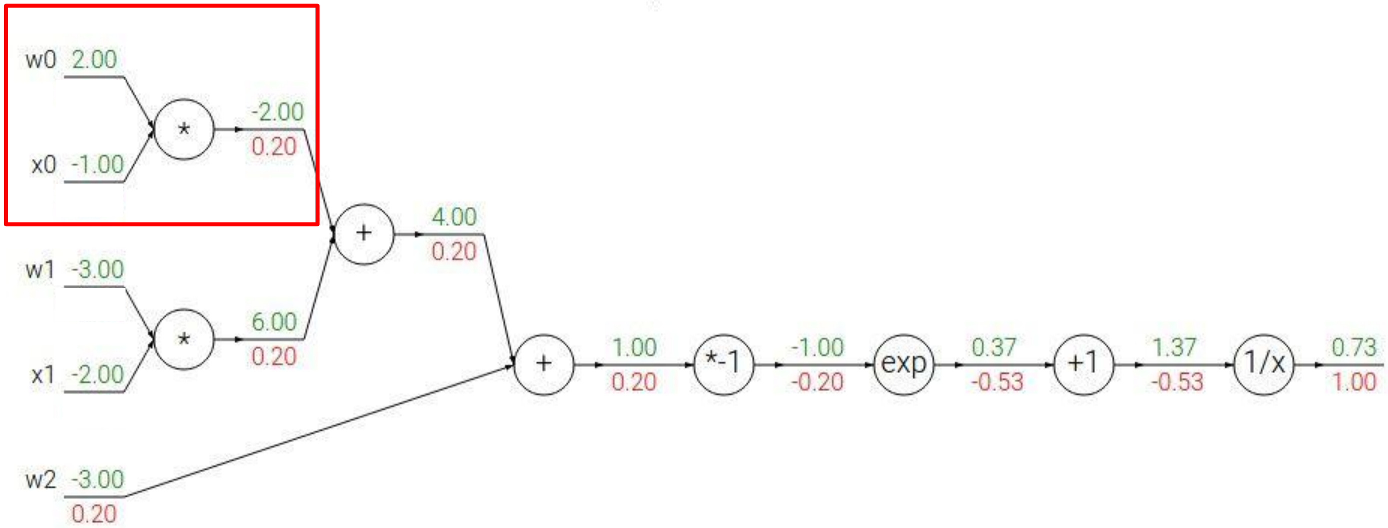


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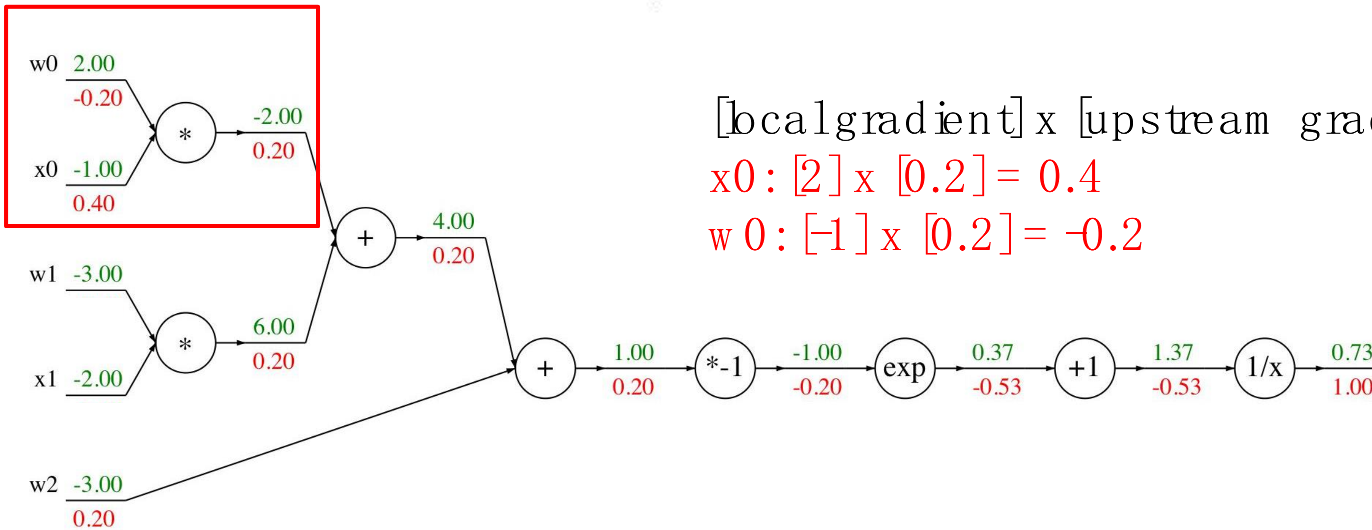



[local gradient] x [upstream gradient]

x0: [2] x [0.2] = 0.4

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

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

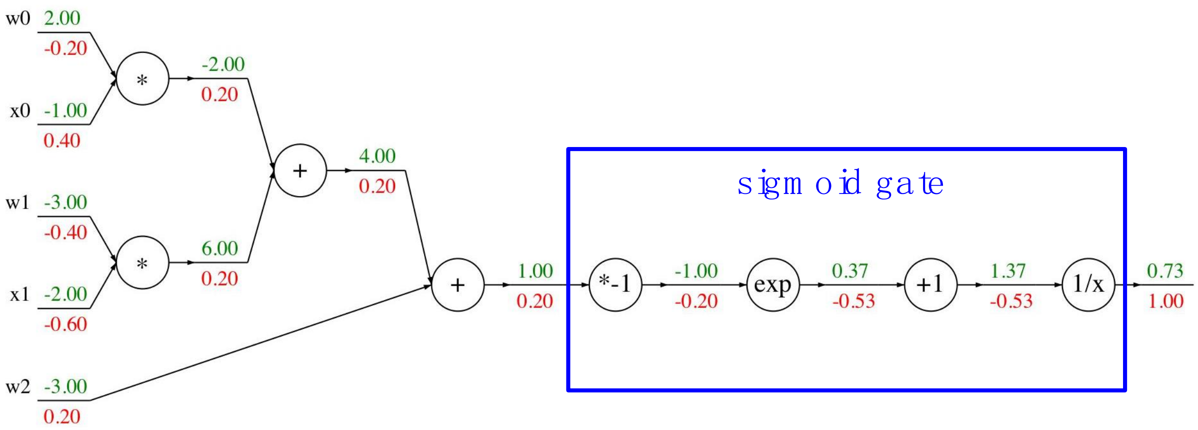
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a \qquad\qquad f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

# Backpropagation: another example

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

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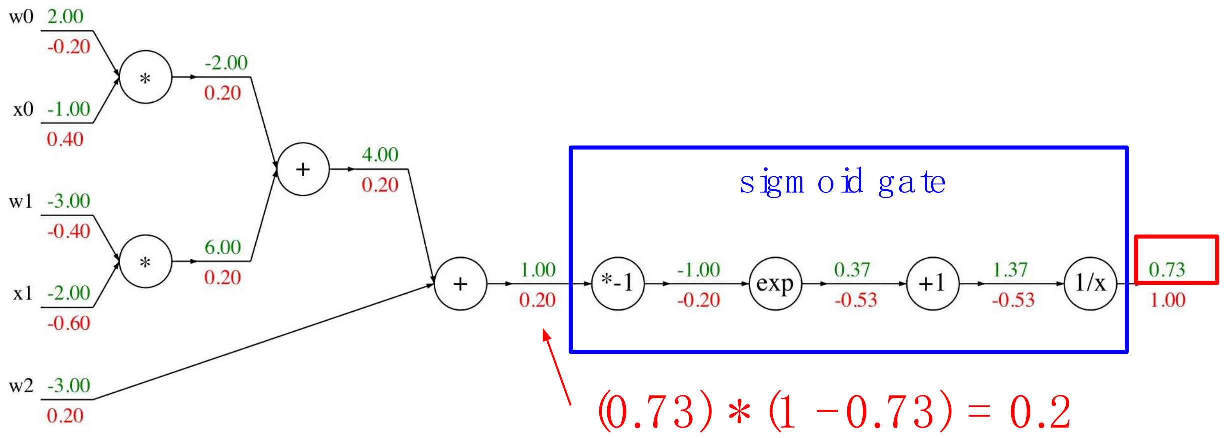
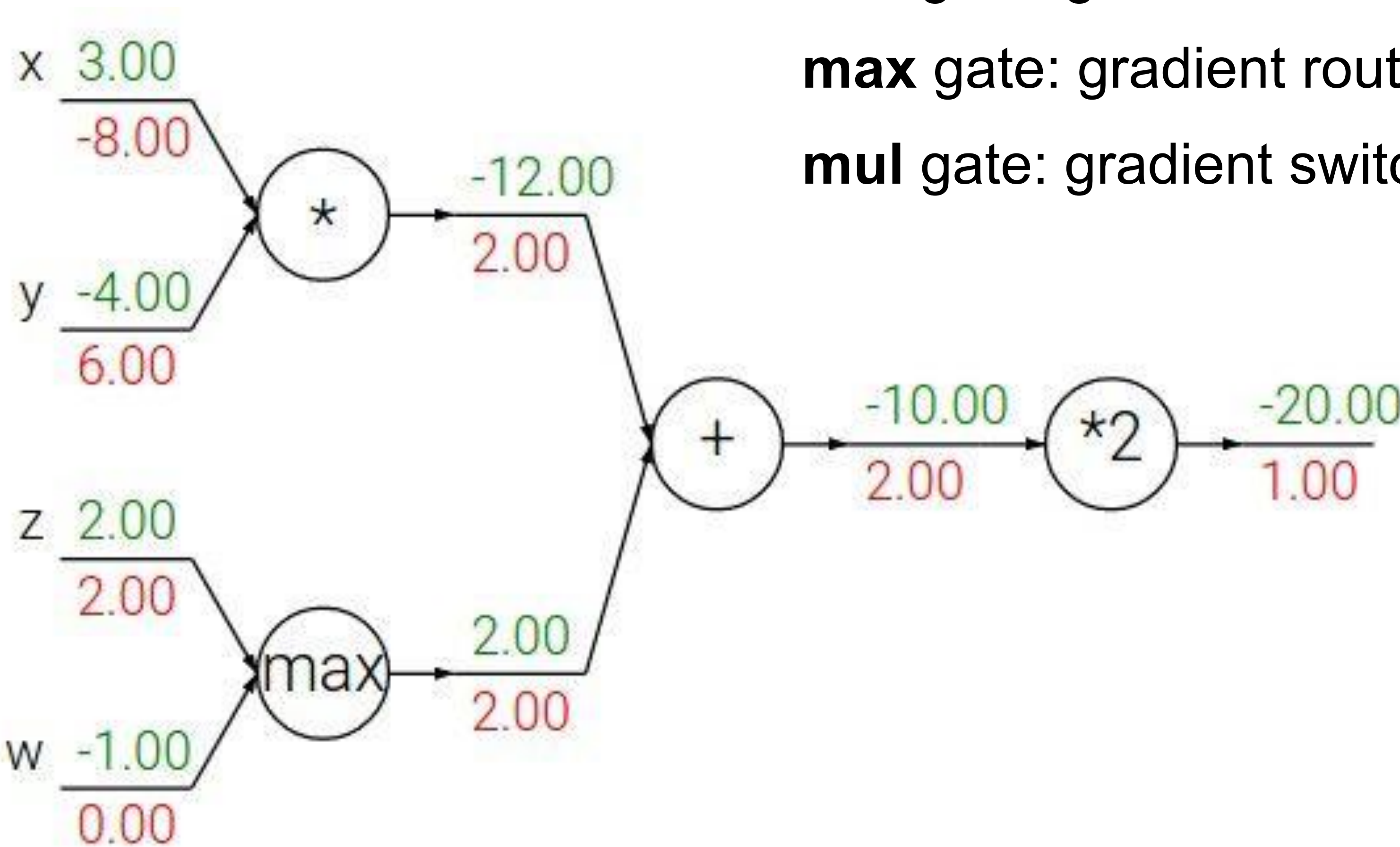


# Patterns in backward flow




**add** gate: gradient distributor

**max** gate: gradient router

**mul** gate: gradient switcher

# Vectorized operation

## Gradients for vectorized code