Today: Outline

- **Neural networks cont'd:** learning via gradient descent; chain rule review; gradient computation using the backpropropagation algorithm

- Reminder: PS2 is due Feb 24

Fei-Fei Li

- Professor, Computer Science, Stanford University
- Co-Director of Stanford's Human-Centered AI Institute
- Previously Vice President at Google and Chief Scientist of AI/ML at Google Cloud
- Co-founder and chairperson of the national non-profit AI4ALL
- Online Deep Learning Course
- **"First, we teach them see, then they help us to see better."**

Image Captioning

A young boy holding a baseball bat

A man riding a horse next to a building

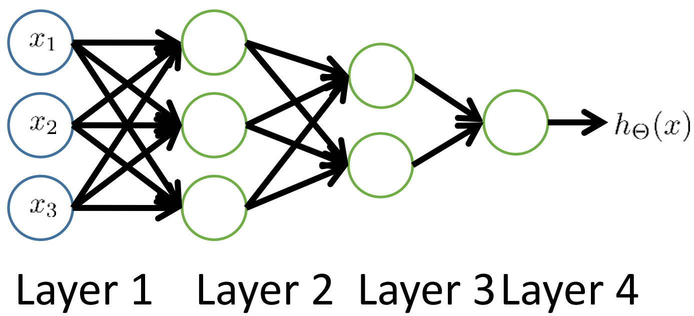
Neural Networks II

Architectures and Learning

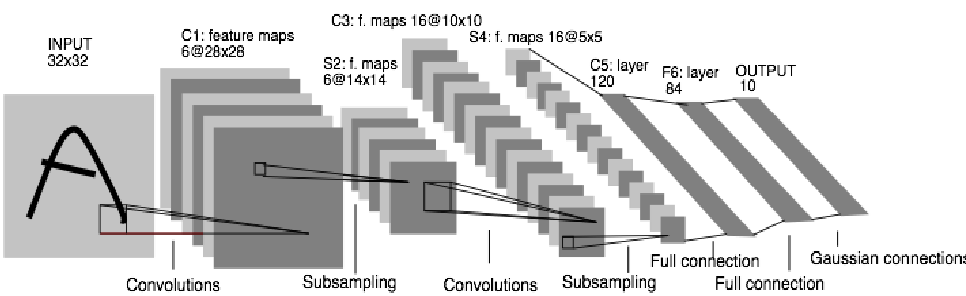
Network architectures

Feed-forward

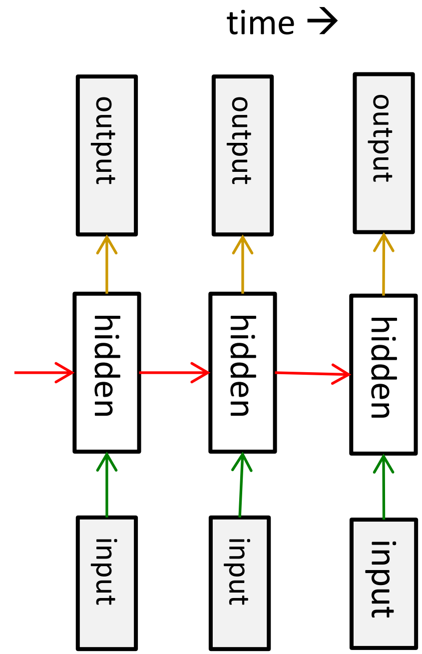
Fully connected



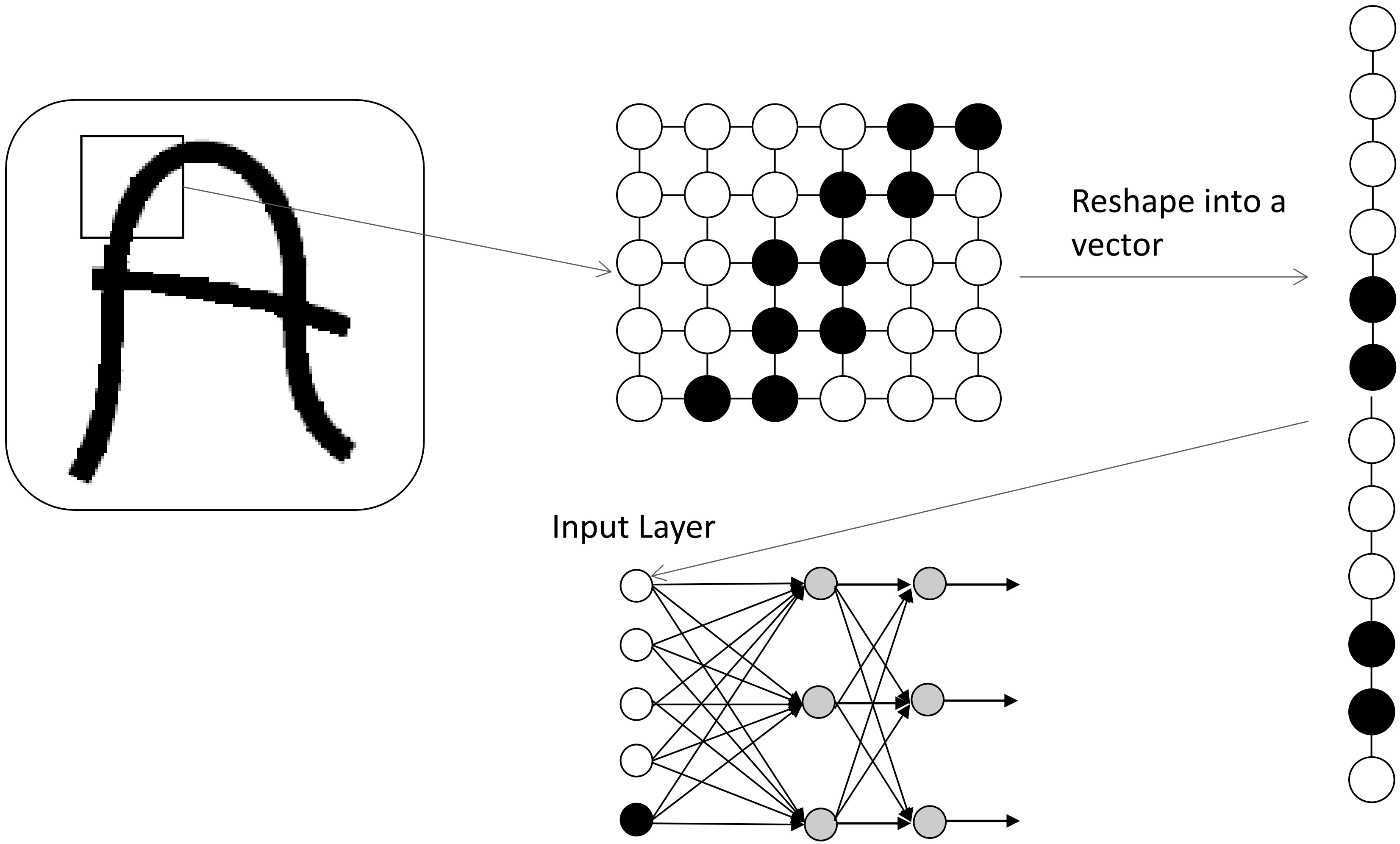
Convolutional



Recurrent



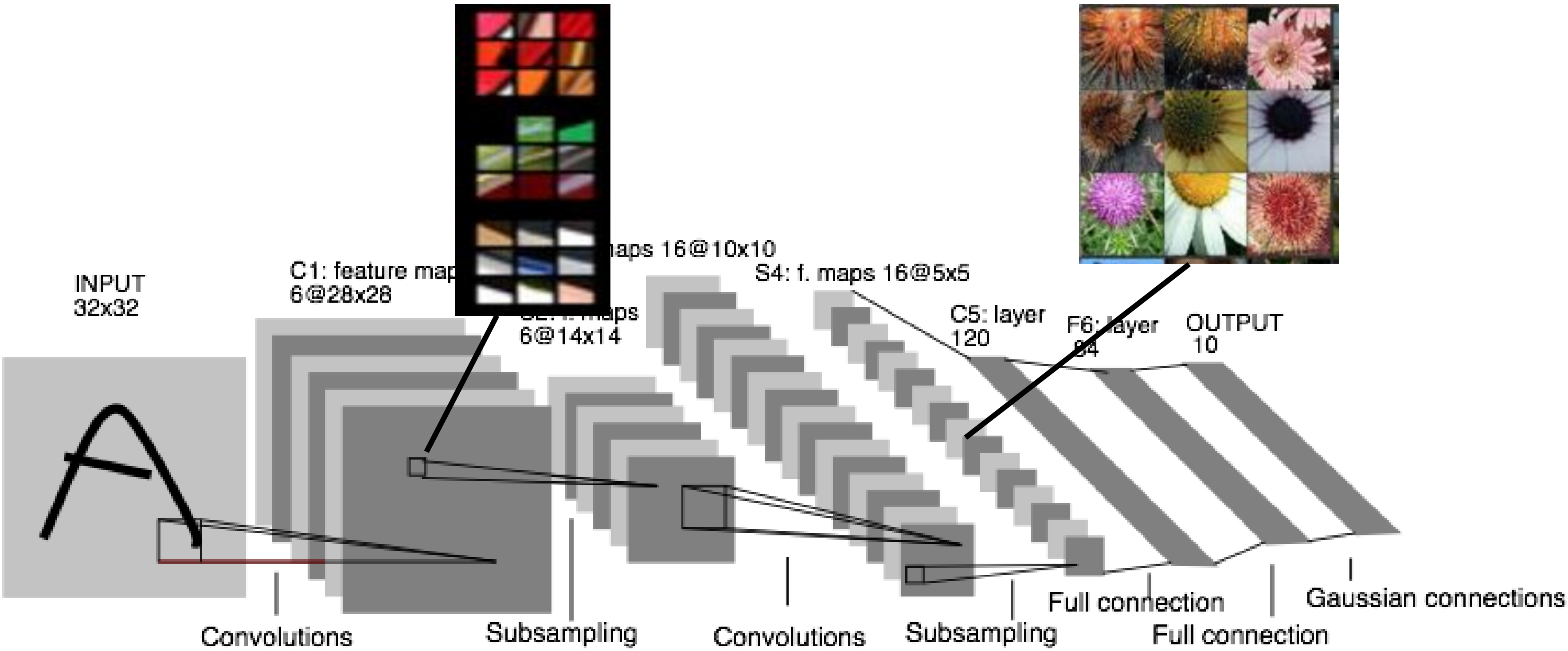
Fully Connected



Not ideal for representing images

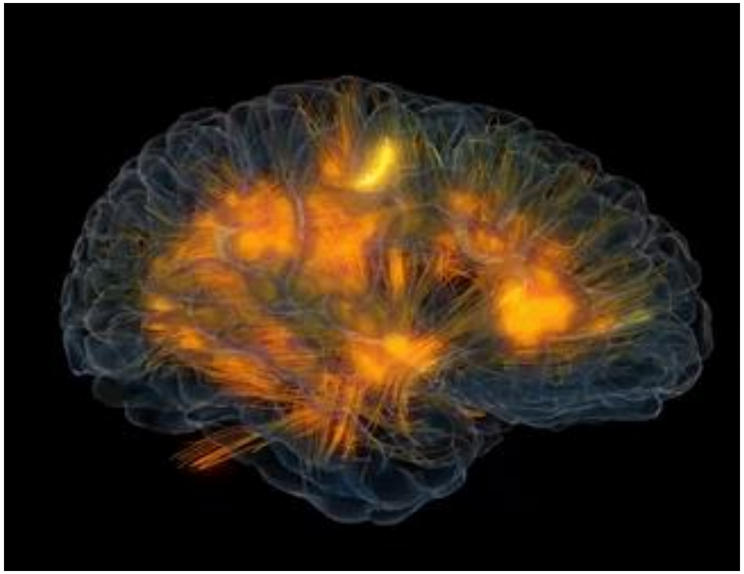
Convolutional Neural Network

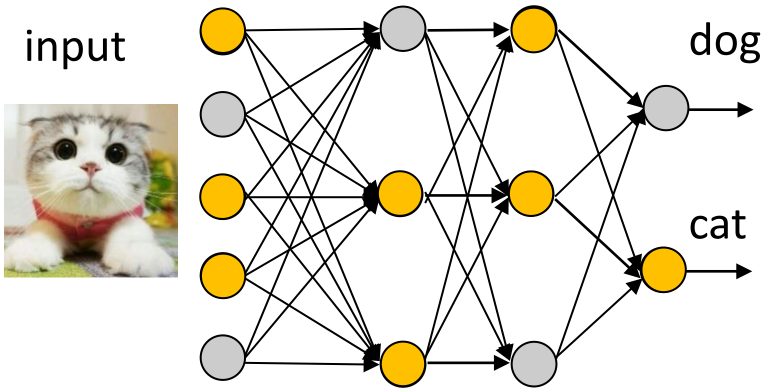
A better architecture for 2d signals



LeNet

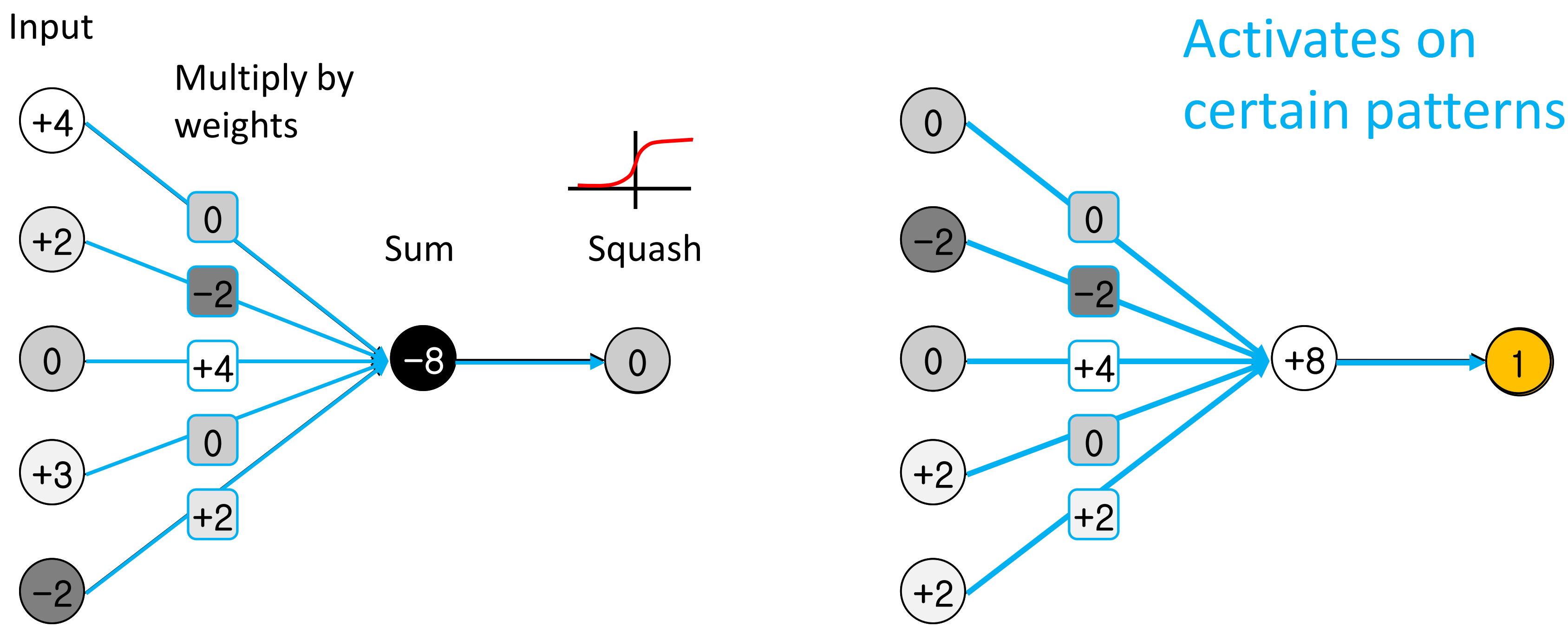
Artificial Neural Network





- **Artificial neural networks:** consist of many inter-connected neurons organized in layers
- **Neurons**: each neuron receives inputs from neurons in previous layer, passes its output to next layer
- **Activation**: neuron's output between 1 (excited) and 0 (not excited) *assuming a sigmoid non-linearity*

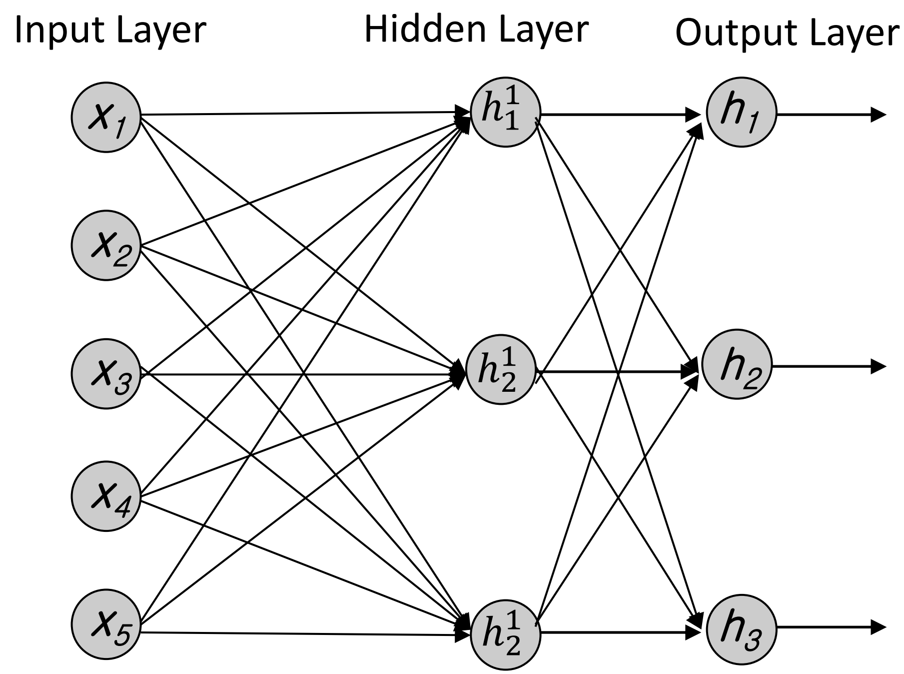
Artificial Neuron: Activation



Artificial Neural Network: notation

input $x = \begin{bmatrix} x_1 \\ \dots \\ x_5 \end{bmatrix}$

hidden layer activations



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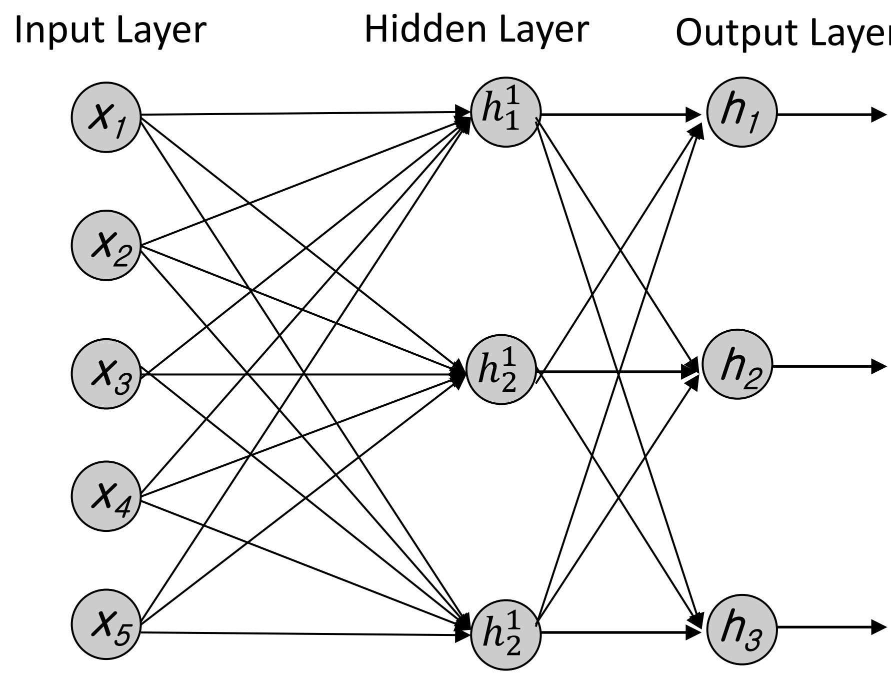
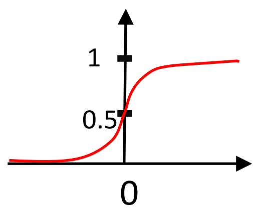


hidden layer activations

$$h^i = g(\Theta^{(i)}x)$$

$$g(z) = \frac{1}{1 + \exp(-z)}$$



output

$$h_\Theta(\mathrm{x}) = g(\Theta^{(2)}h^i)$$

weights $\Theta^{(1)} = \begin{pmatrix} \theta_{11} & \cdots & \theta_{15} \\ \vdots & \ddots & \vdots \\ \theta_{31} & \cdots & \theta_{35} \end{pmatrix}$ $\Theta^{(2)} = \begin{pmatrix} \theta_{11} & \cdots & \theta_{13} \\ \vdots & \ddots & \vdots \\ \theta_{31} & \cdots & \theta_{33} \end{pmatrix}$

Cost function

Neural network: $h_\Theta(x) \in \mathbb{R}^K \quad (h_\Theta(x))_i = i^{th} \text{ output}$

training error

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log(h_\Theta(x^{(i)}))_k + (1-y_k^{(i)}) \log(1-(h_\Theta(x^{(i)}))_k)\right]$$

$$+\frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}(\Theta_{ji}^{(l)})^2$$

regularization

Gradient computation

$$J(\Theta) = -\frac{1}{m}\left[\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)} \log h_\theta(x^{(i)})_k + (1 - y_k^{(i)}) \log(1 - h_\theta(x^{(i)})_k)\right]$$
$$+\frac{\lambda}{2m}\sum_{l=1}^{L-1}\sum_{i=1}^{s_l}\sum_{j=1}^{s_{l+1}}(\Theta_{ji}^{(l)})^2$$

$$\min_{\Theta} J(\Theta)$$

Need code to compute:

- $J(\Theta)$
- $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$

Use "***Backpropagation algorithm***"

- Efficient way to compute $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$
- Computes gradient incrementally by "propagating" backwards through the network

Neural Networks II

Backpropagation

Chain Rule

- Need to compute gradient of

$$\log(h_\Theta(\mathrm{x})) = \log(g(\Theta^{(2)} g(\Theta^{(1)} x))) \quad \text{w.r.t } \Theta$$

- How can we compute the gradient of several chained functions?

$$f(\theta) = f_1(f_2(\theta)) \qquad f'(\theta) = f_1'(f_2(\theta)) * f_2{}'(\theta)$$

$$f'(\theta) = \frac{\partial f}{\partial \theta} = \frac{\partial f_1}{\partial f_2} \frac{\partial f_2}{\partial \theta}$$

- What about functions of multiple variables?

$$f(\theta_1, \theta_2) = f_1(f_2(\theta_1, \theta_2)) \qquad \frac{\partial f}{\partial \theta_1} = \qquad \frac{\partial f}{\partial \theta_2} =$$

https://www.khanacademy.org/math/multivariable-calculus/multivariable-derivatives/multivariable-chain-rule/v/multivariable-chain-rule

Backpropagation: Efficient Chain Rule

- Partial gradient computation via chain rule:

$$\frac{\partial f}{\partial \theta_1} = \frac{\partial f_1}{\partial f_2}(f_2(f_3(\theta))) * \frac{\partial f_2}{\partial f_3}(f_3(\theta)) * \frac{\partial f_3}{\partial \theta_1}(\theta)$$

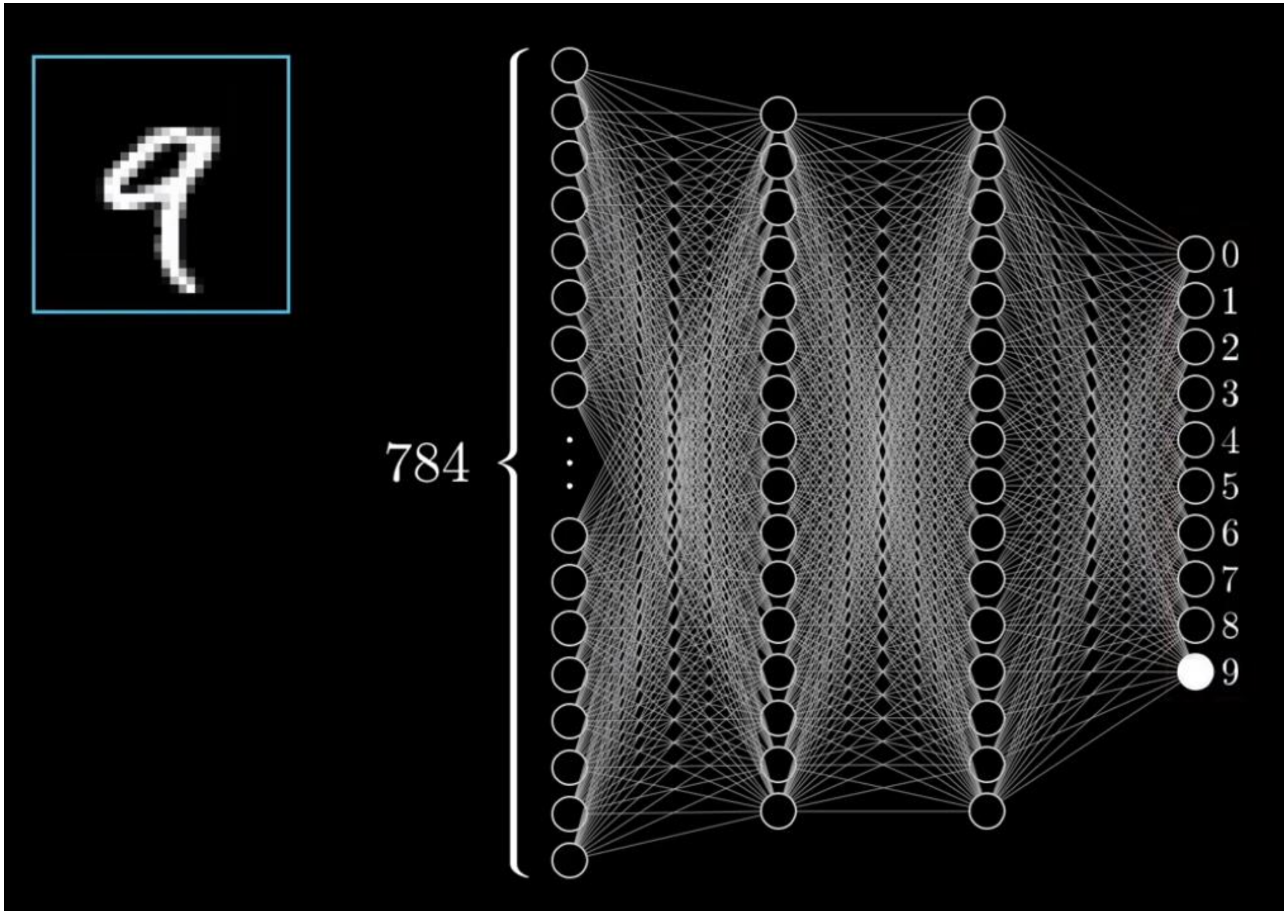
$$\frac{\partial f}{\partial \theta_2} = \frac{\partial f_1}{\partial f_2}(f_2(f_3(\theta))) * \frac{\partial f_2}{\partial f_3}(f_3(\theta)) * \frac{\partial f_3}{\partial \theta_2}(\theta)$$

$$\frac{\partial f}{\partial \theta_3} = \frac{\partial f_1}{\partial f_2}(f_2(f_3(\theta))) * \frac{\partial f_2}{\partial f_3}(f_3(\theta)) * \frac{\partial f_3}{\partial \theta_3}(\theta)$$

- need to re-evaluate functions many times
- Very inefficient! E.g. 100,000-dim parameters

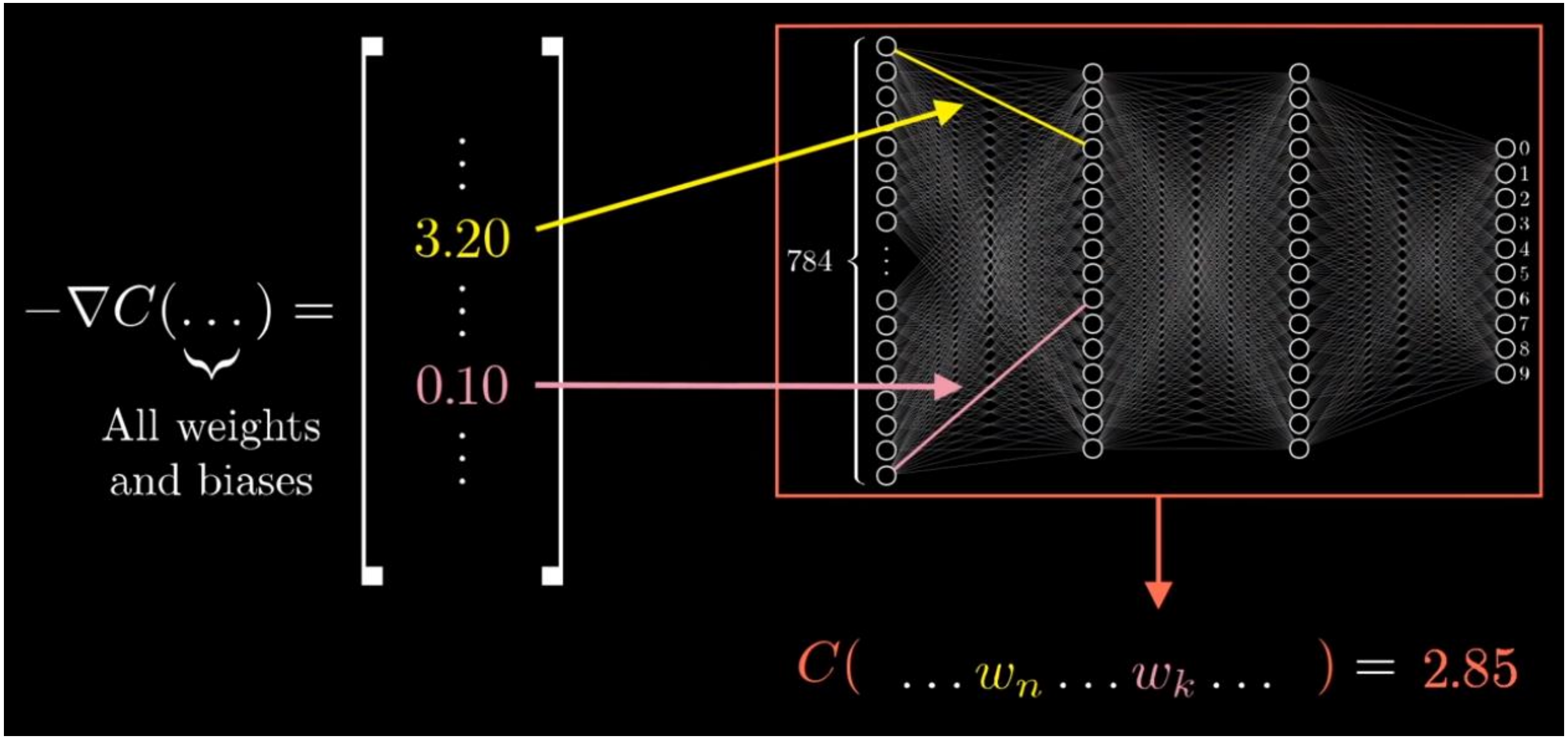
Example: Classification

- A deep network is a massive composite function!



BLUE1BROWN SERIES

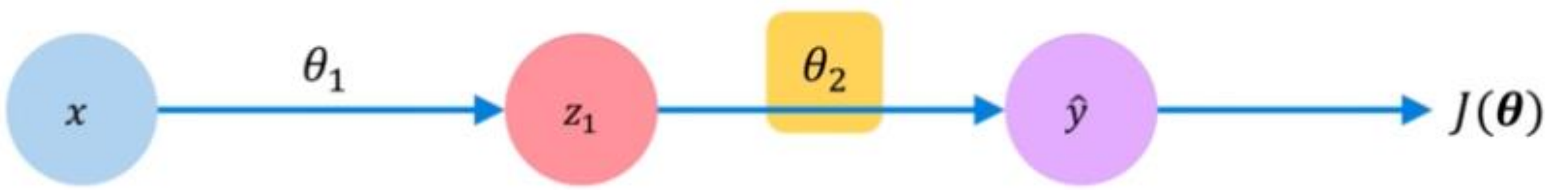
Interpretation of Computed Gradients



- The cost function is 32 times more sensitive to changes in the yellow weight *vs.* the pink weight.

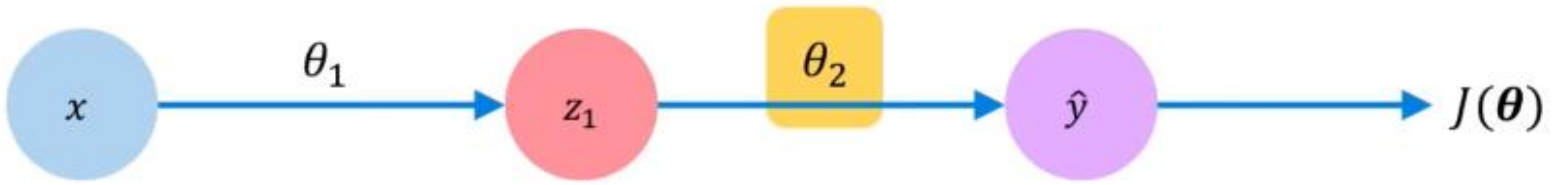
BLUE1BROWN SERIES

Computing Gradients: Backpropagation



How does a small change in one weight (ex. $\boldsymbol{\theta_2}$*) affect the final loss* $\boldsymbol{J(\theta)}$*?*

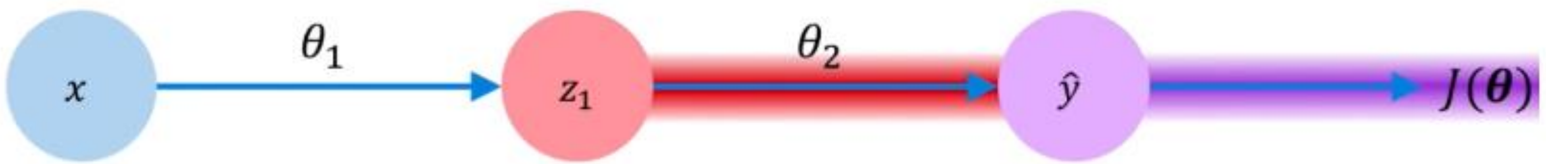
Computing Gradients: Backpropagation



$$\frac{\partial J(\boldsymbol{\theta})}{\partial \theta_2} =$$

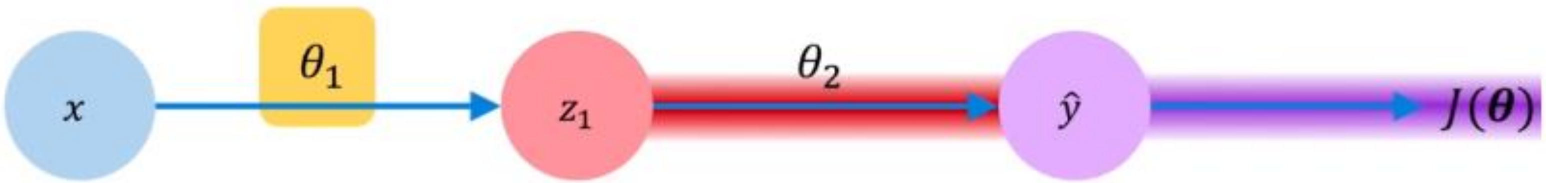
Let's use the chain rule!

Computing Gradients: Backpropagation



$$\frac{\partial J(\boldsymbol{\theta})}{\partial \theta_2} = \frac{\partial J(\boldsymbol{\theta})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial \theta_2}$$

Computing Gradients: Backpropagation

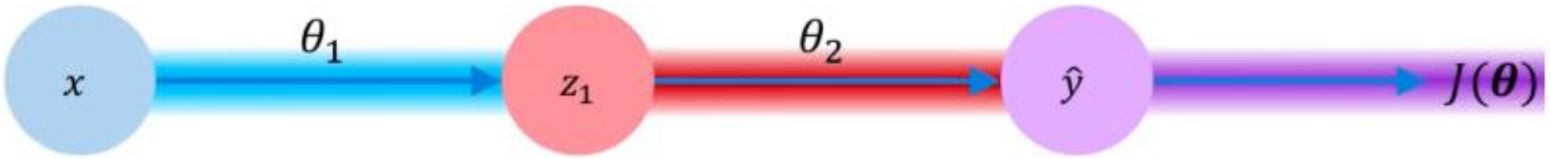


$$\frac{\partial J(\boldsymbol{\theta})}{\partial \theta_1} = \frac{\partial J(\boldsymbol{\theta})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial \theta_1}$$

Apply chain rule!

Apply chain rule!

Computing Gradients: Backpropagation



$$\frac{\partial J(\boldsymbol{\theta})}{\partial \theta_1} = \frac{\partial J(\boldsymbol{\theta})}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial z_1} * \frac{\partial z_1}{\partial \theta_1}$$

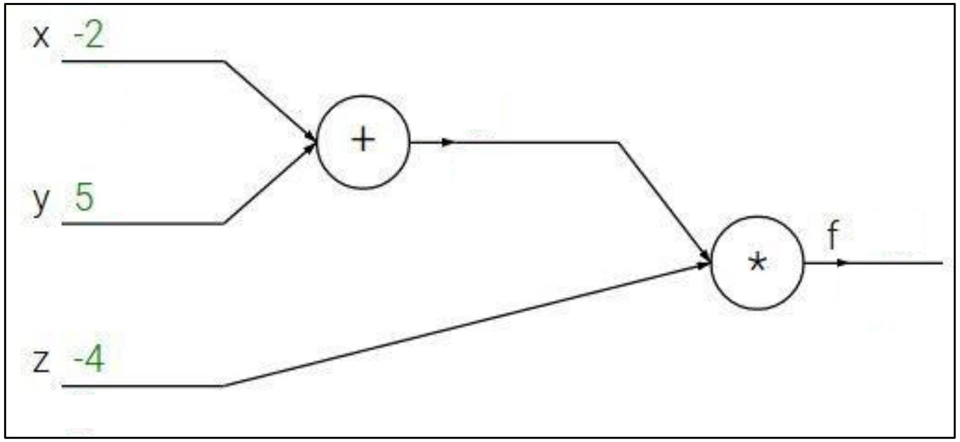
Neural Networks II

Analytical Gradients with Computational Graphs

Chain Rule with a Computational Graph

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

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



Chain Rule with a Computational Graph

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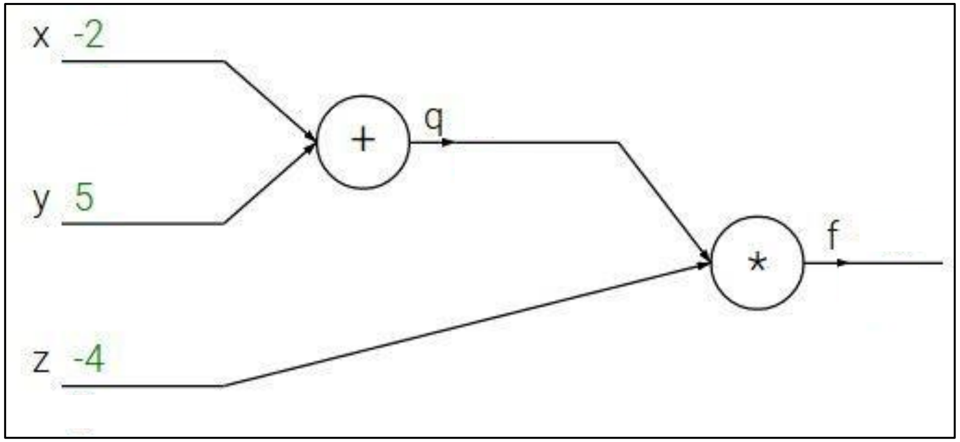

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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

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

Computation Graph: Forward

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

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

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

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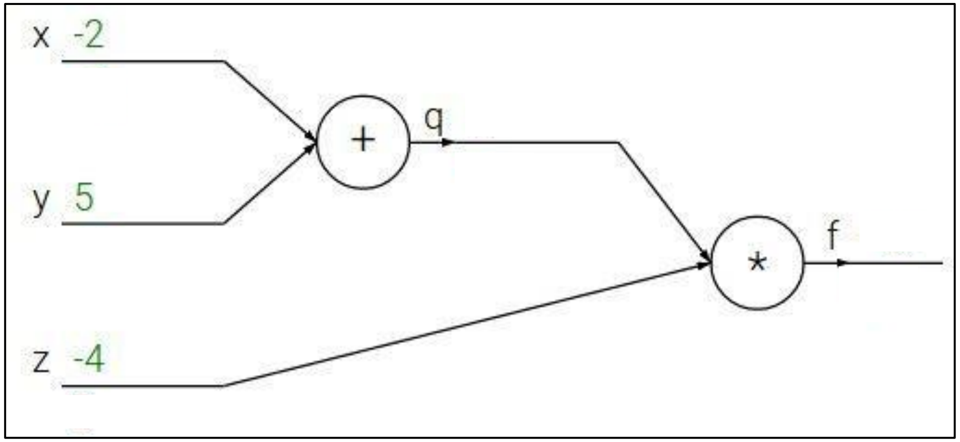
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



compute values

Computation Graph: Backward

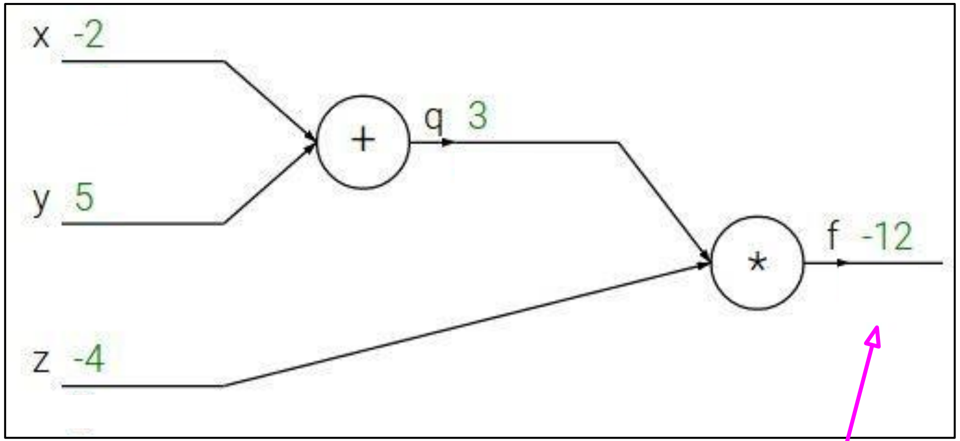
$$f(x,y,z) = (x+y)z$$

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

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

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

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



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

compute gradients

Computation Graph: Backward

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

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

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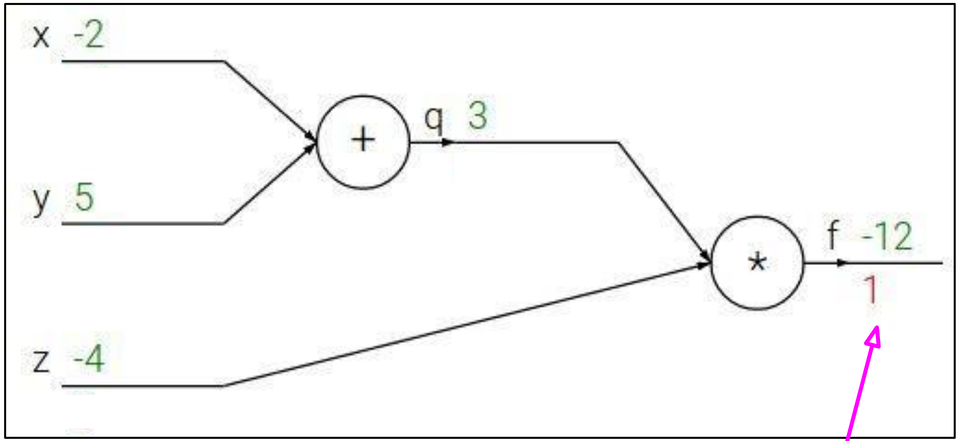

$$\frac{\partial f}{\partial f}$$

Computation Graph: Backward

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

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

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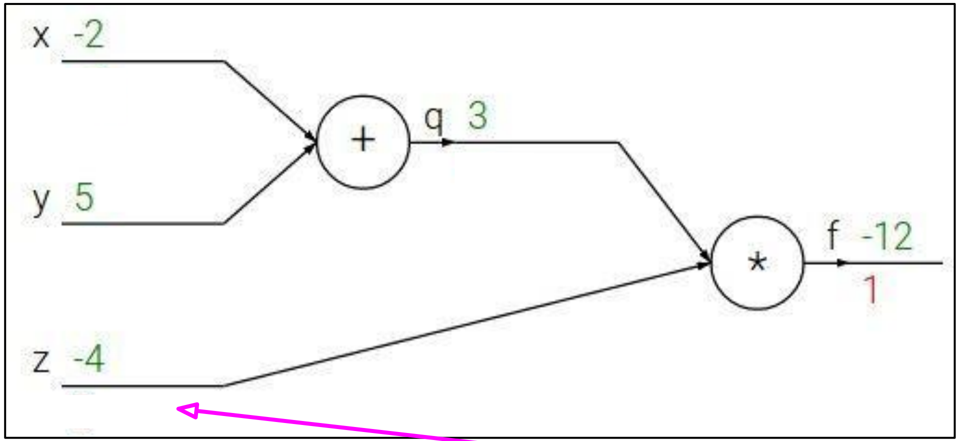
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

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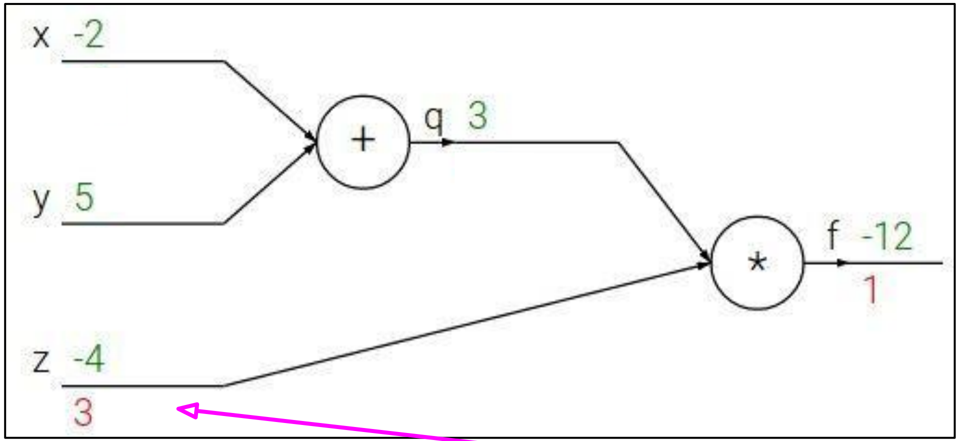

$$\frac{\partial f}{\partial z}$$

Computation Graph: Backward

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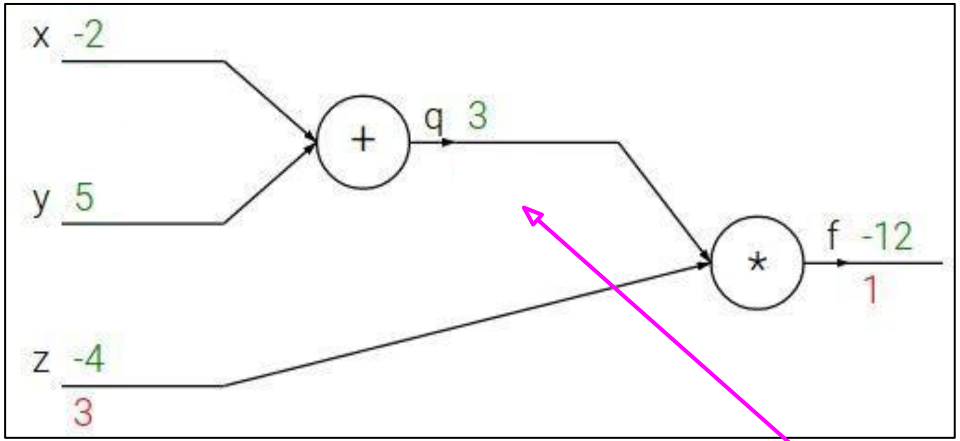
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

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

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

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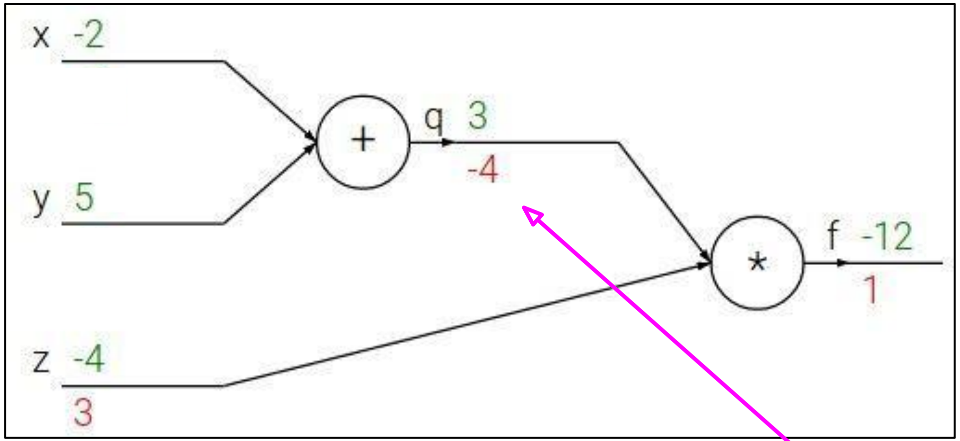

$$\frac{\partial f}{\partial q}$$

Computation Graph: Backward

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

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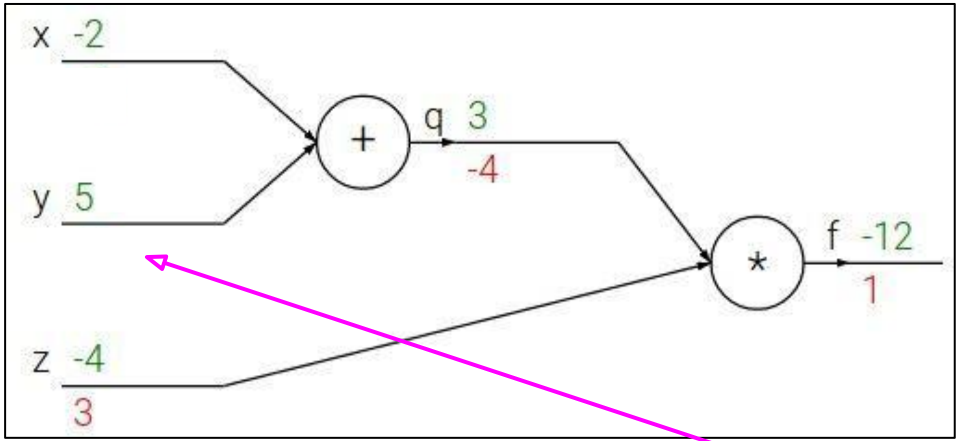
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

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

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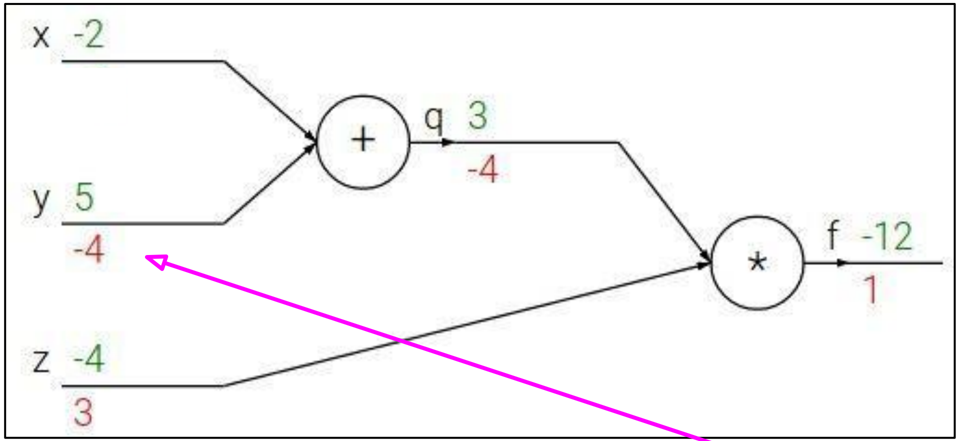
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Chain rule:

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

Computation Graph: Backward

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

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

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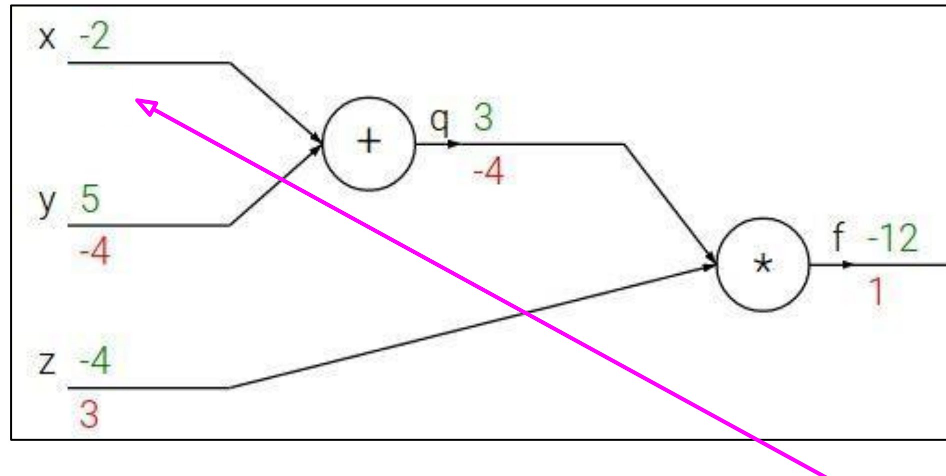

$$\boxed{\frac{\partial f}{\partial x}}$$

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

Computation Graph: Backward

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

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

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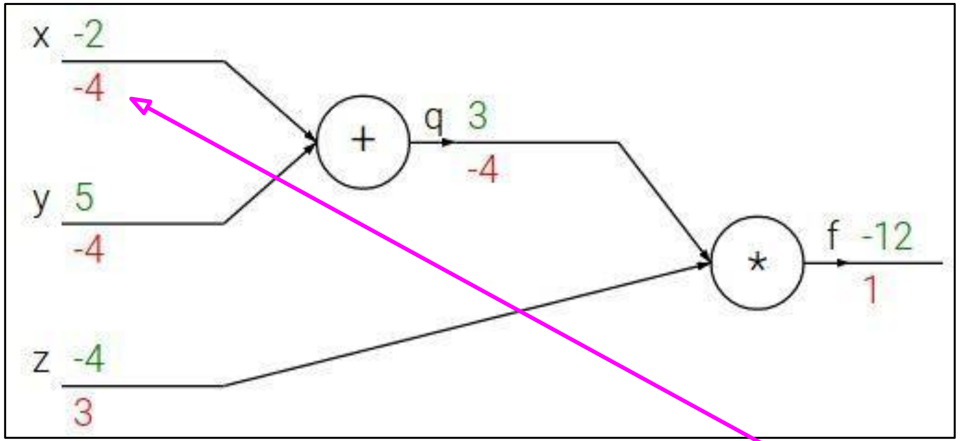
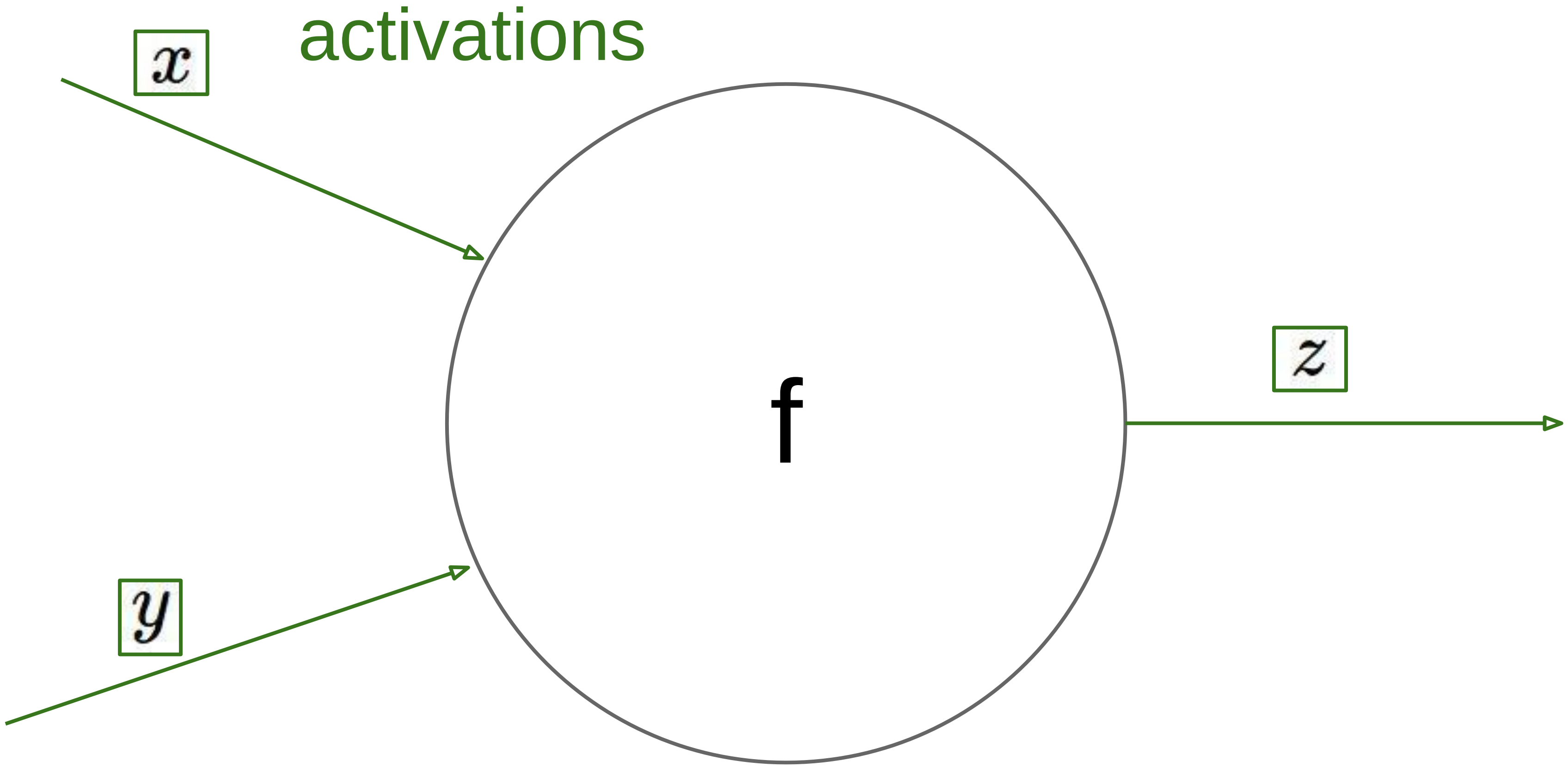
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

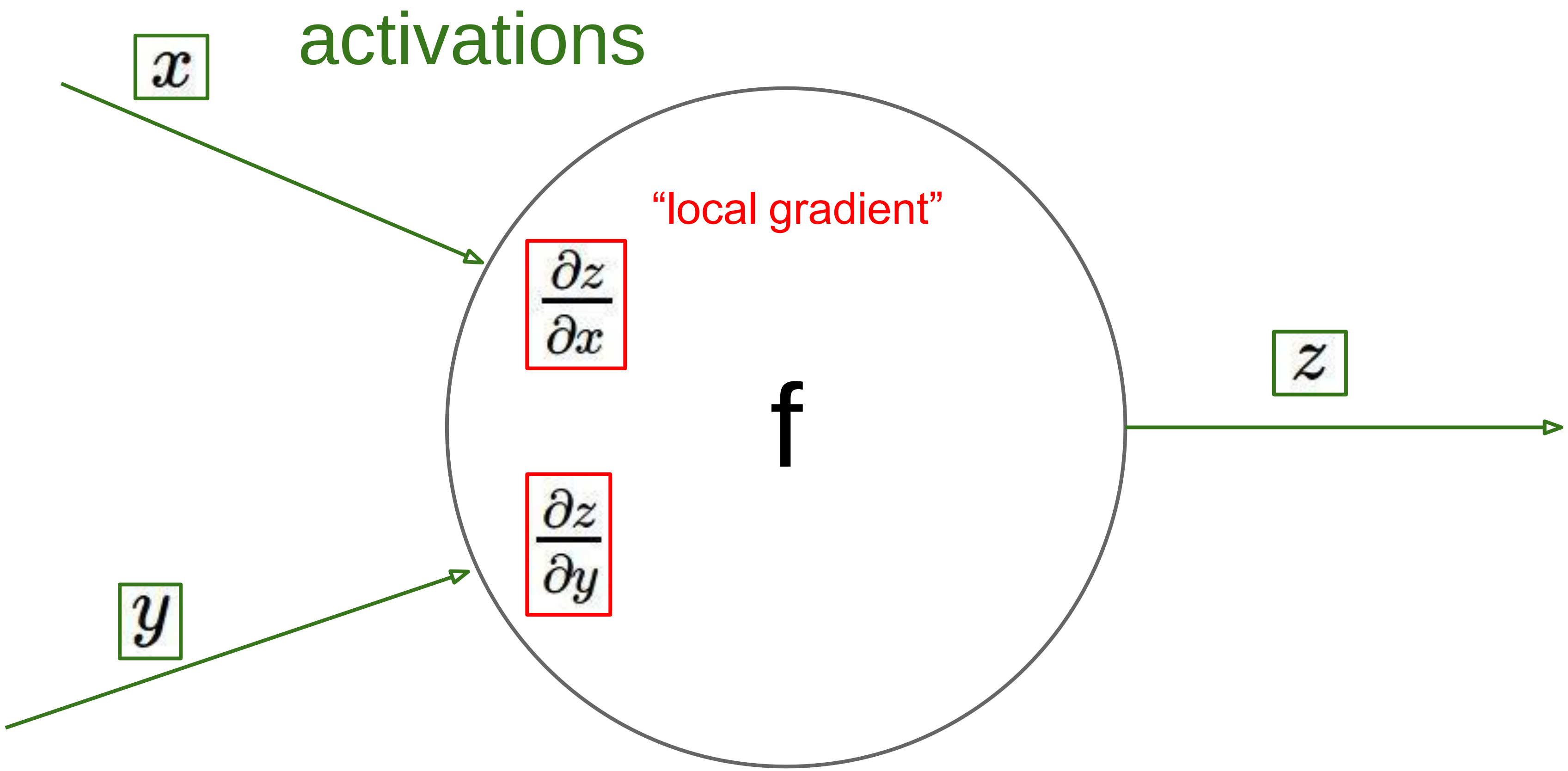


$$\frac{\partial f}{\partial x}$$

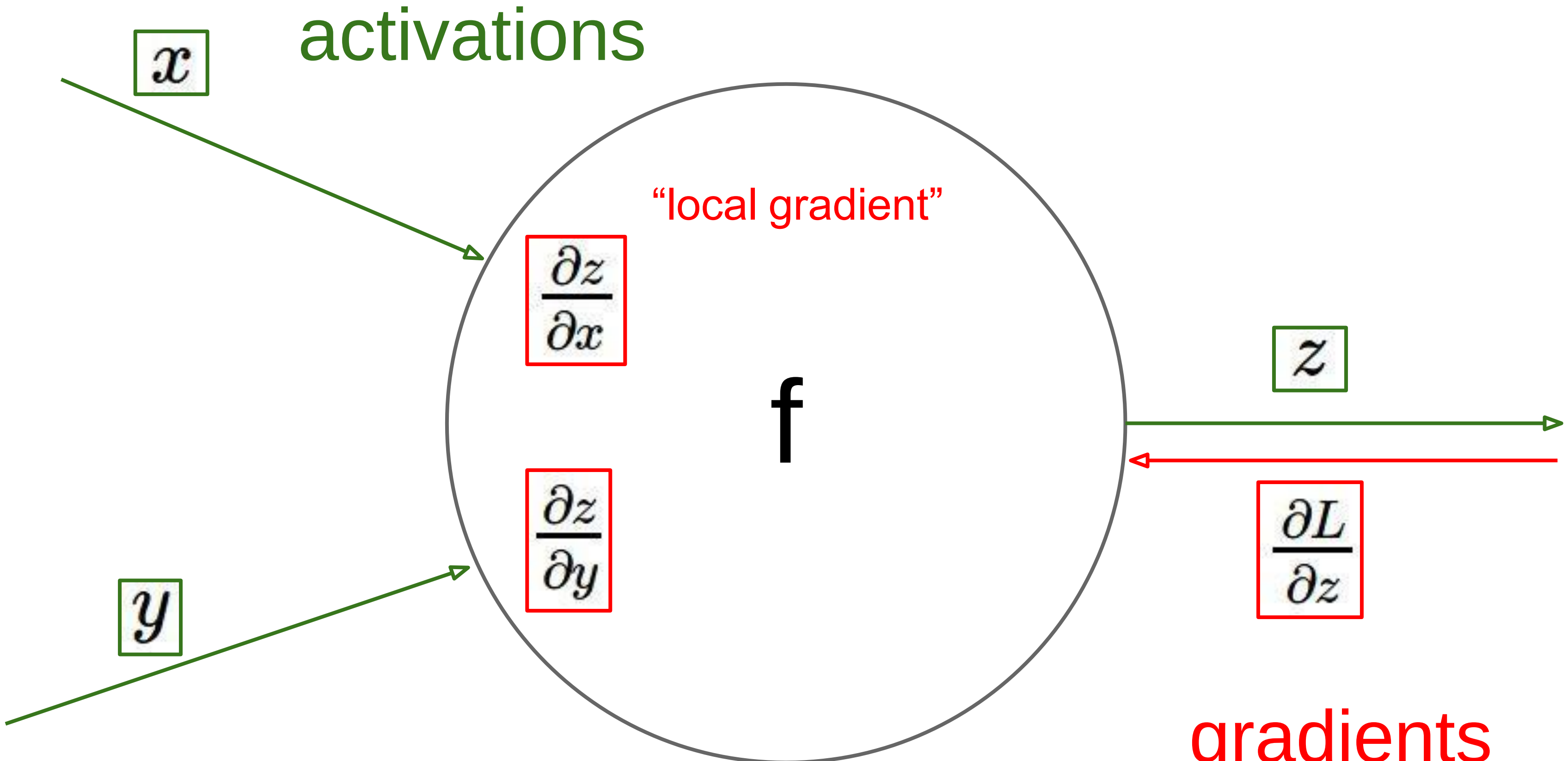
Chain rule:

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

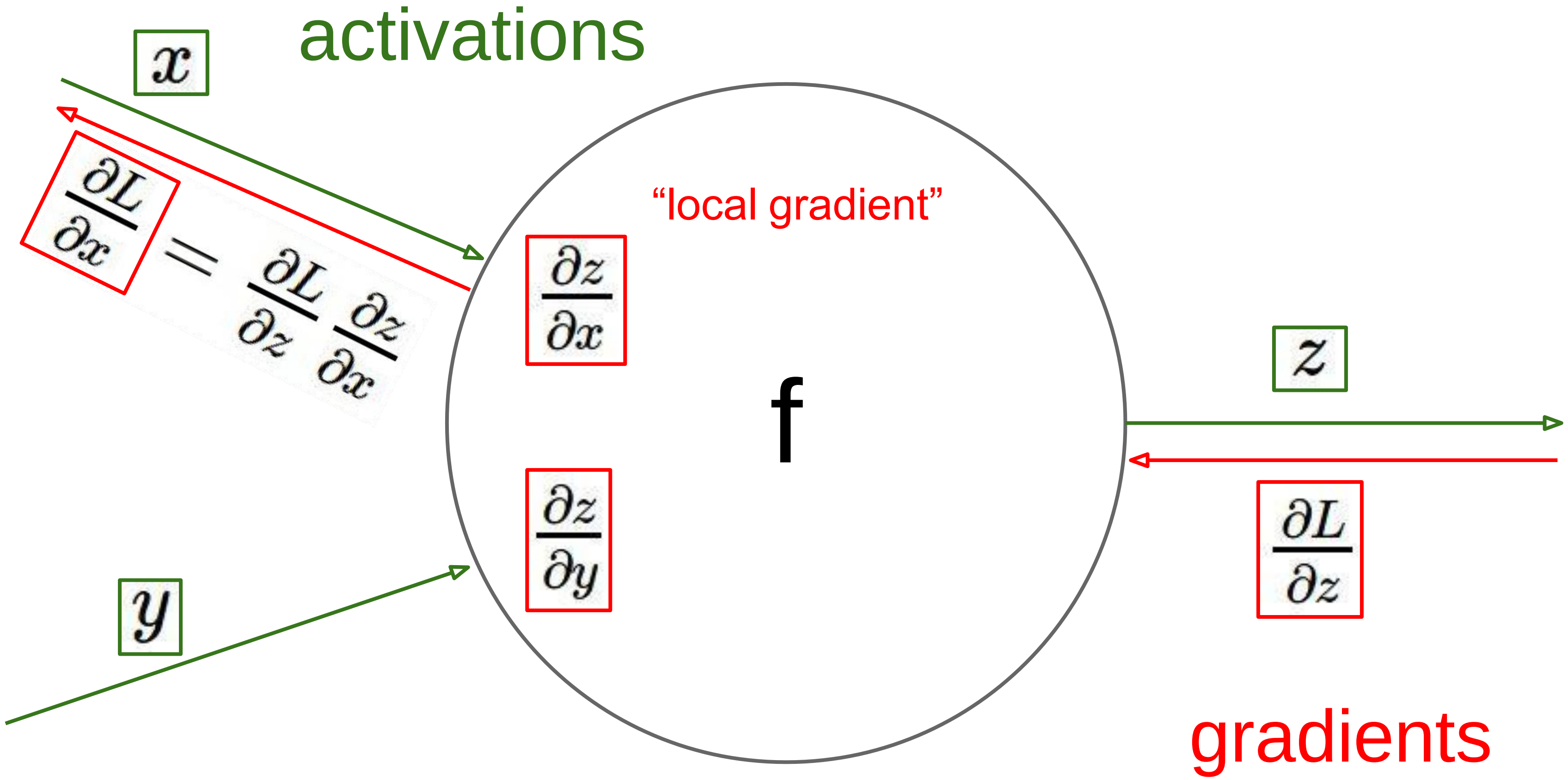

activations
x
y
z
f



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



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


activations
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$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
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z
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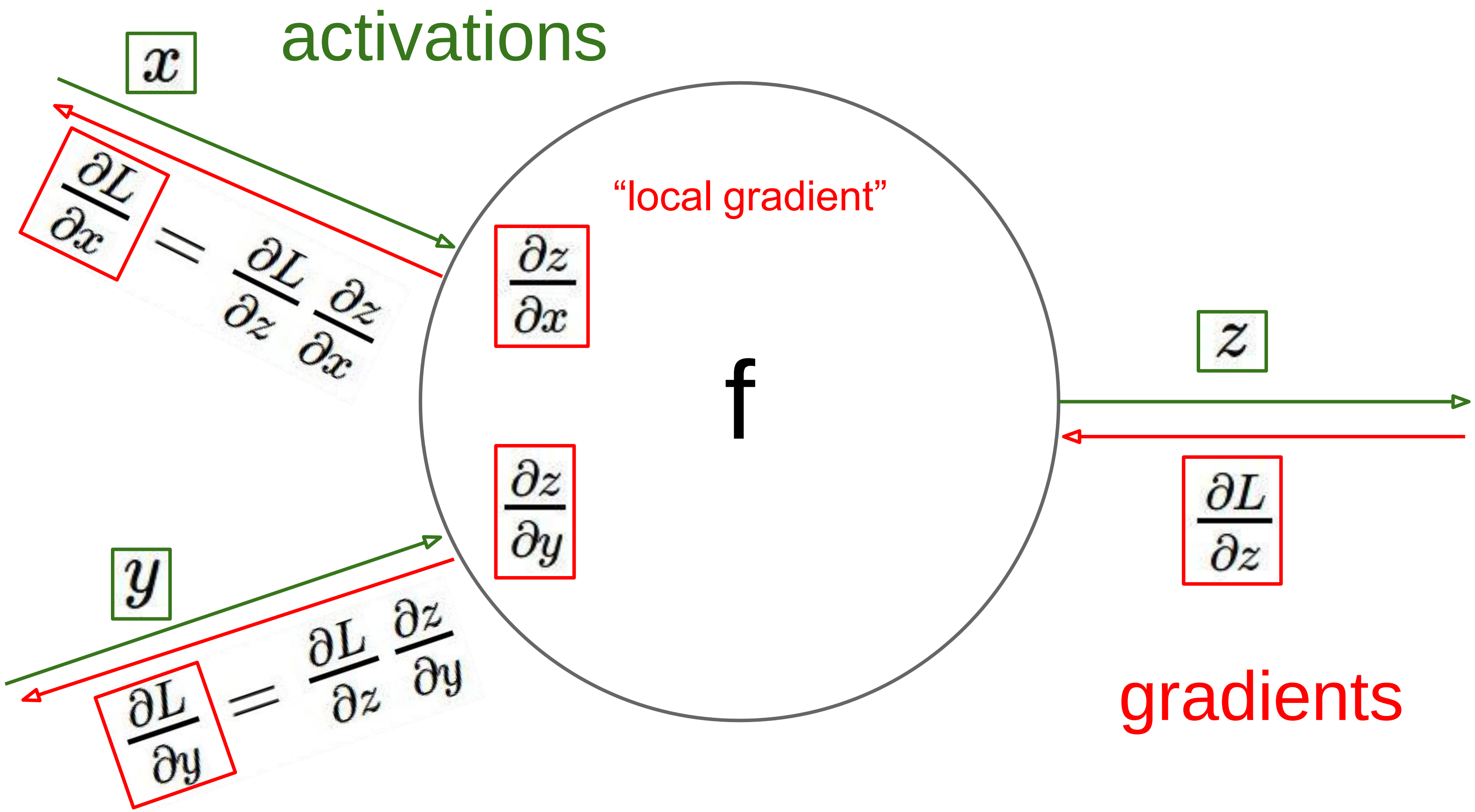
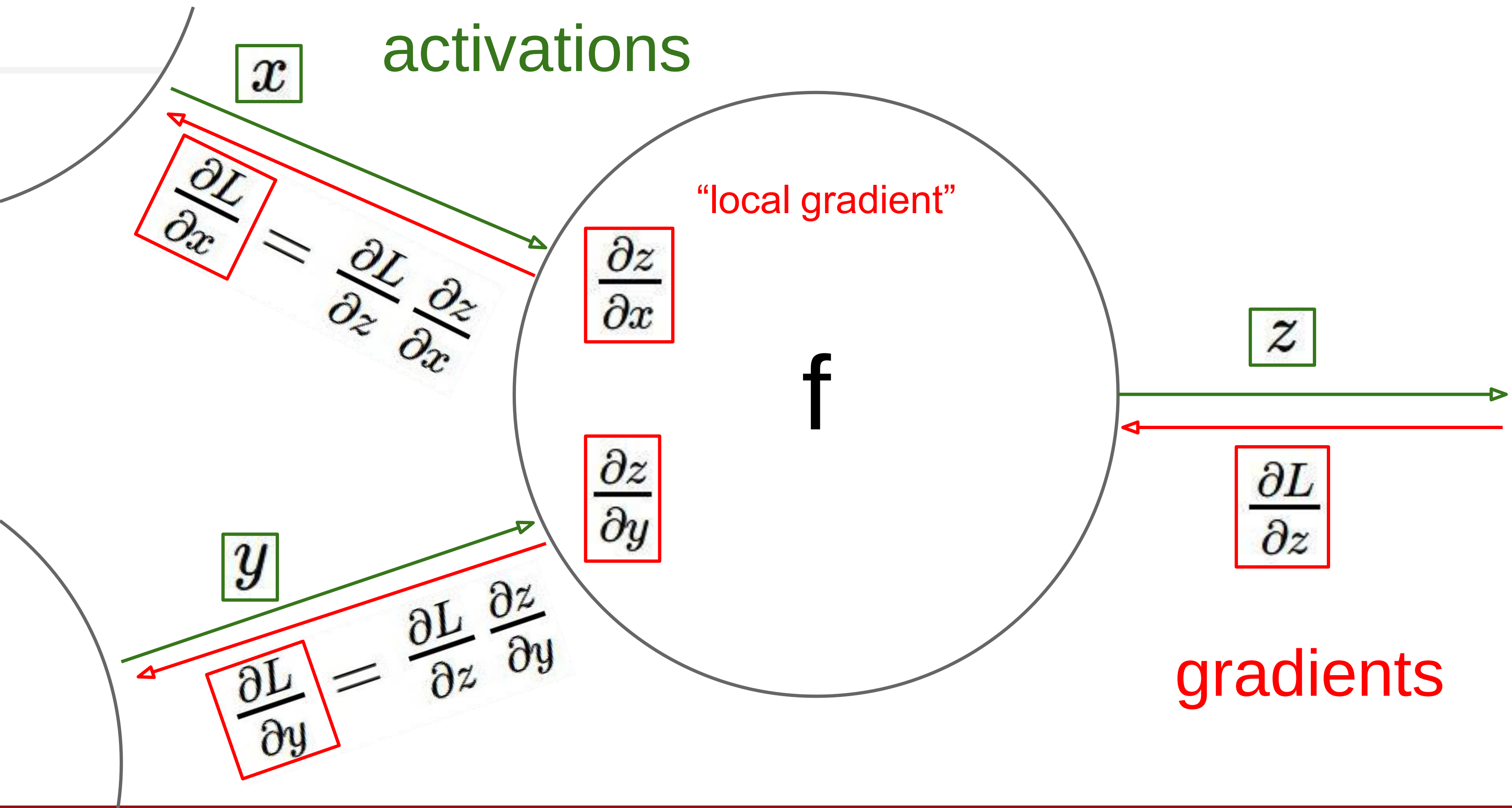
y
gradients



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
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients



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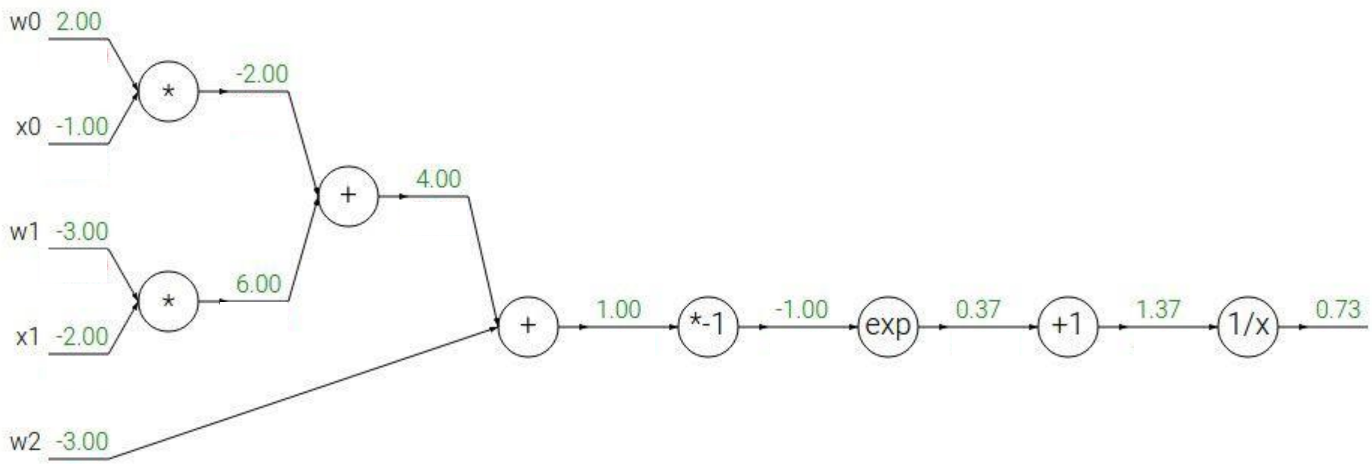
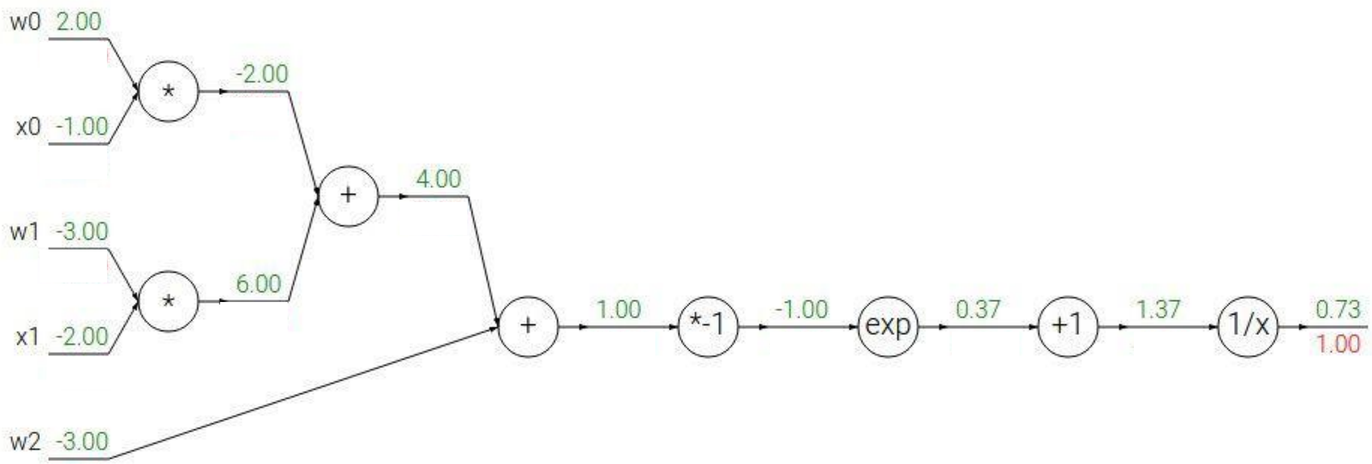
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients

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



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

Computing a 2D Sigmoid Neuron!



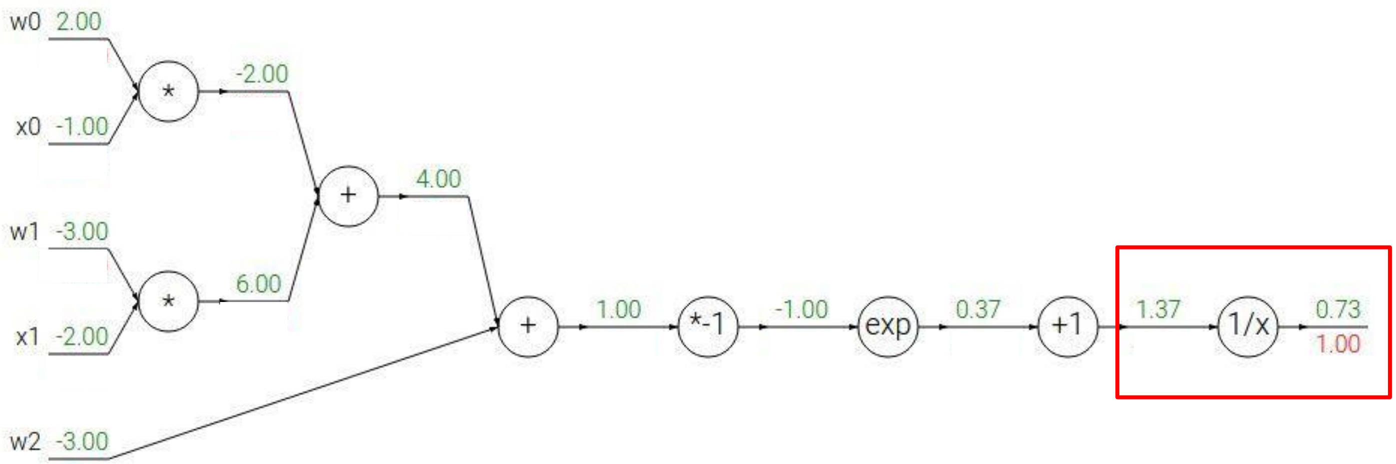
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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



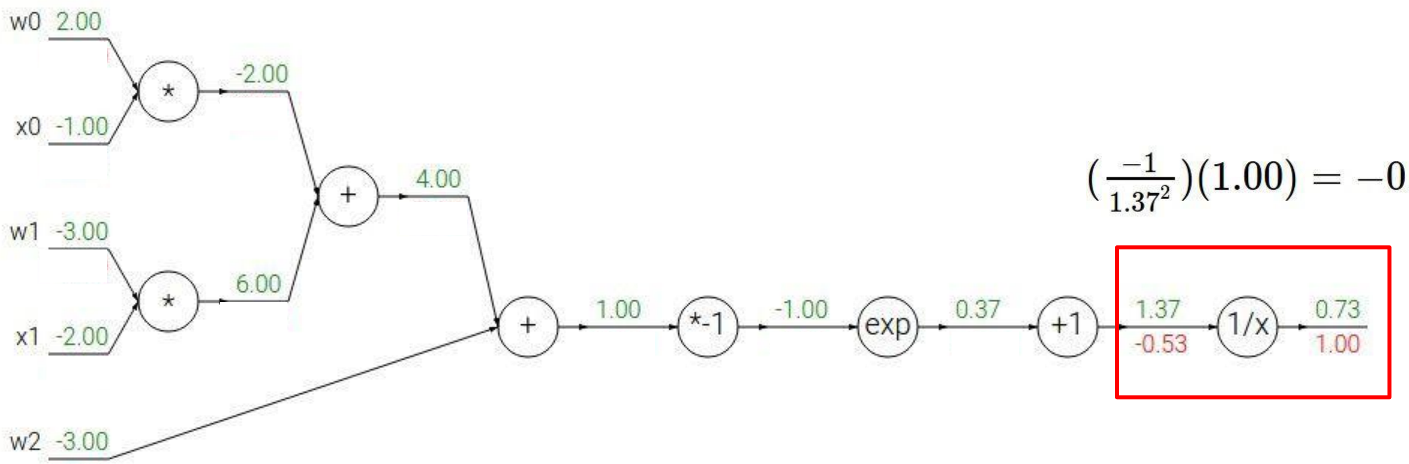
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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



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

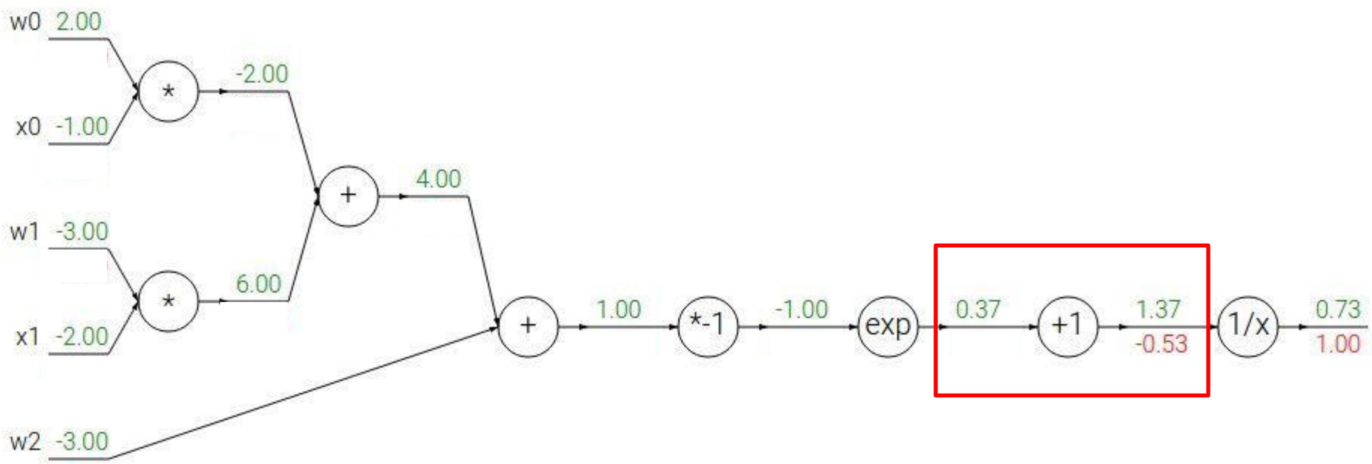
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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



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

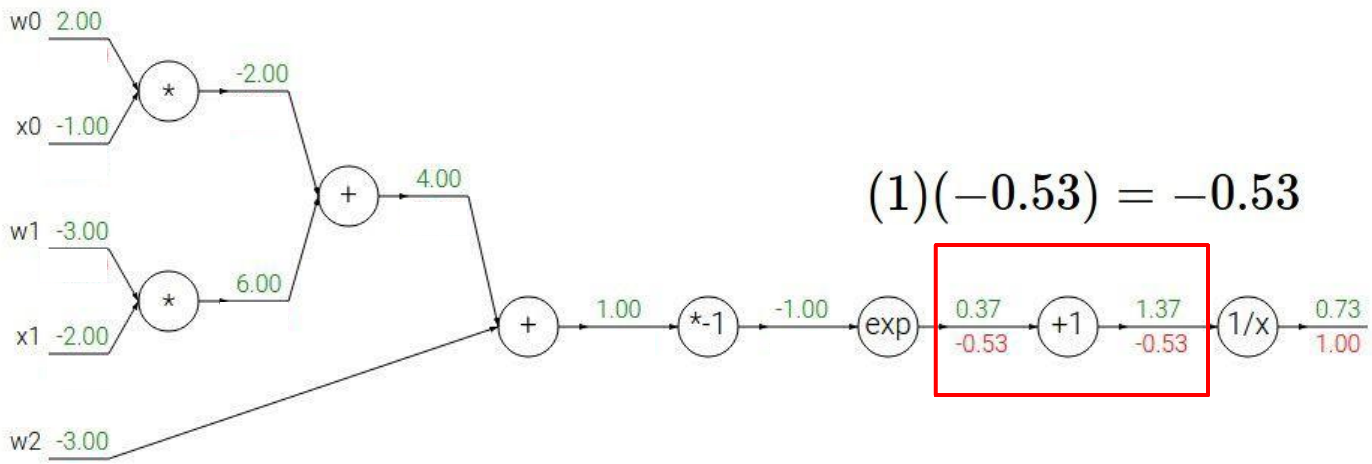
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

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

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

Another example:

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



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

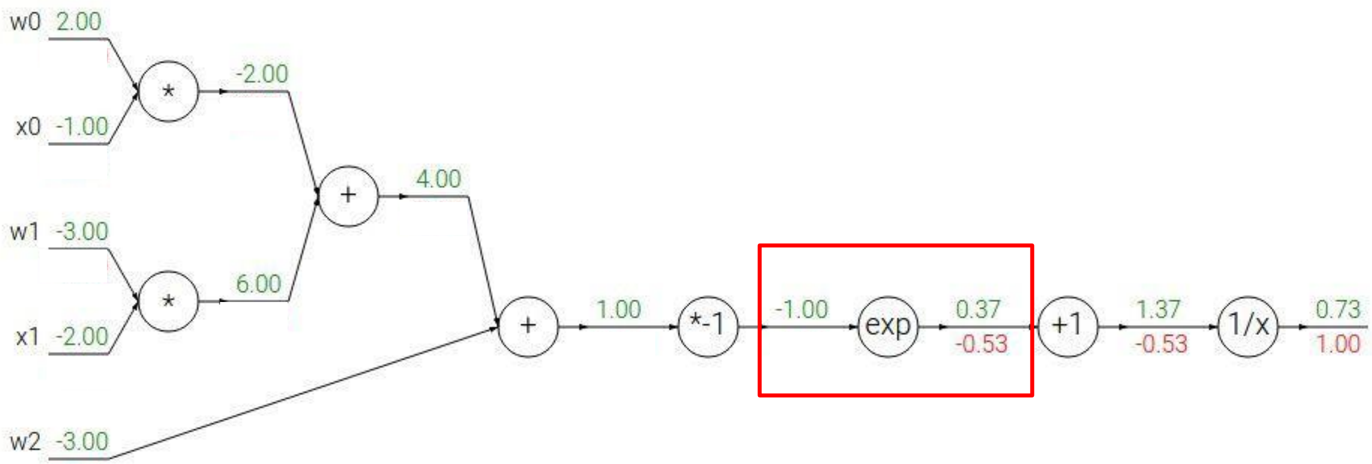
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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



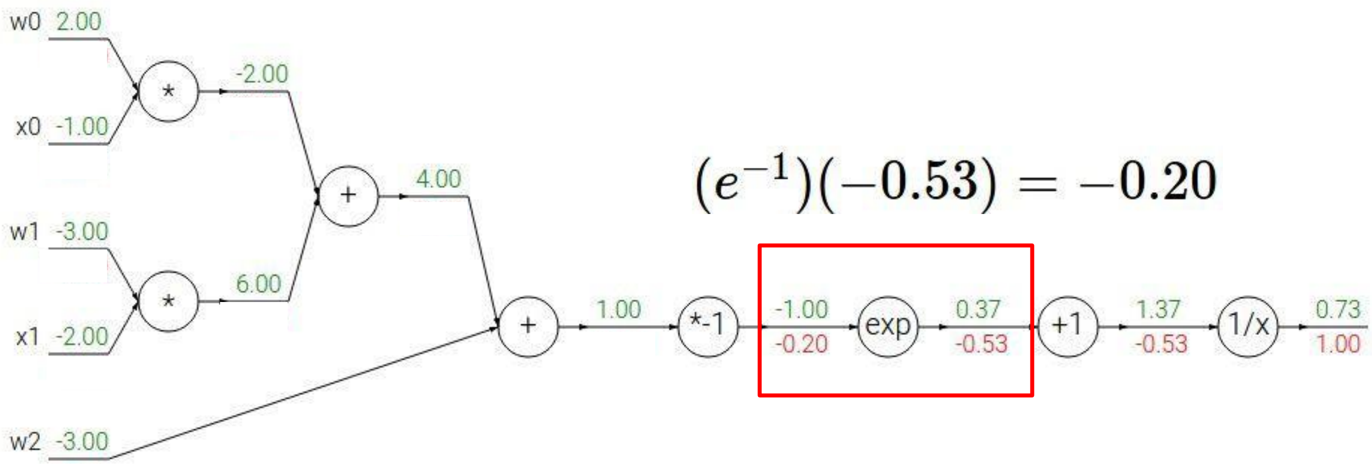
$$\boxed{f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x}$$

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

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

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

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



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

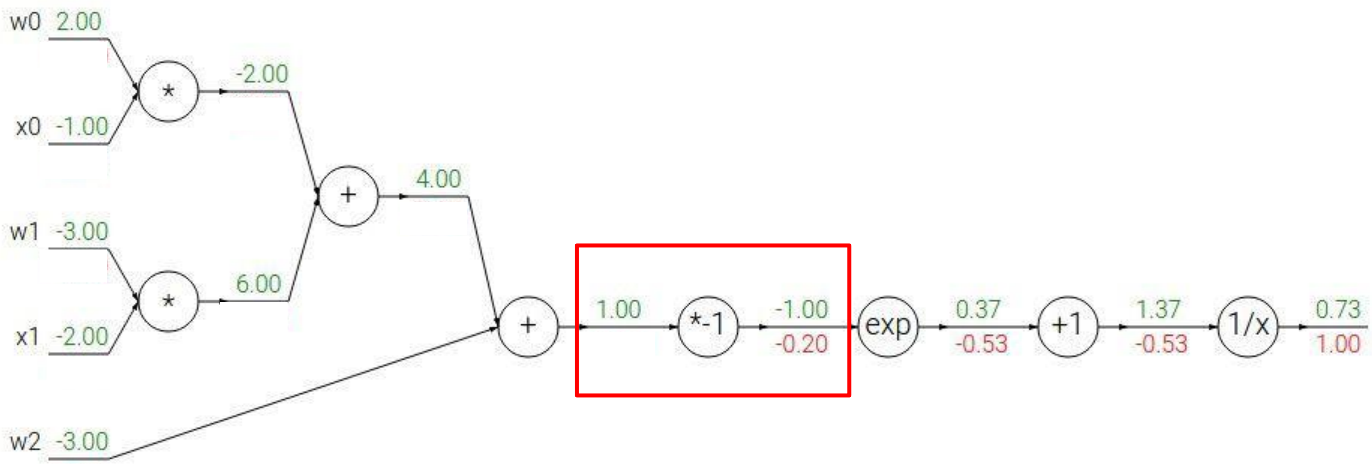
$$\boxed{f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x}$$

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

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

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

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



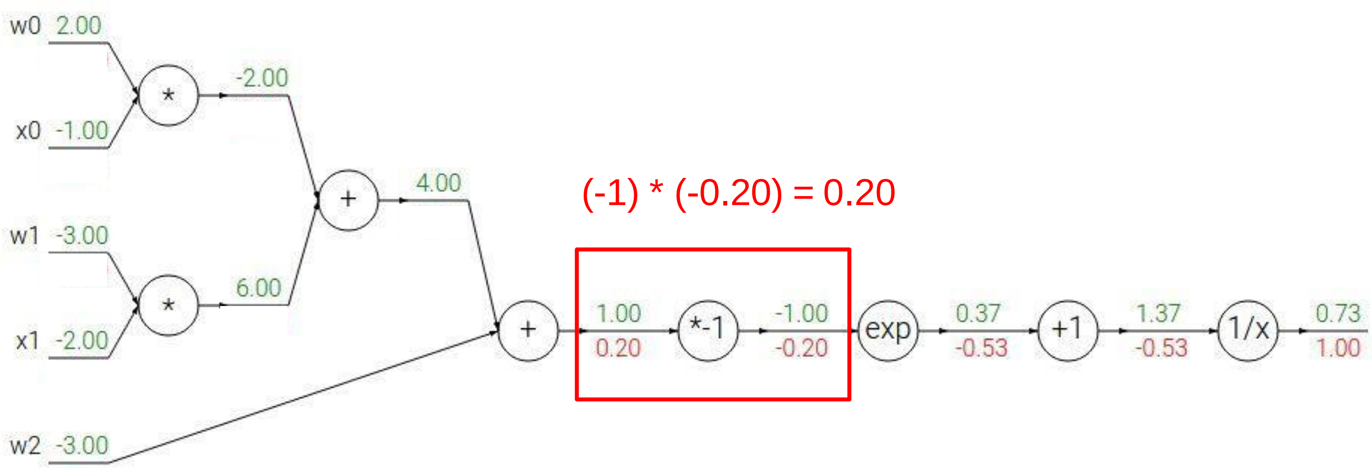
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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



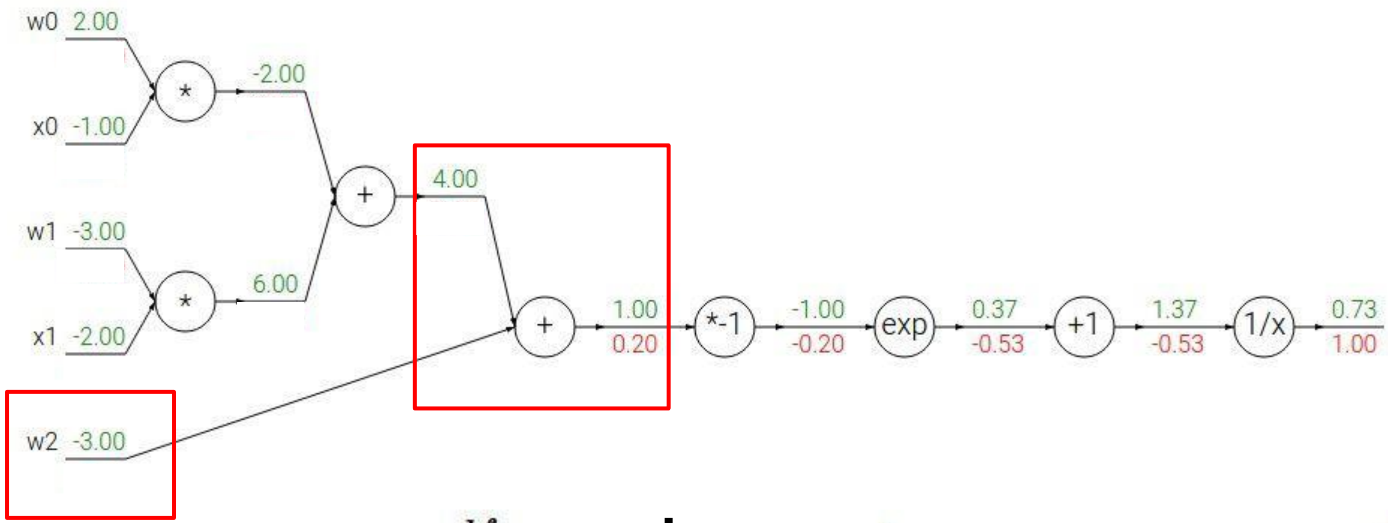
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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



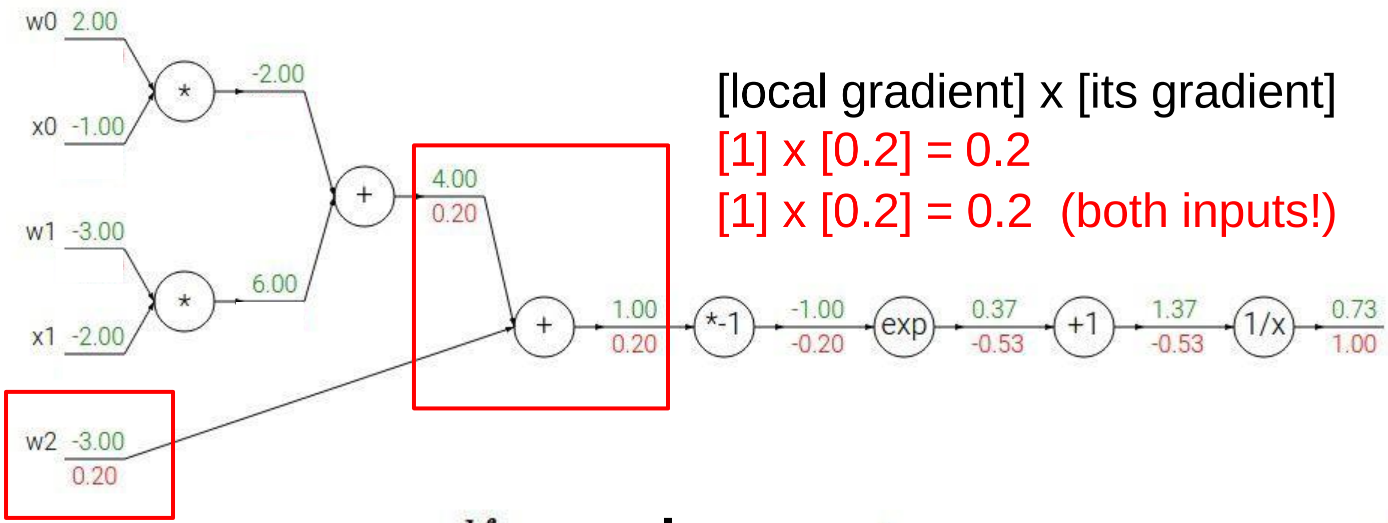
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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

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



[local gradient] x [its gradient]

[1] x [0.2] = 0.2

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

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

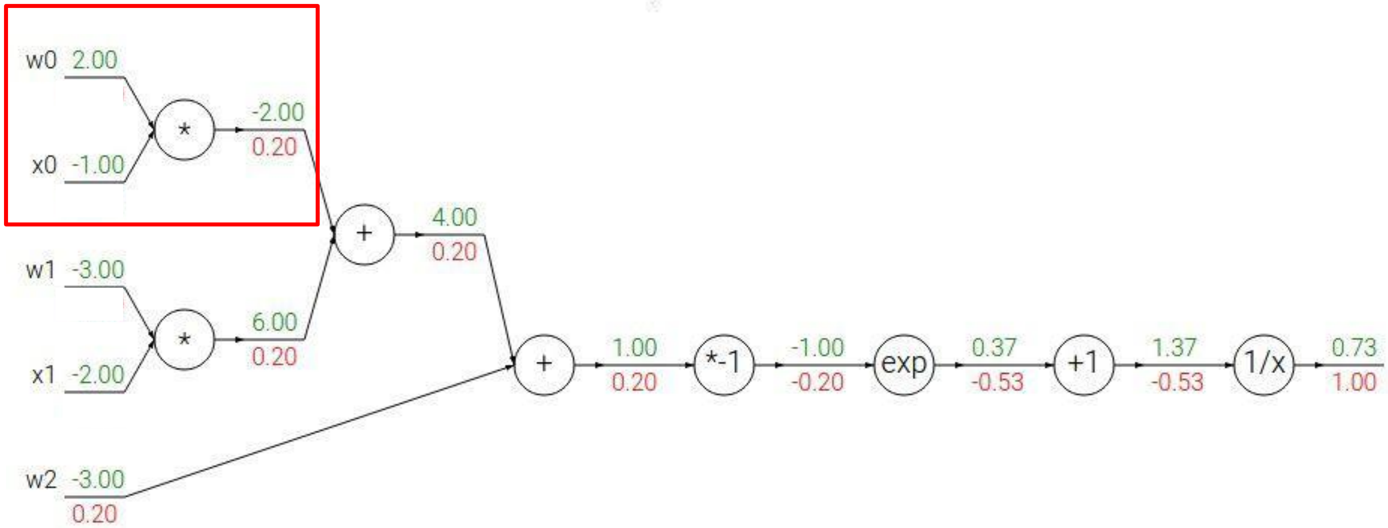
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

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

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

Another example:

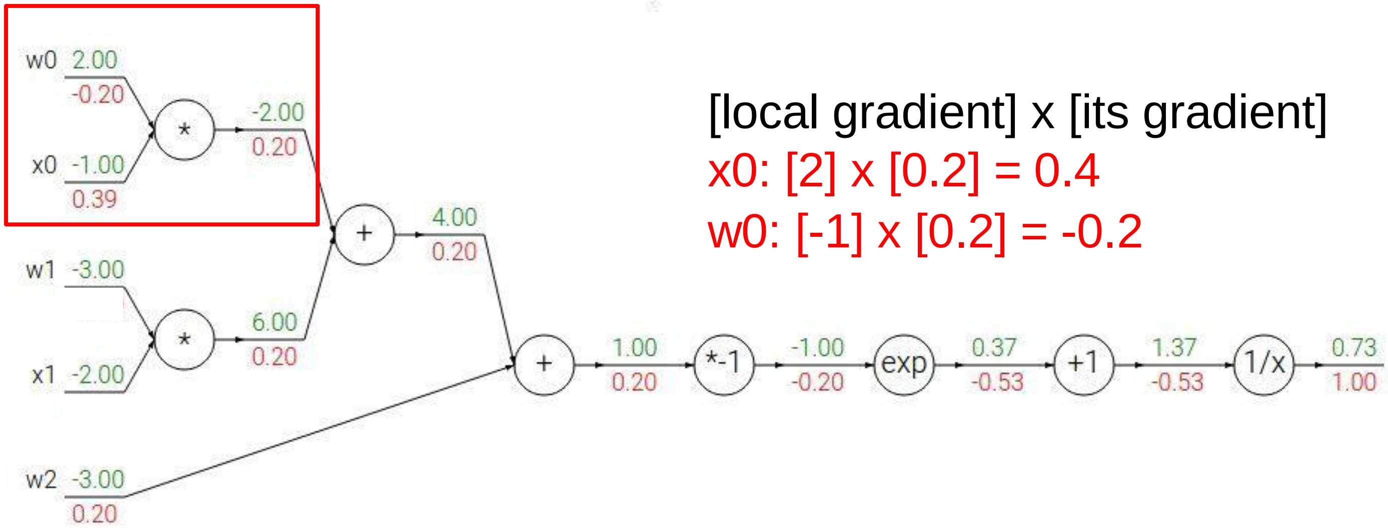
$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



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

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

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



[local gradient] x [its gradient]

x0: [2] x [0.2] = 0.4

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

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

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

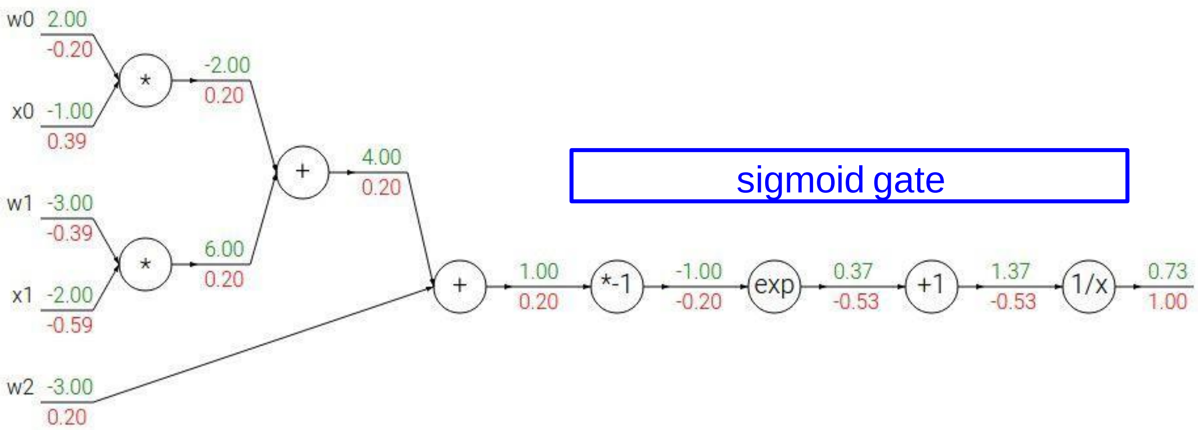
$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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

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

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

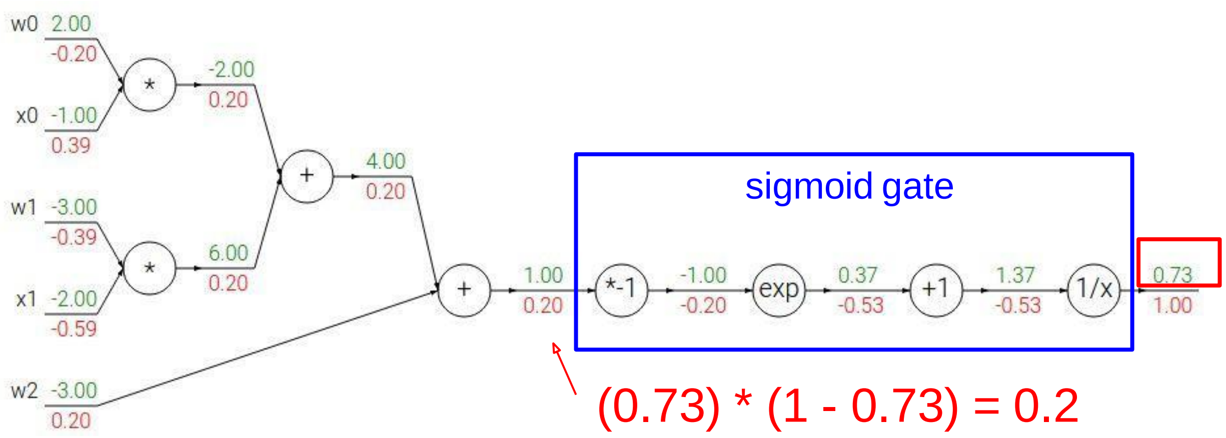
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



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

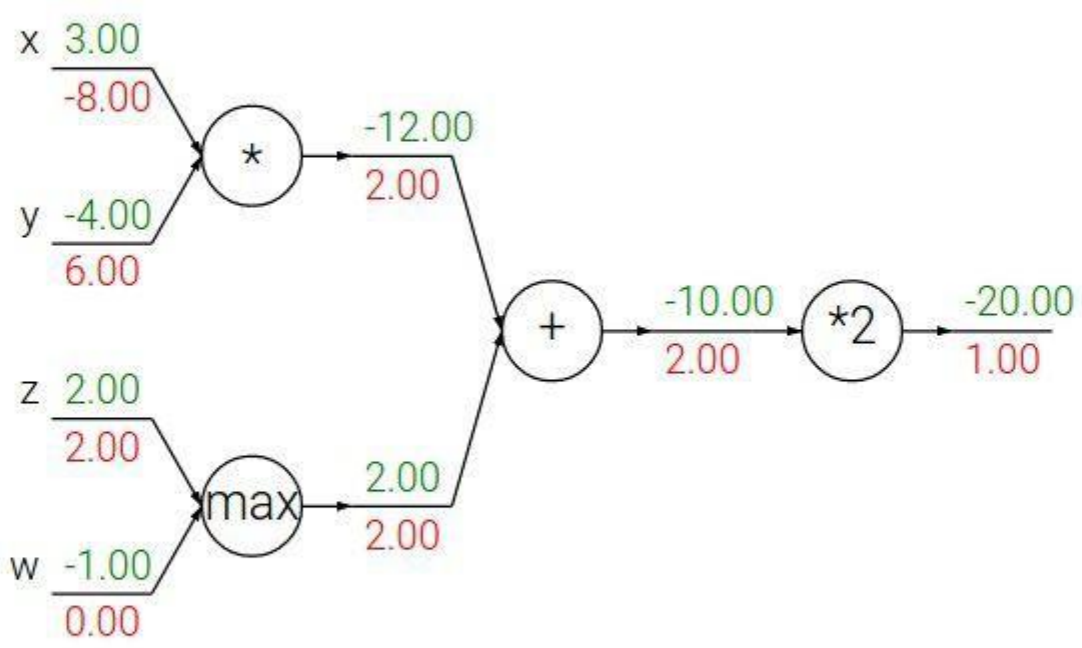
$$\boxed{\sigma(x) = \frac{1}{1+e^{-x}}}$$ sigmoid function

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

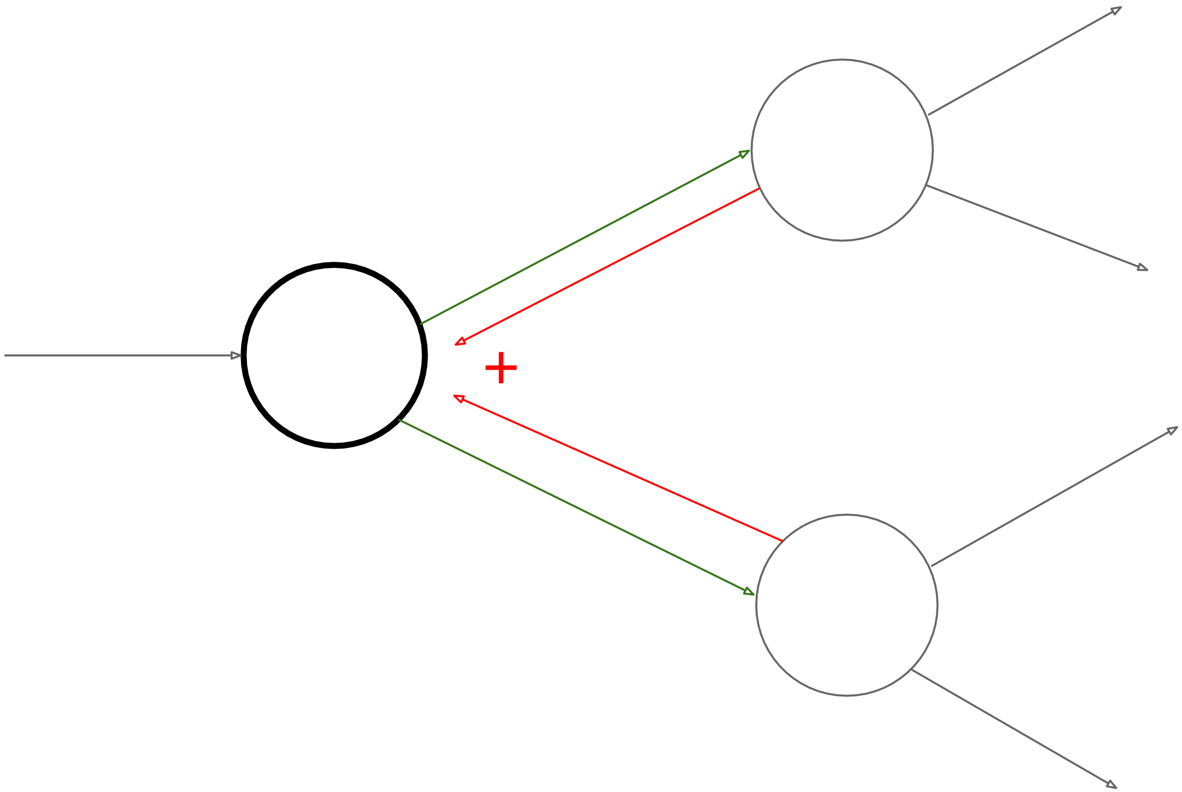


Patterns in backward flow

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

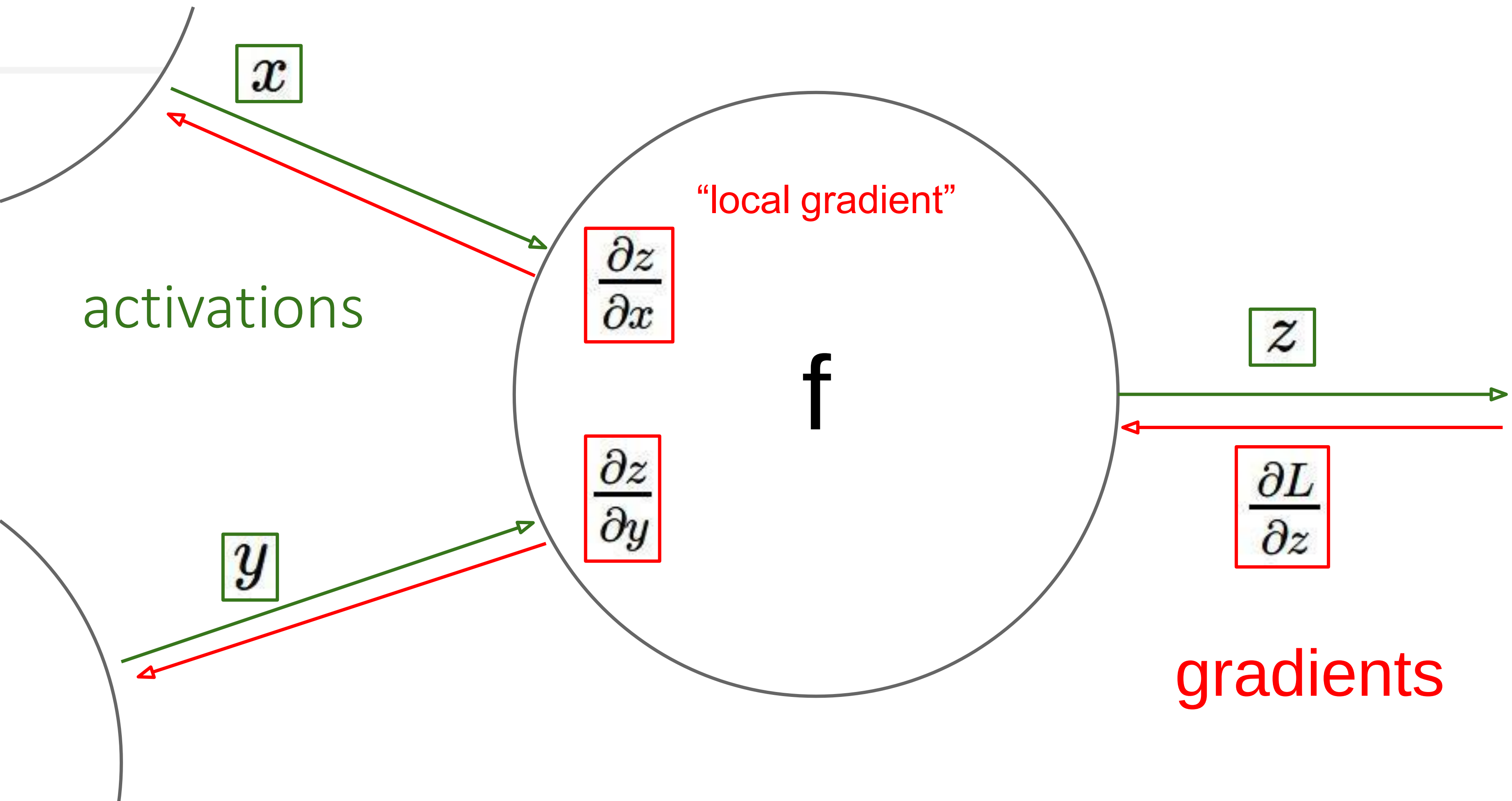


Gradients add at branches

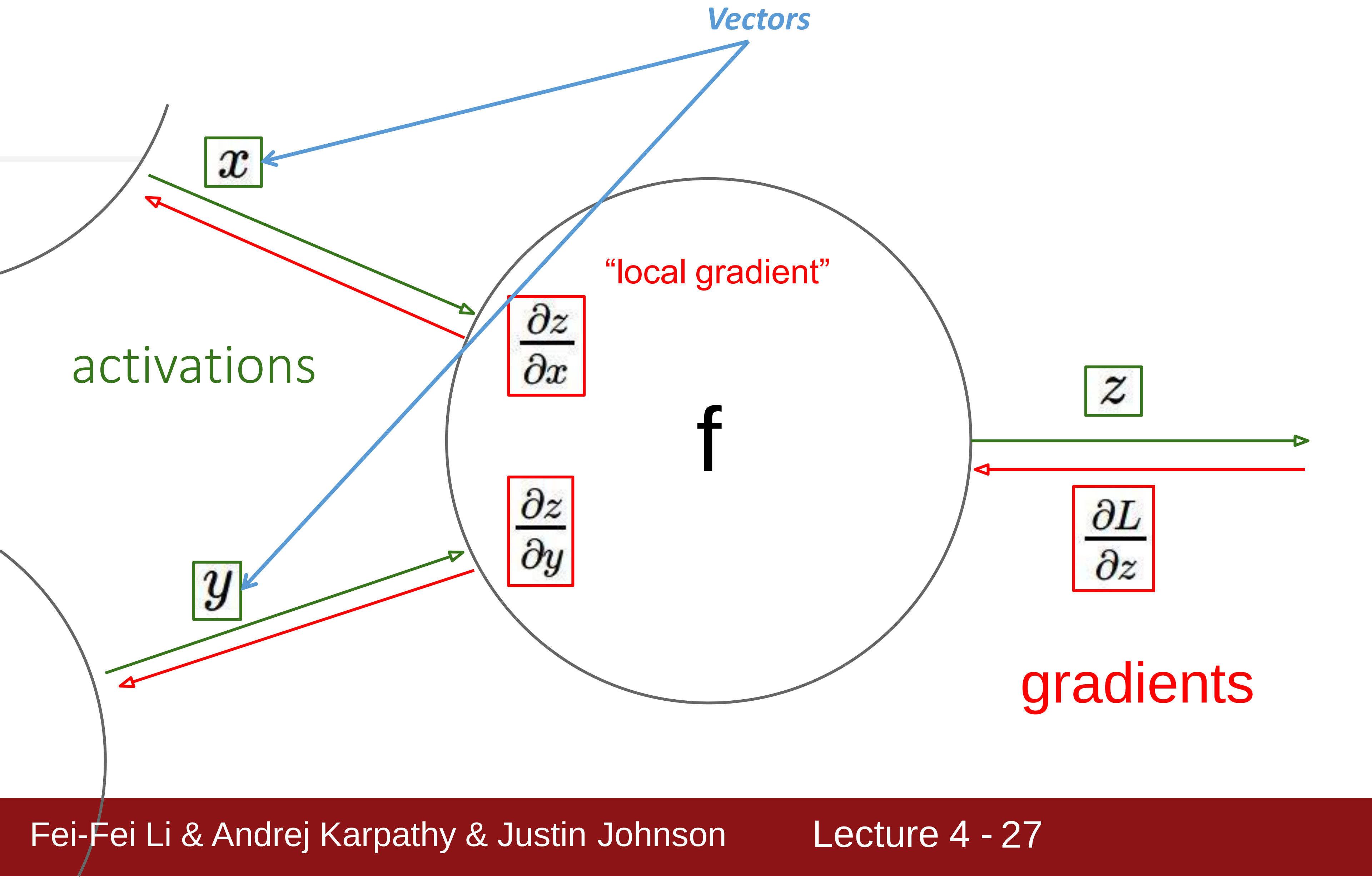


Neural Networks II

Vectorized Backpropagation



https://web.stanford.edu/class/cs224n/readings/gradient-notes.pdf



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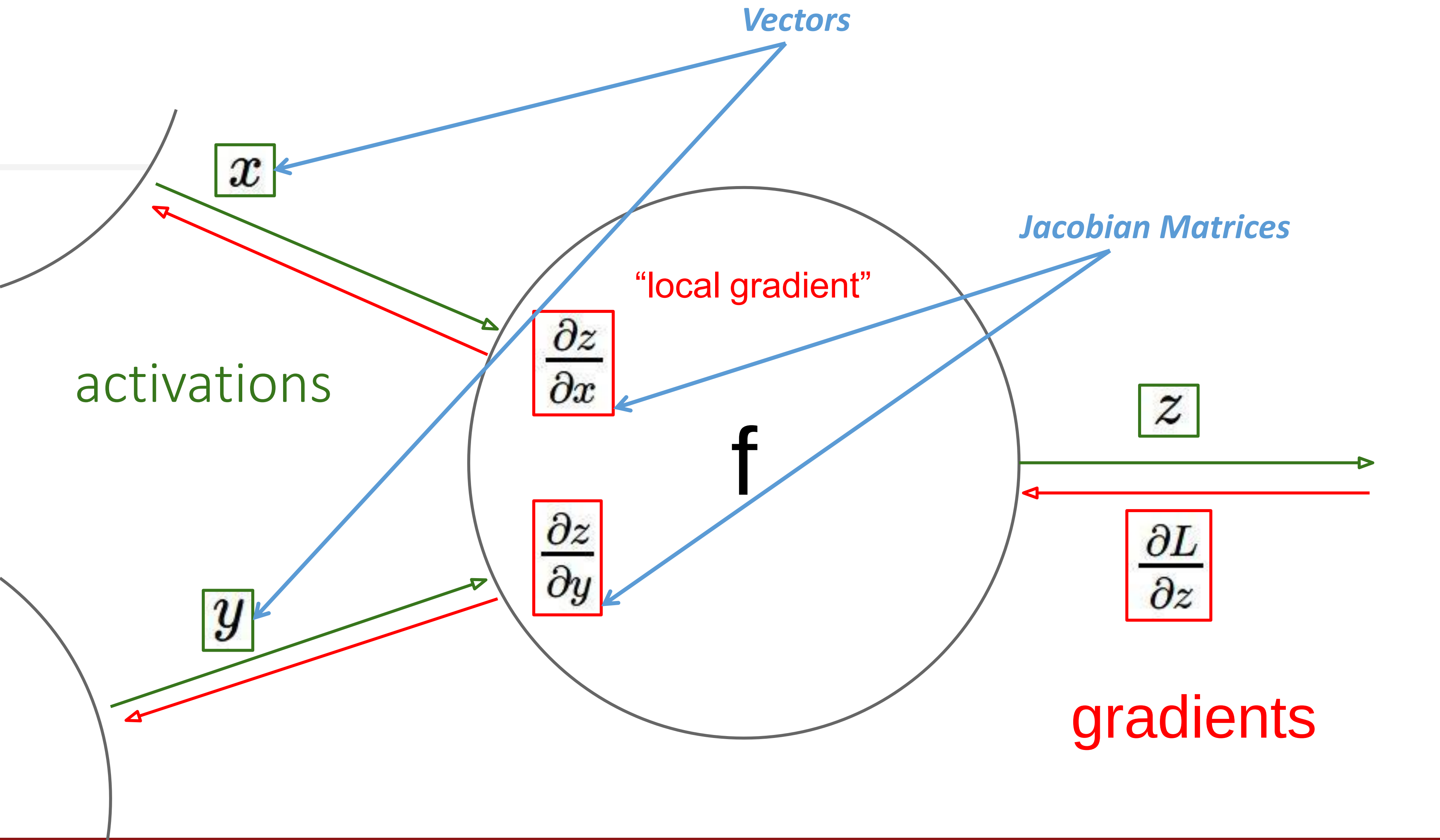

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