

Today: Outline

- Dropout
- Data Augmentation
- Backpropagation
- **Reminders:** *Pre-lec Material 1 posted,
due: Mon May 31*

*Last day to email me any dates
you cannot make to lecture
due: Fri May 28*



Neural Networks

Dropout

Dropout: A Classical Regularization Technique

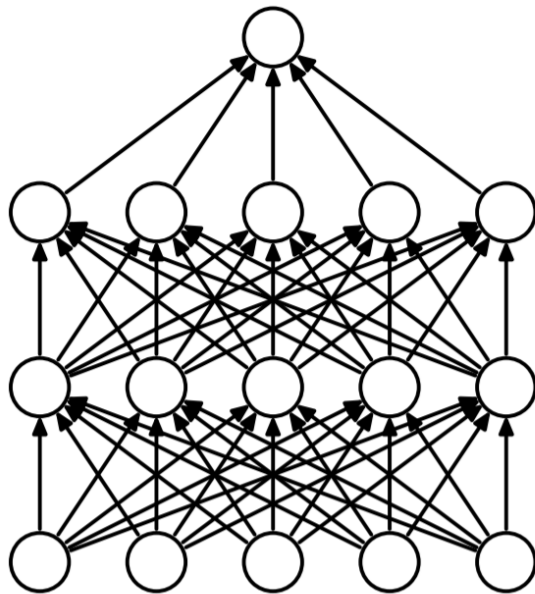
- Combining the predictions of many different models is a very successful way to reduce test errors.
- But it appears to be too expensive for big neural networks that already take several days to train.
- There is, however, a very efficient version of model combination that only costs about a factor of two during training: **Dropout**

Dropout: A Classical Regularization Technique

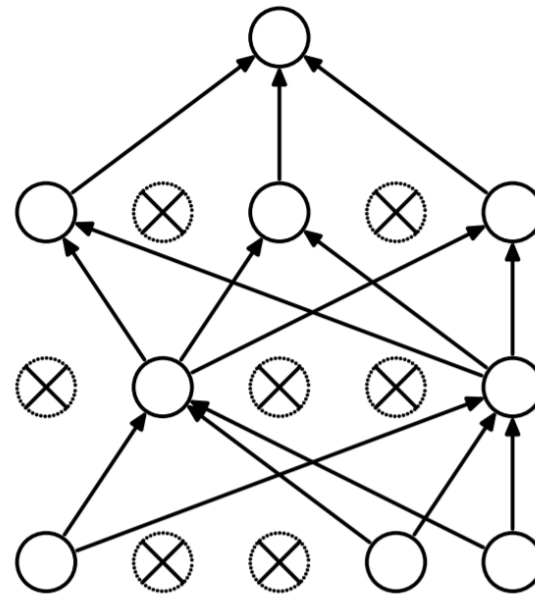
- Setting to zero the output of each hidden neuron with a specific dropout probability, *e.g.* 0.5.
- The neurons which are “dropped out” in this way
 - do not contribute to the forward pass, and
 - do not participate in backpropagation.
- So every time an input is presented, the neural network samples a different architecture, but all these architectures share weights.

Dropout: A Classical Regularization Technique

- Many Deep Models employ dropout at training time to avoid overfitting, allowing for better generalization.



(a) Standard Neural Net



(b) After applying dropout.

Dropout: A Classical Regularization Technique

- Dropout can be thought of as a model averaging technique.
- Dropout can be applied to fully-connected layers or convolutional layers.
- It has so far been observed to give higher performance gains when applied to fully-connected layers.

Dropout Variants

- Several variants of dropout have been introduced:
 - How much dropout is applied to neurons/weights?
 - Information Dropout
 - DropConnect
 - Curriculum Dropout
 - Which neurons to drop out?
 - Adaptive Dropout
 - DropBlock
 - Excitation Dropout



Neural Networks

Data Augmentation

Data Augmentation

- Another technique that prevents overfitting.
- How?
By artificially enlarging the dataset using label-preserving transformations.
- Examples:
 - generating image translations and horizontal reflections
 - altering the intensities of the RGB channels in training images: add perturbations to each RGB image pixel
$$I_{xy} = [I_{xy}^R, I_{xy}^G, I_{xy}^B]$$

Data Augmentation

- Could be computed “on the fly,” and do not necessarily need to be stored on disk.
- How?
The transformed images are generated in Python code on the CPU while the GPU is training on the previous batch of images.
- So these data augmentation schemes can be, in effect, computationally free.



Neural Networks

General Notation

Artificial Neural Network:

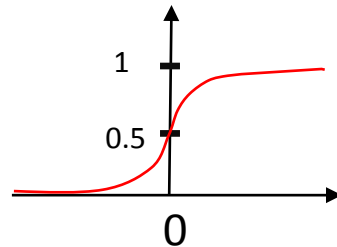
general notation

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

hidden layer activations

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

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



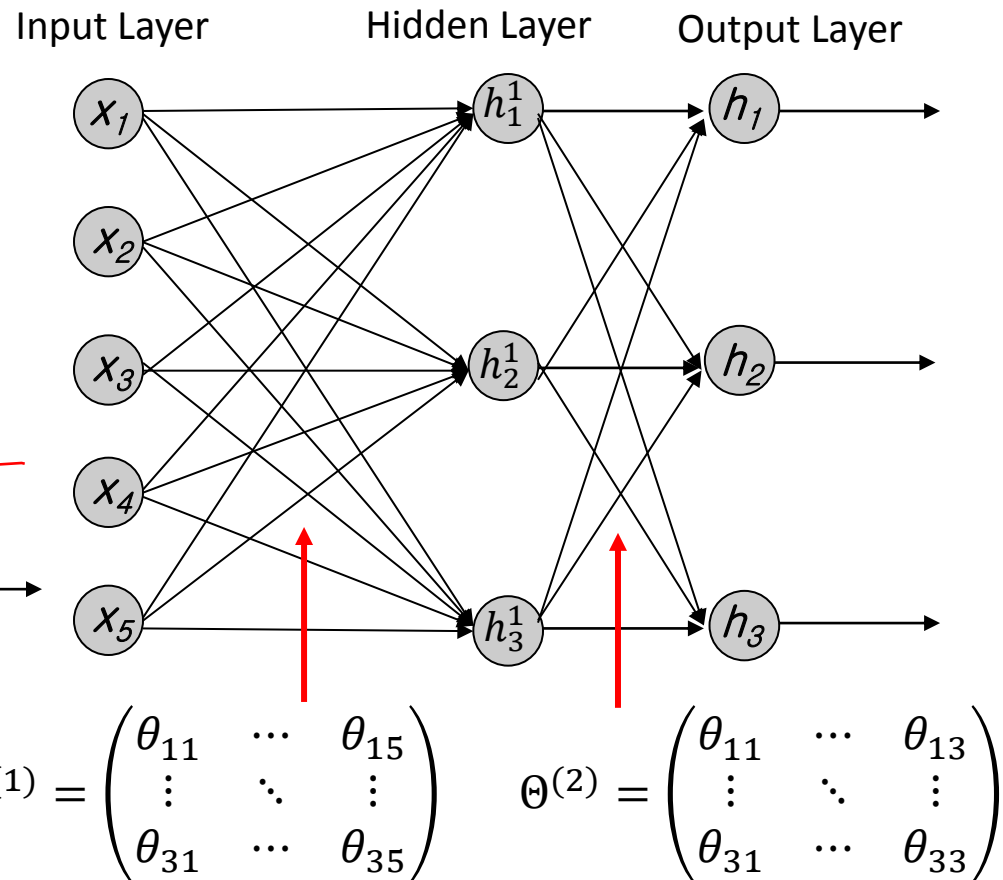
output

$$h_{\Theta}(x) = g(\Theta^{(2)}a)$$

weights

$$\Theta^{(1)} = \begin{pmatrix} \theta_{11} & \dots & \theta_{15} \\ \vdots & \ddots & \vdots \\ \theta_{31} & \dots & \theta_{35} \end{pmatrix}$$

$$\Theta^{(2)} = \begin{pmatrix} \theta_{11} & \dots & \theta_{13} \\ \vdots & \ddots & \vdots \\ \theta_{31} & \dots & \theta_{33} \end{pmatrix}$$



Cost function

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

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

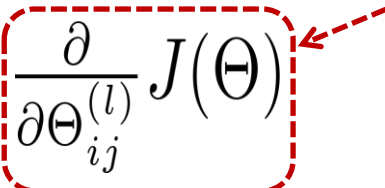
Gradient computation

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

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

Need code to compute:

- $J(\Theta)$

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

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

Backpropagation

Chain Rule

- Need to compute gradient of

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

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

$$f(\theta) = f_1(f_2(\theta)) \quad f'(\theta) = f_1'(f_2(\theta)) * f_2'(\theta)$$

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

- What about functions of multiple variables?

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

Backpropagation: Efficient Chain Rule

- Partial gradient computation via chain rule:

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

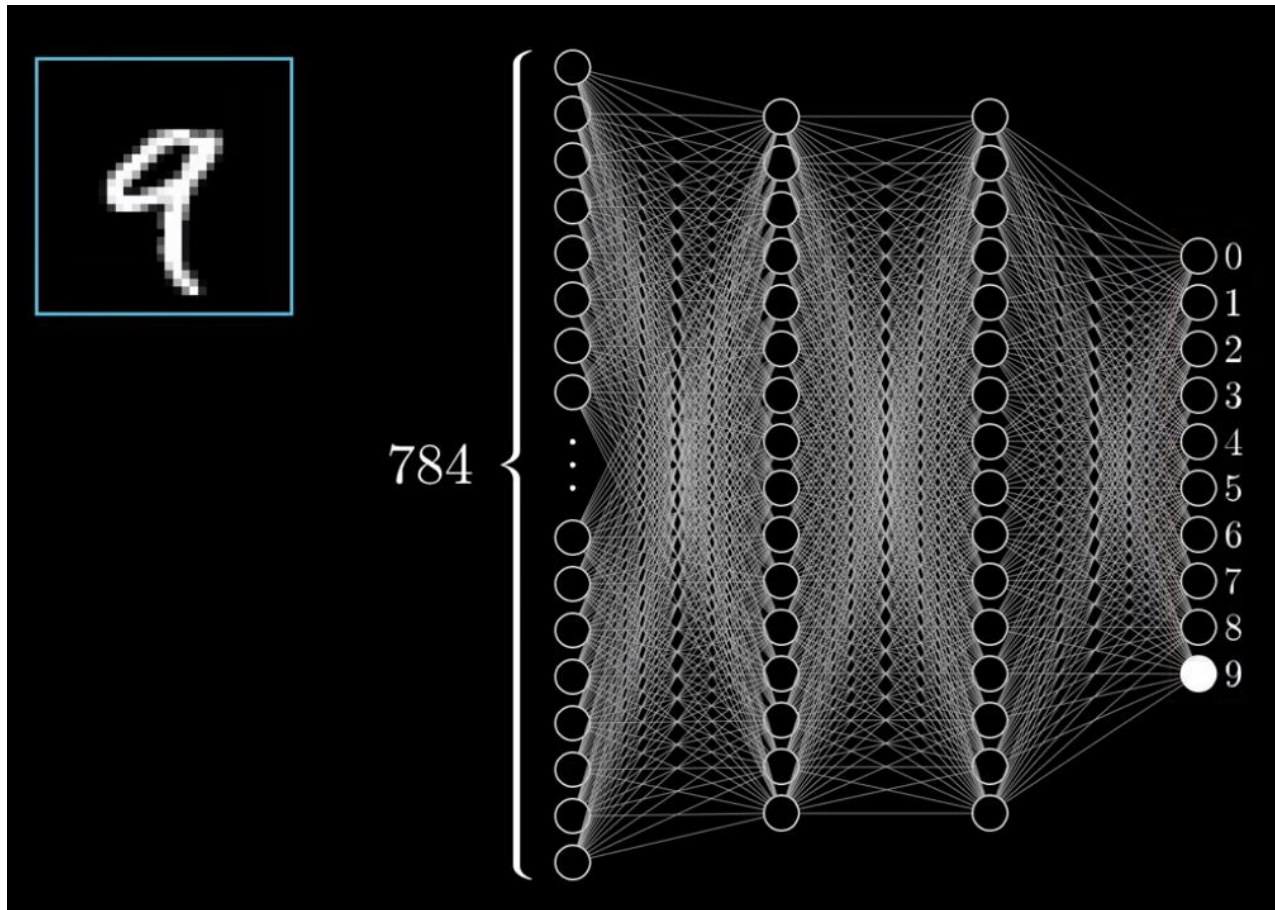
$$\frac{\partial f}{\partial \theta_2} = \frac{\partial f_1}{\partial f_2}(f_2(f_3(\theta))) * \frac{\partial f_2}{\partial f_3}(f_3(\theta)) * \frac{\partial f_3}{\partial \theta_2}(\theta)$$

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

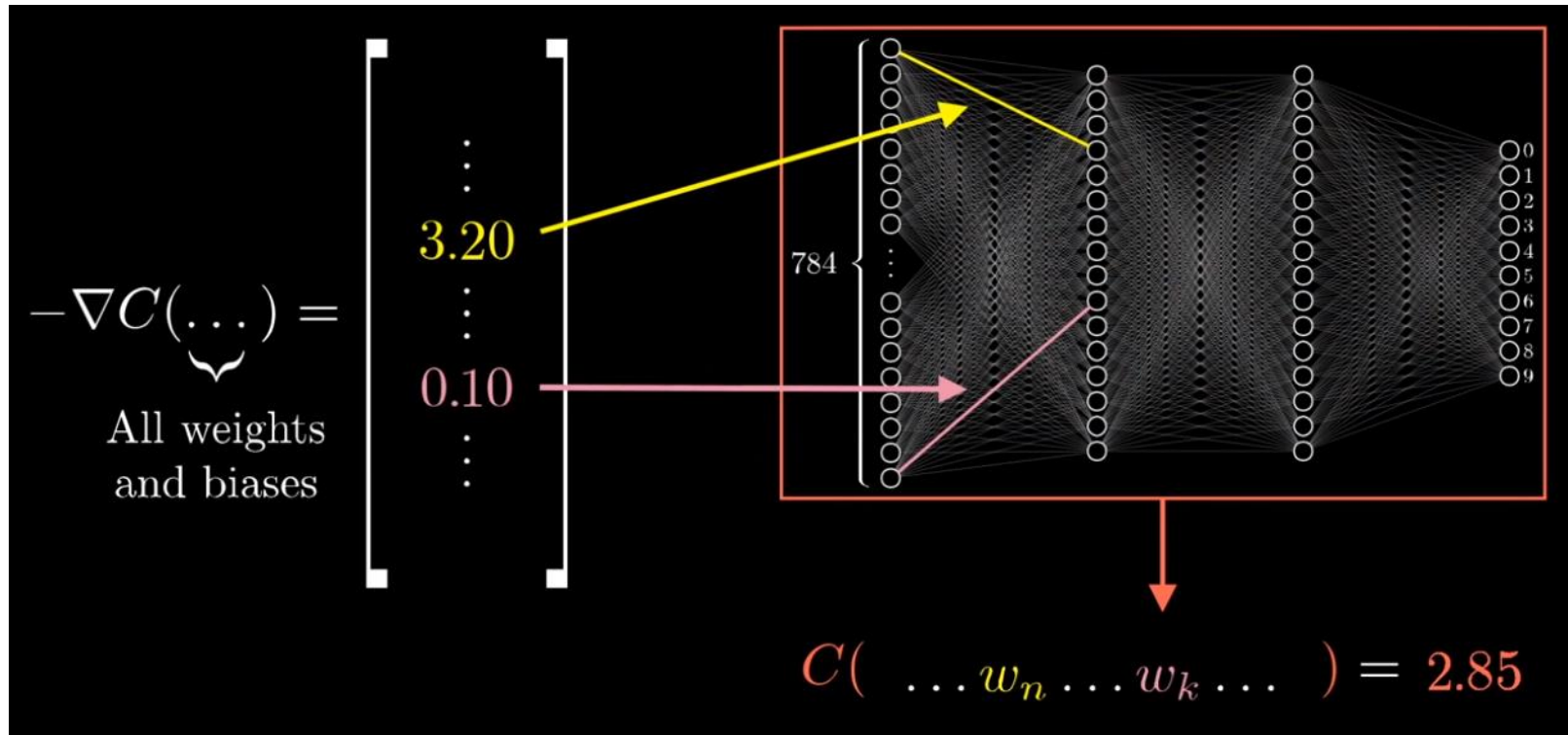
- need to re-evaluate functions many times
- Very inefficient! E.g. 100,000-dim parameters

Example: Classification

- A deep network is a massive composite function!

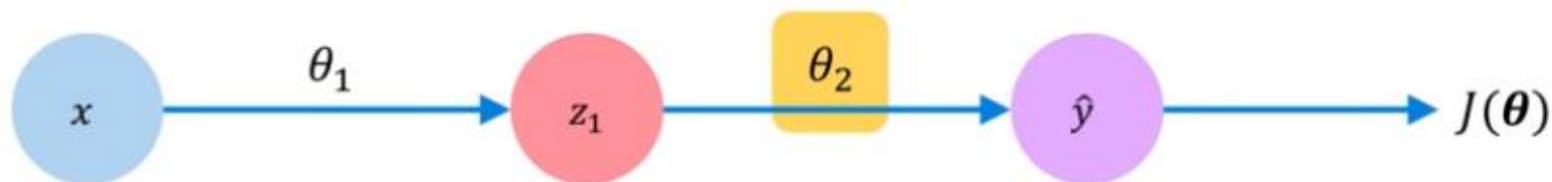


Interpretation of Computed Gradients



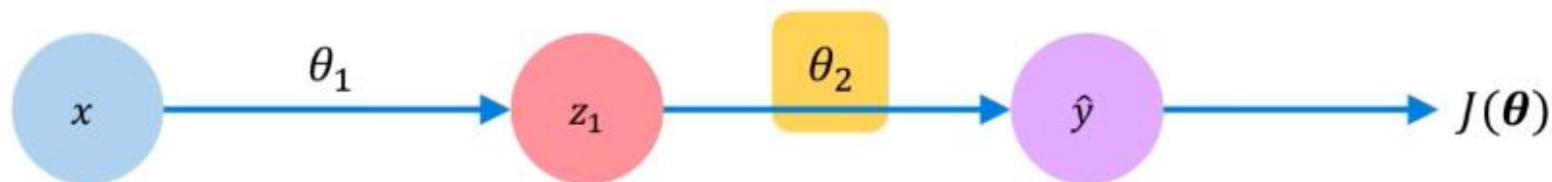
- The cost function is 32 times more sensitive to changes in the yellow weight vs. the pink weight.

Computing Gradients: Backpropagation



How does a small change in one weight (ex. θ_2) affect the final loss $J(\theta)$?

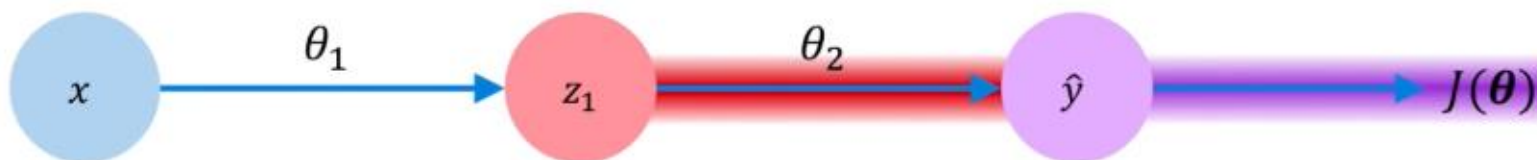
Computing Gradients: Backpropagation



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

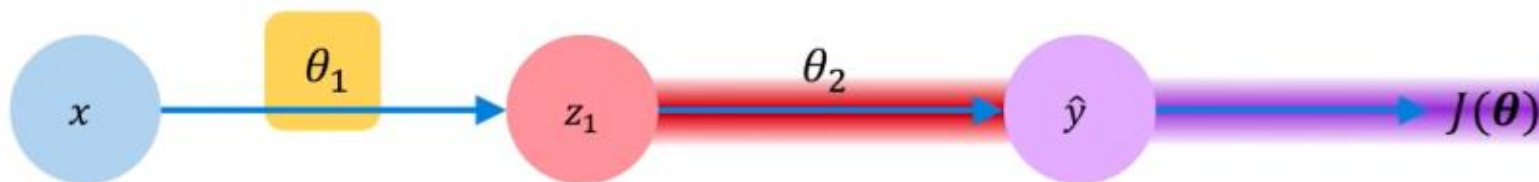
Let's use the chain rule!

Computing Gradients: Backpropagation



$$\frac{\partial J(\theta)}{\partial \theta_2} = \underbrace{\frac{\partial J(\theta)}{\partial \hat{y}}}_{\text{purple}} * \underbrace{\frac{\partial \hat{y}}{\partial \theta_2}}_{\text{red}}$$

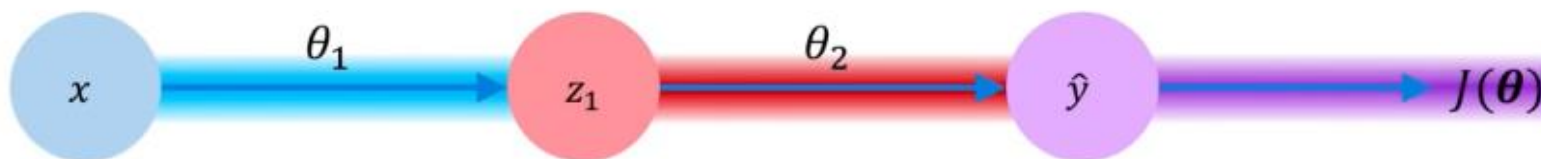
Computing Gradients: Backpropagation



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

Apply chain rule! Apply chain rule!

Computing Gradients: Backpropagation



$$\frac{\partial J(\theta)}{\partial \theta_1} = \underbrace{\frac{\partial J(\theta)}{\partial \hat{y}}}_{\text{purple}} * \underbrace{\frac{\partial \hat{y}}{\partial z_1}}_{\text{red}} * \underbrace{\frac{\partial z_1}{\partial \theta_1}}_{\text{blue}}$$



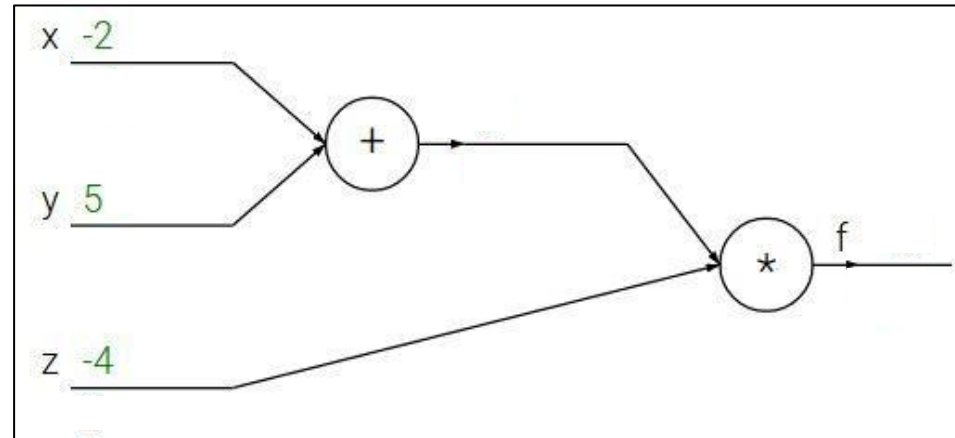
Neural Networks

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

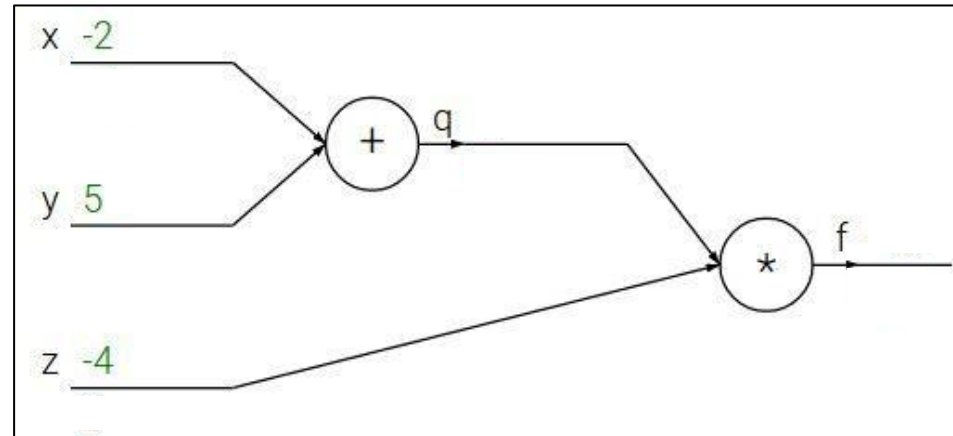
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e.g. $x = -2, y = 5, z = -4$

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

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

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



Computation Graph: Forward

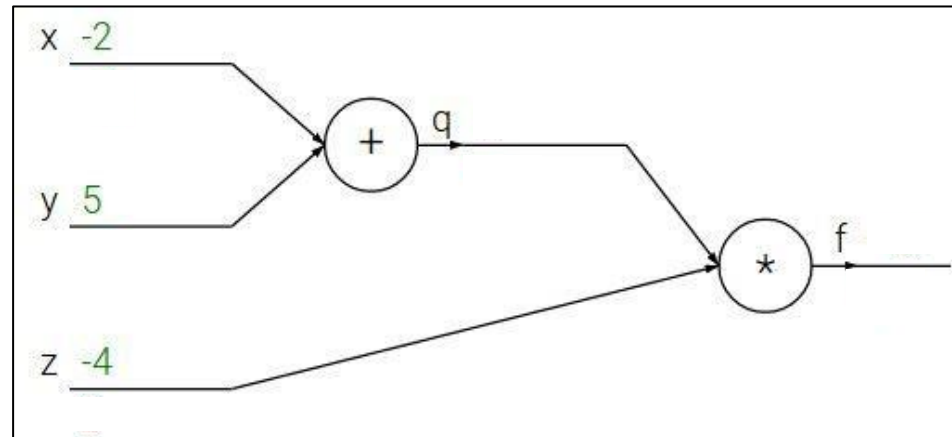
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



compute values



Computation Graph: Backward

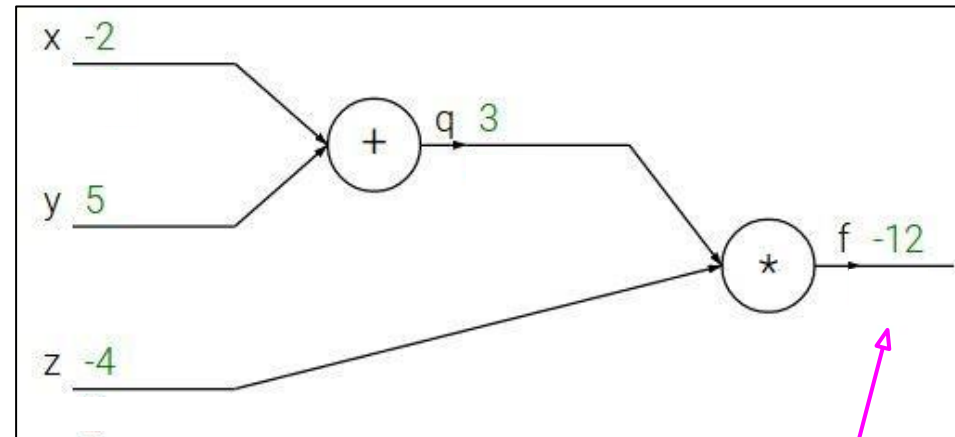
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

compute gradients



Computation Graph: Backward

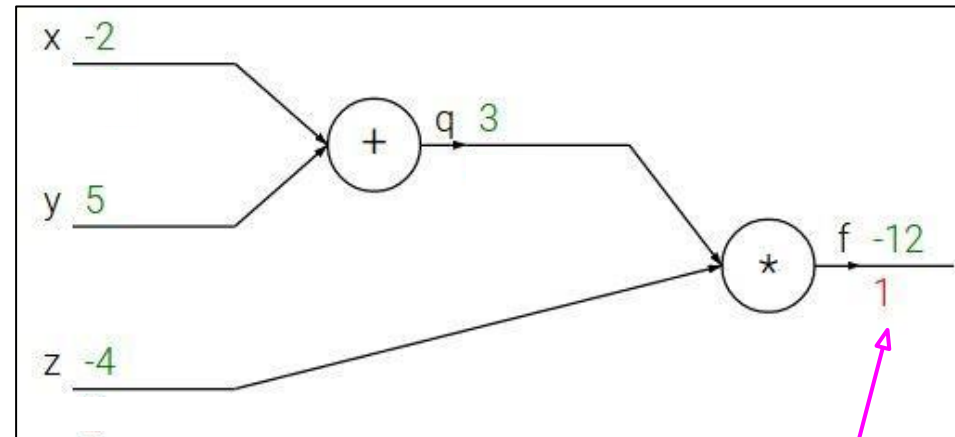
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

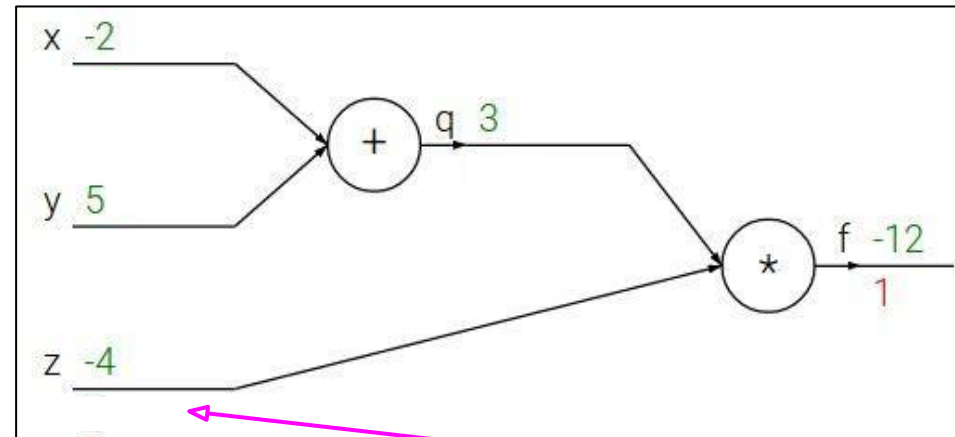
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

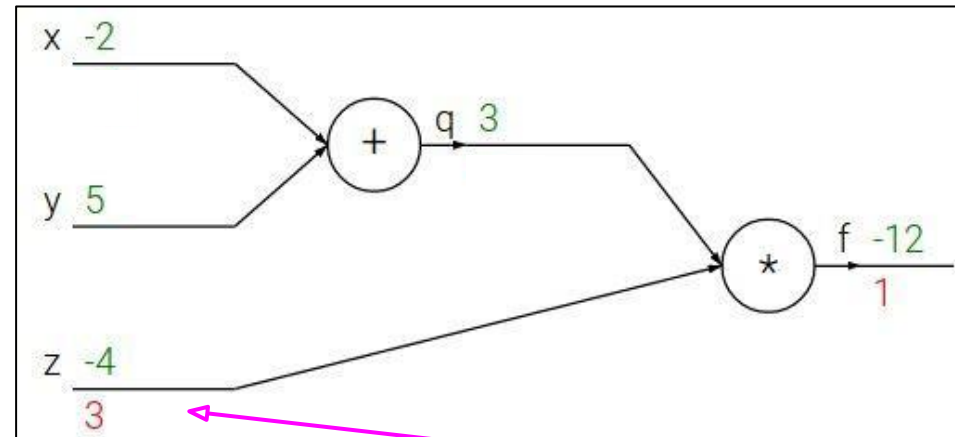
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

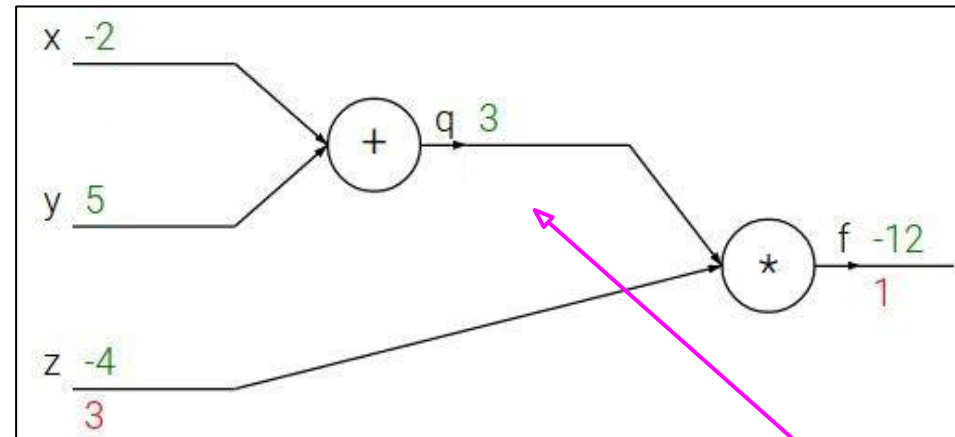
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

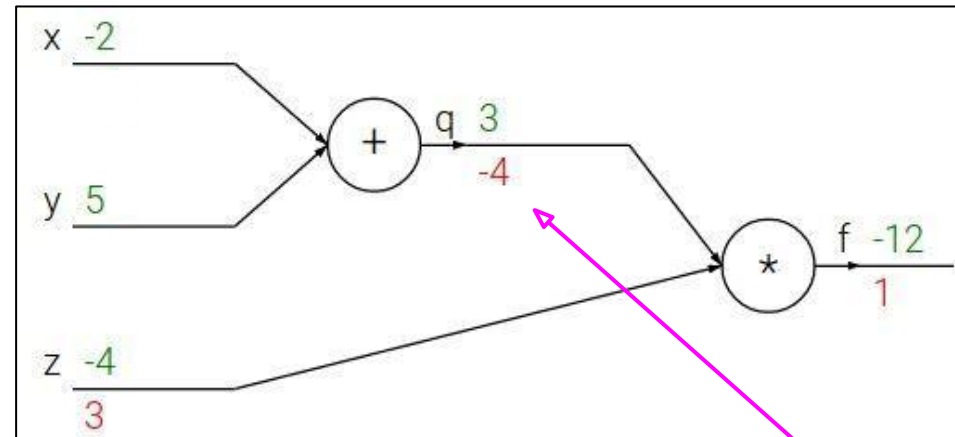
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

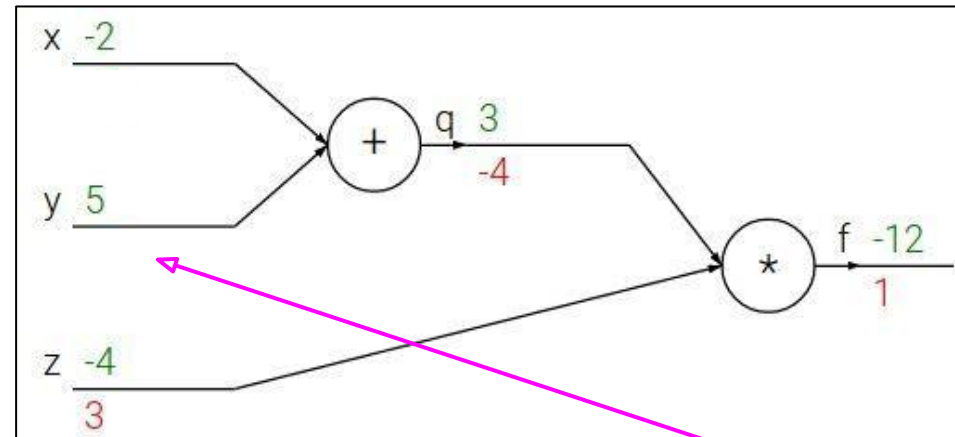
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

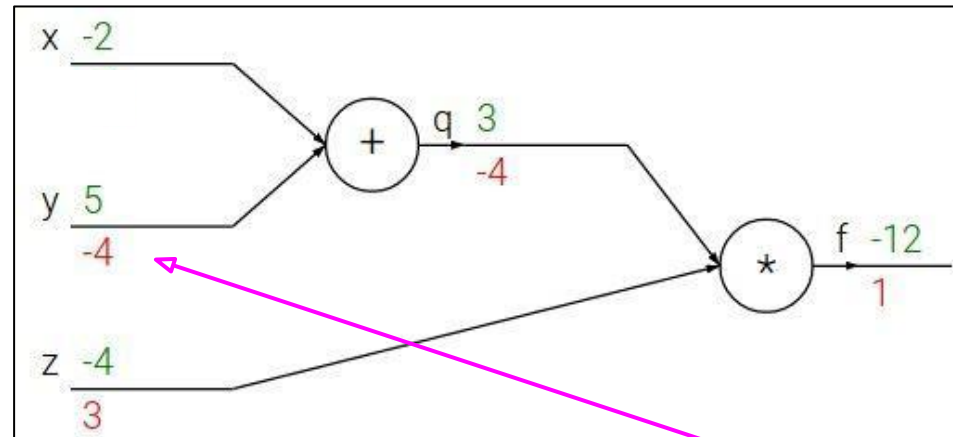
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Chain rule:

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

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

Computation Graph: Backward

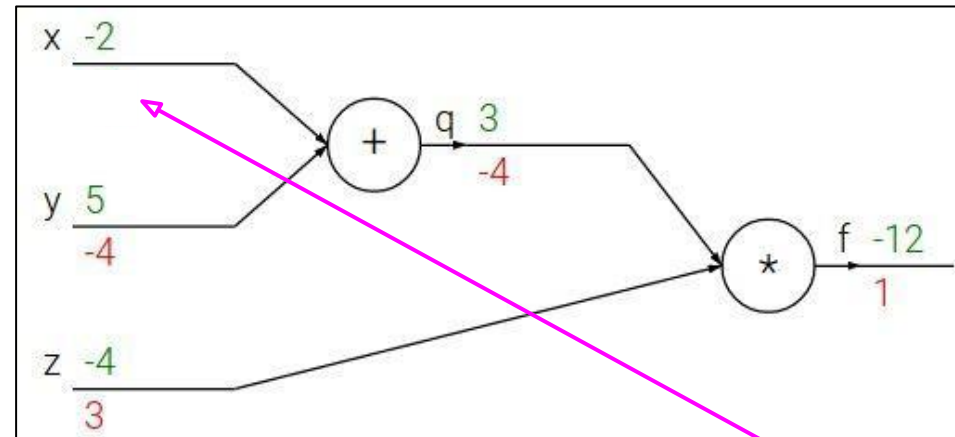
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

Computation Graph: Backward

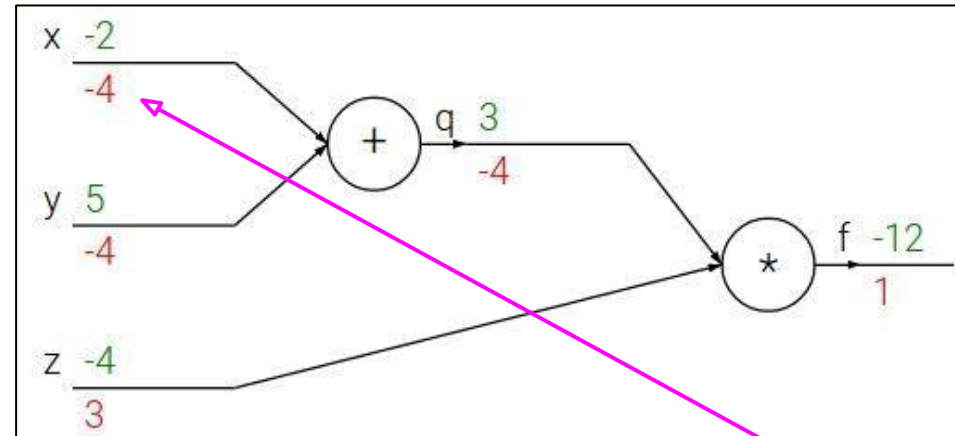
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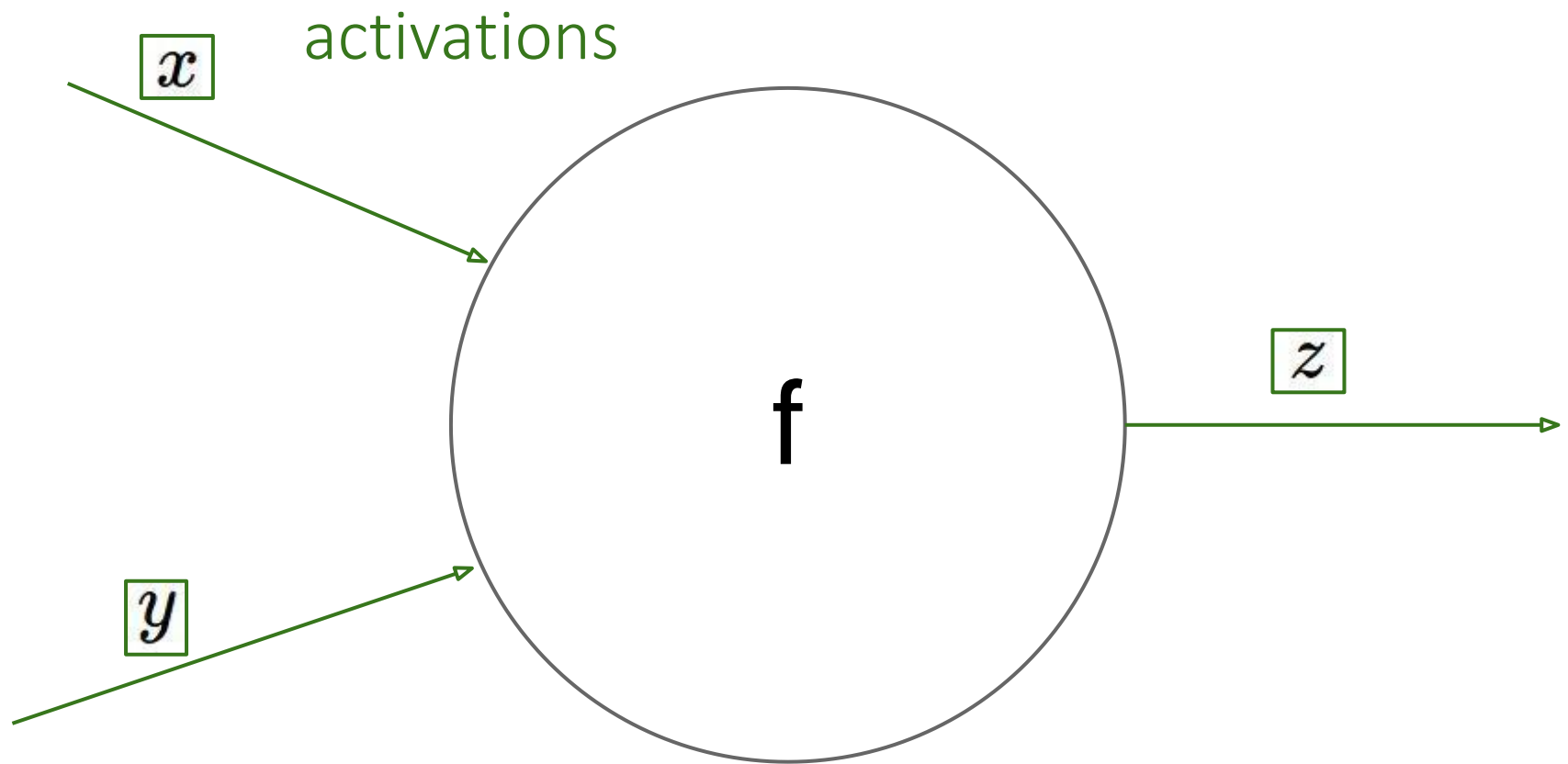
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

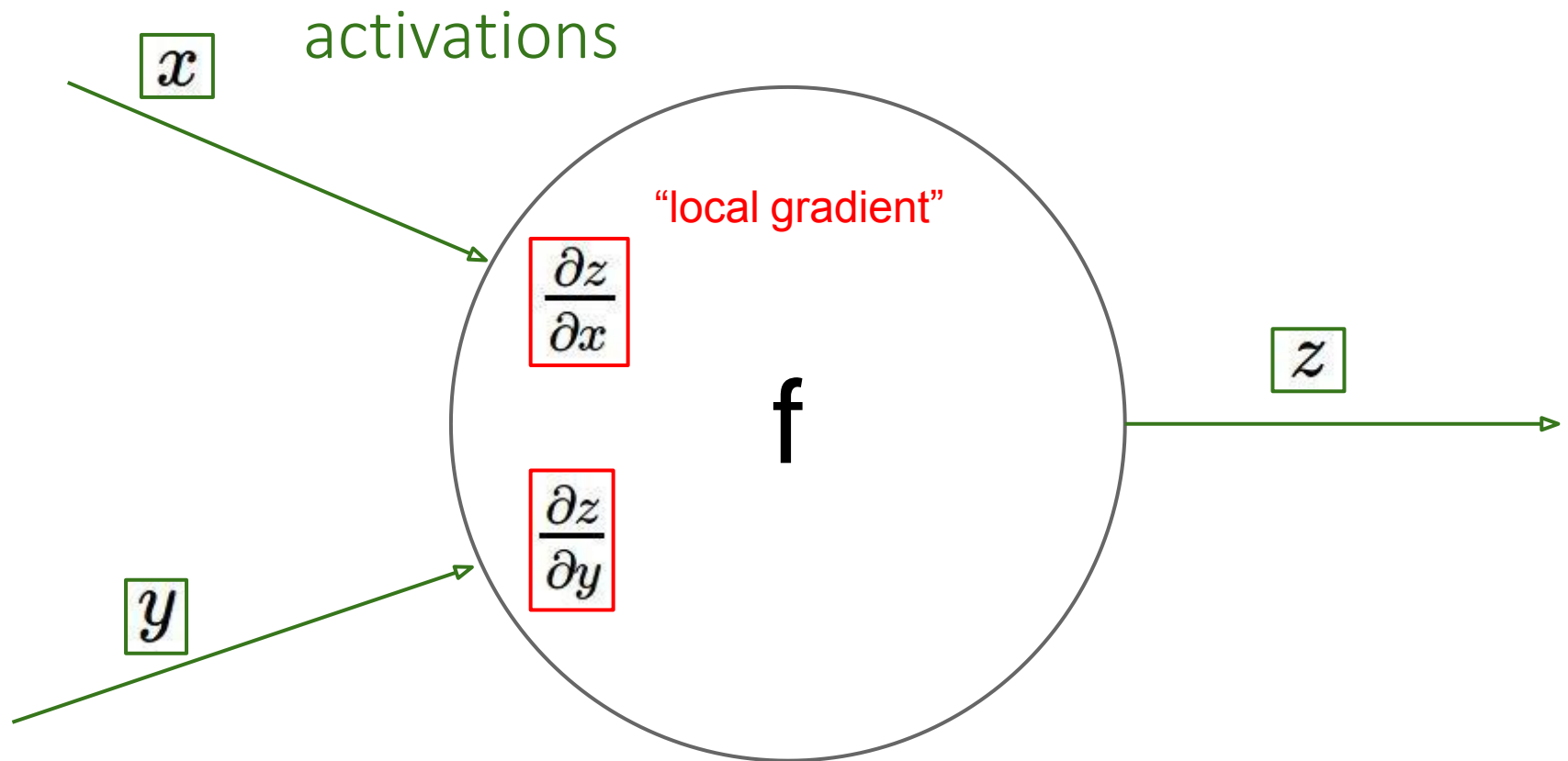


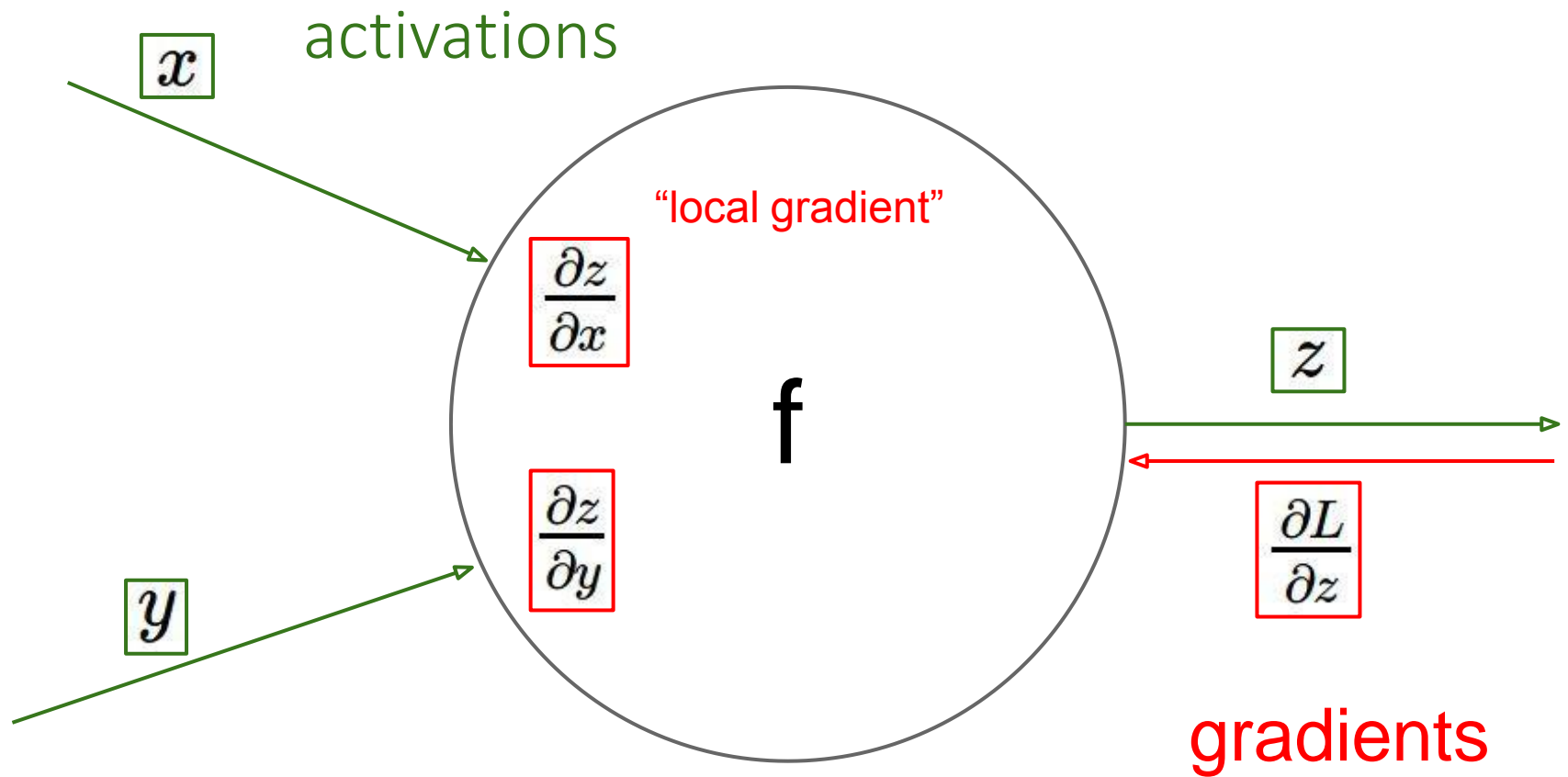
Chain rule:

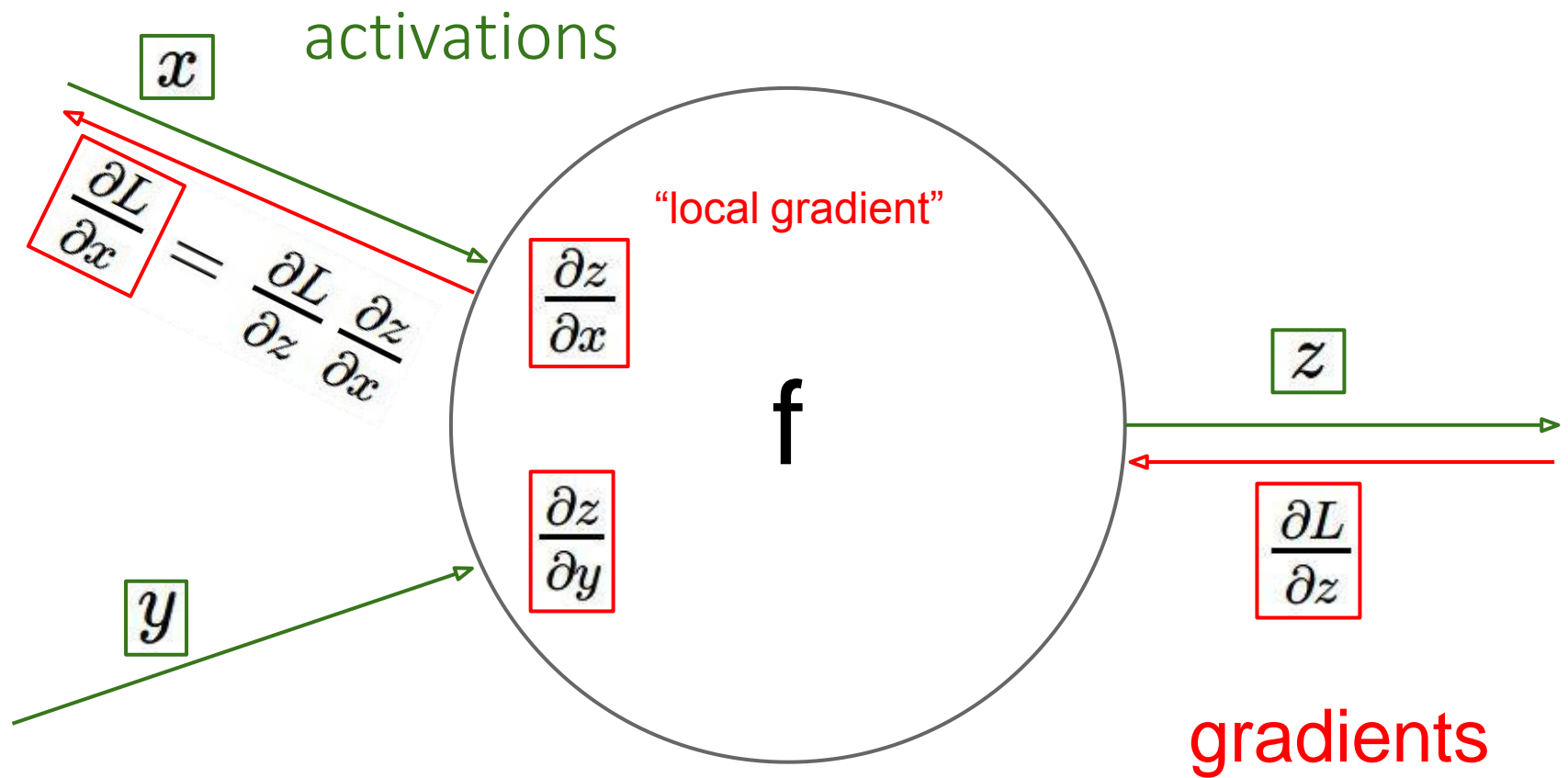
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

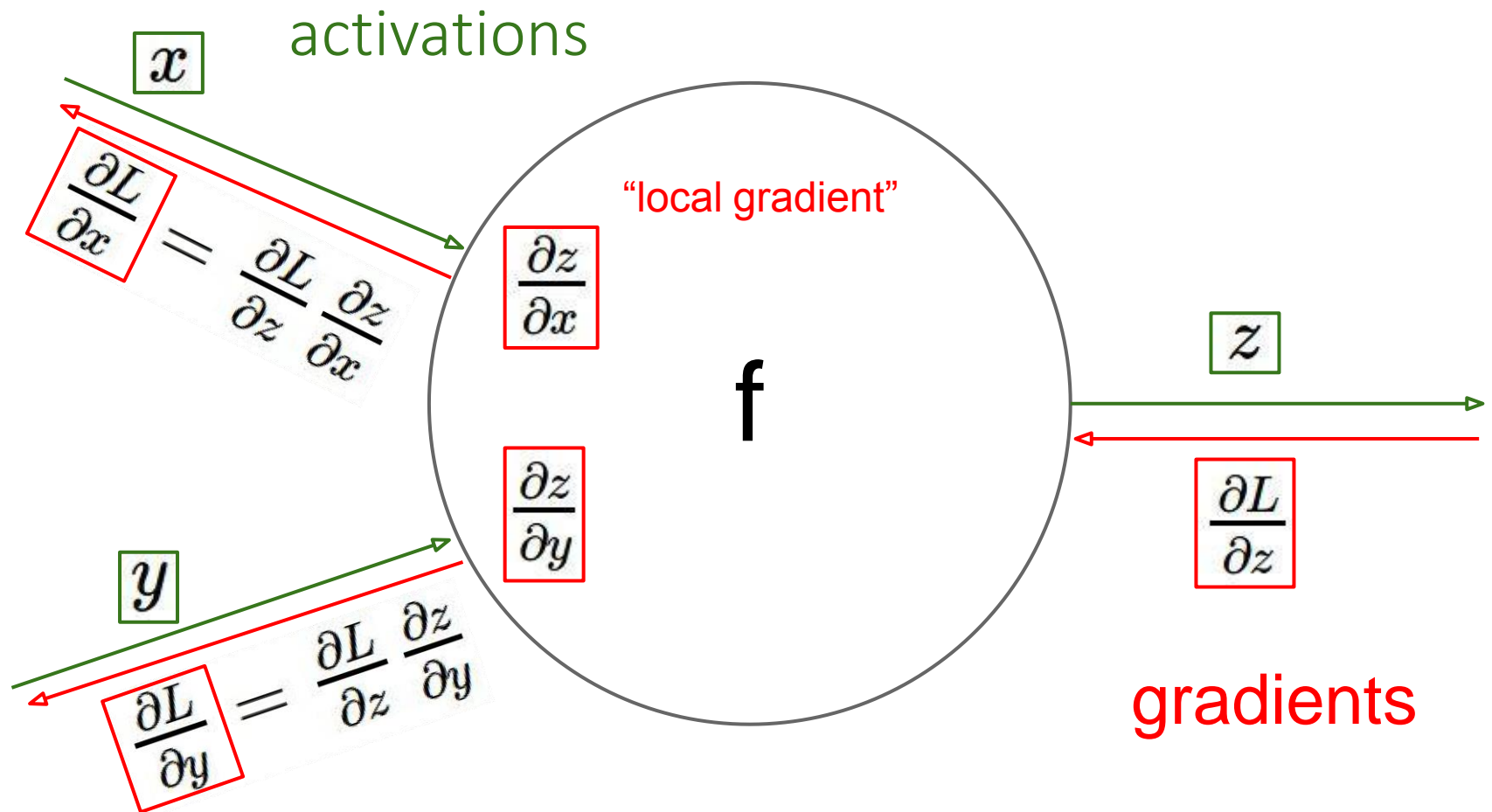
$$\frac{\partial f}{\partial x}$$

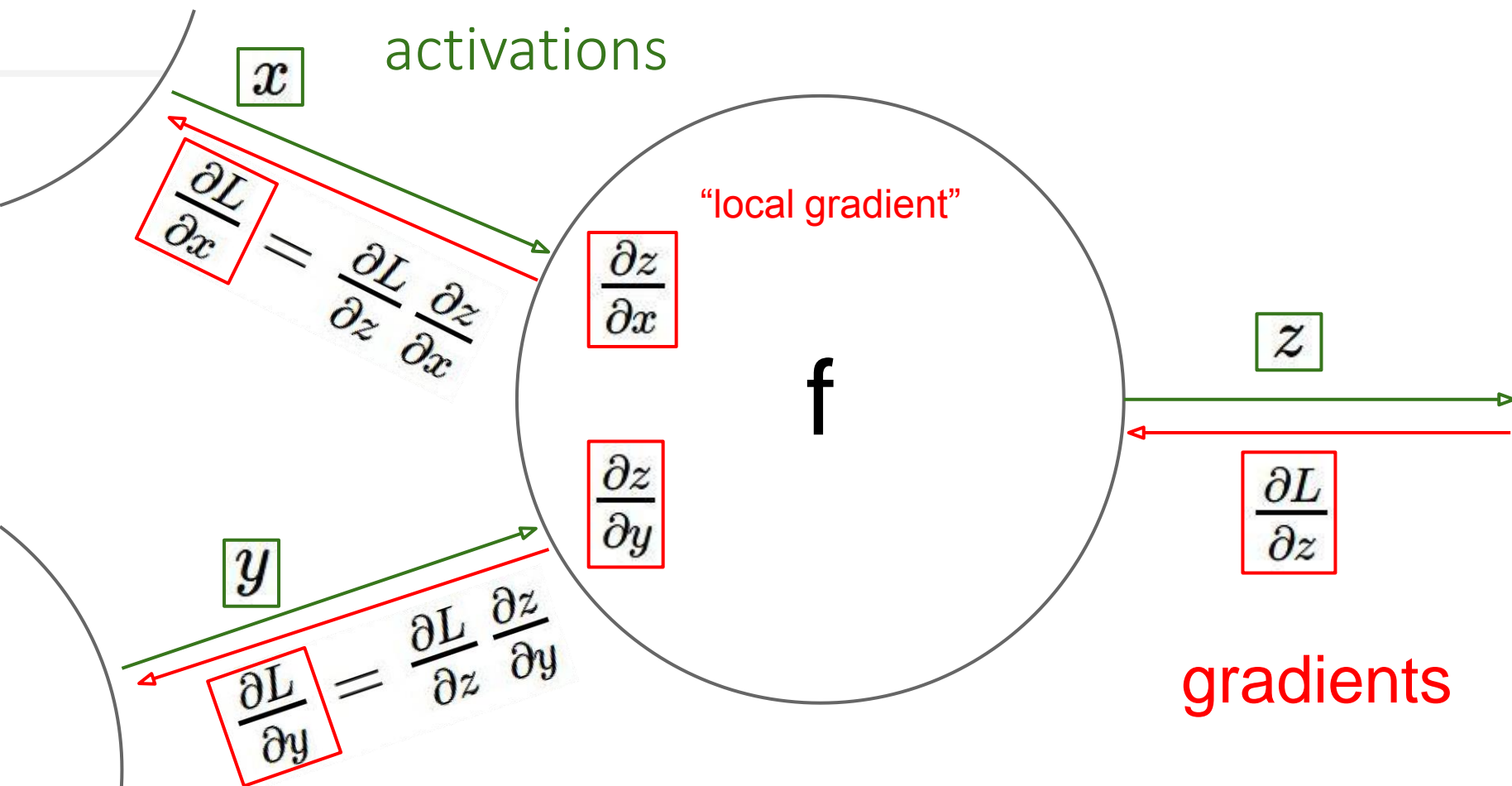






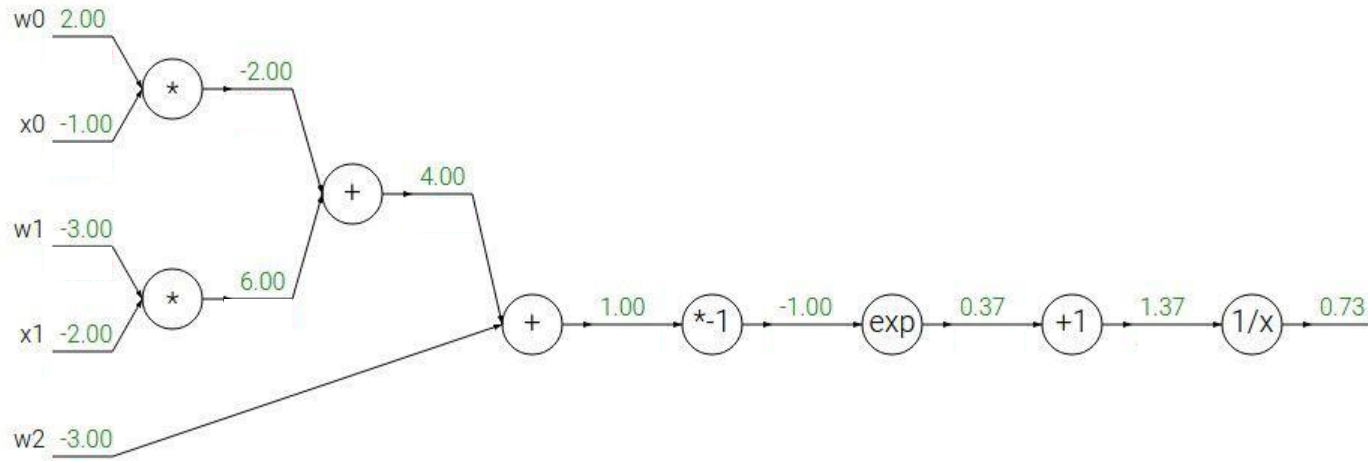






Another example:

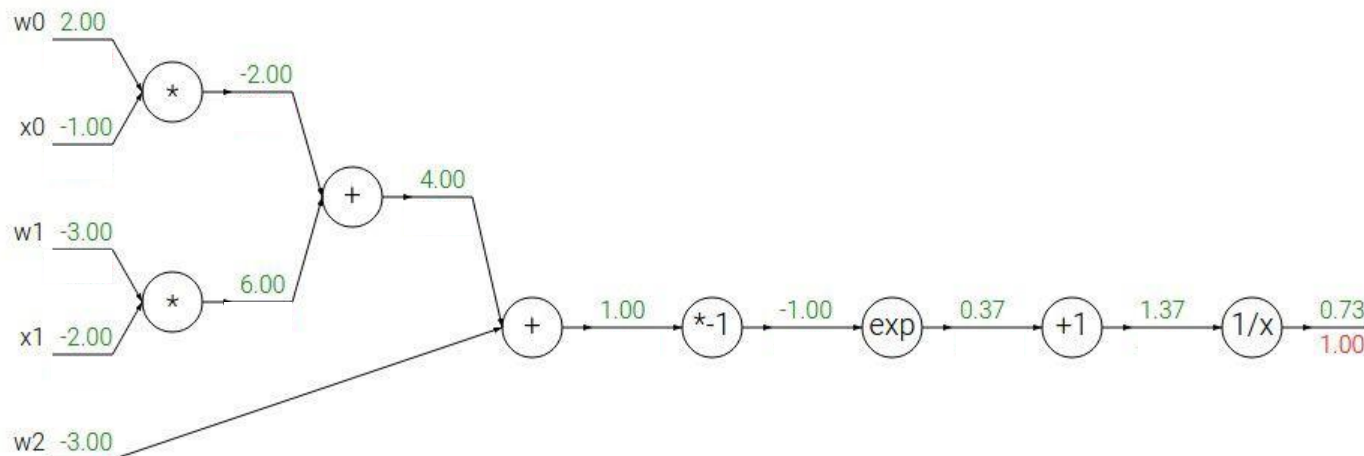
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



Another example:

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

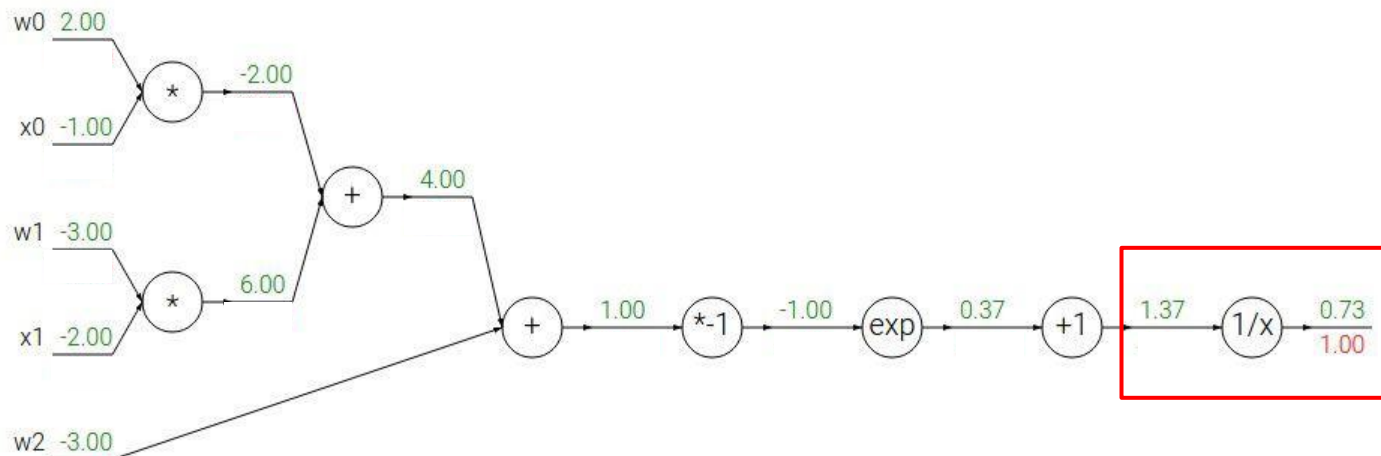
Computing a 2D Sigmoid Neuron!



$f(x) = e^x$	\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	$\frac{df}{dx} = 1$

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

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

$$f(x) = \frac{1}{x}$$

→

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

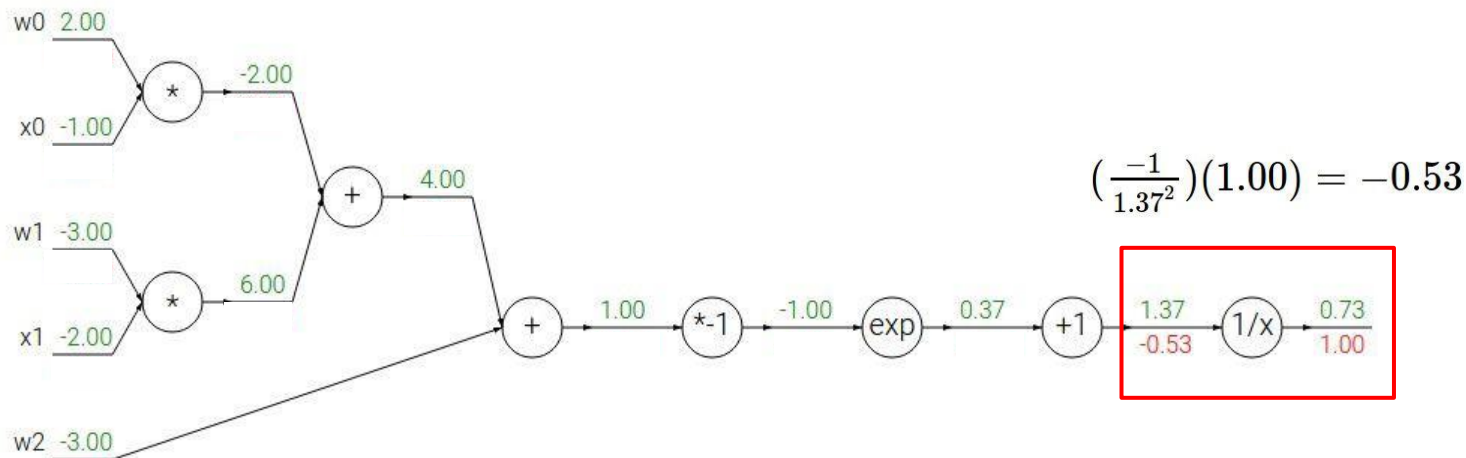
$$f_c(x) = c + x$$

→

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

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

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

$$f(x) = \frac{1}{x}$$

→

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

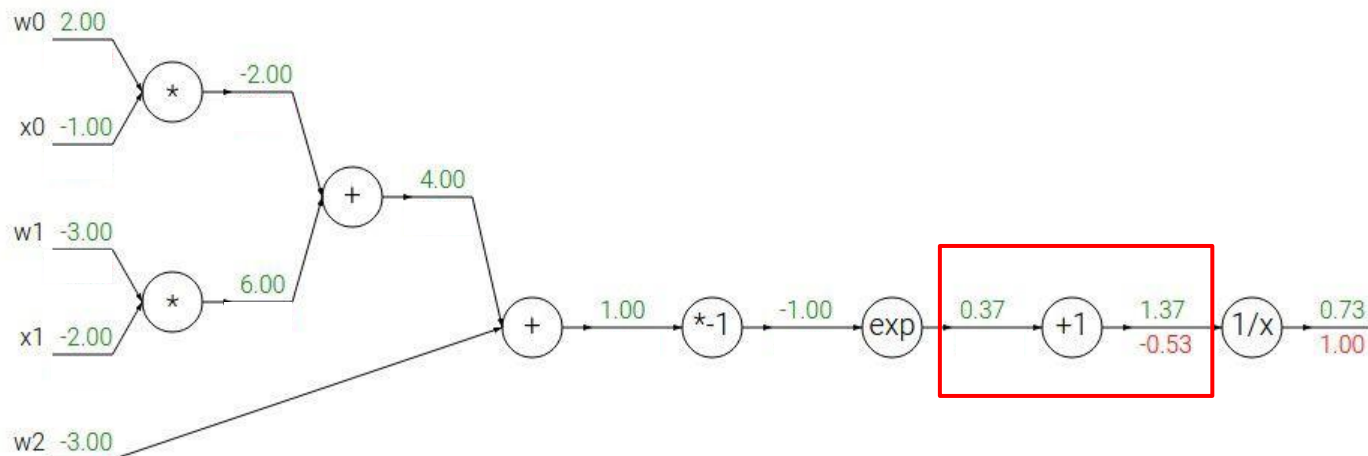
$$f_c(x) = c + x$$

→

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

Another example:

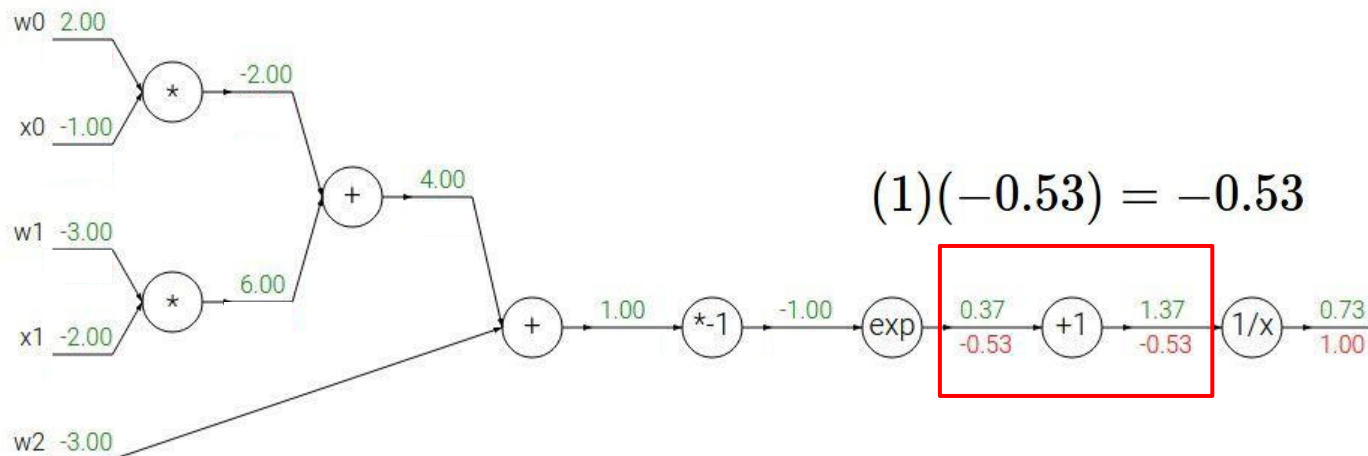
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

Another example:

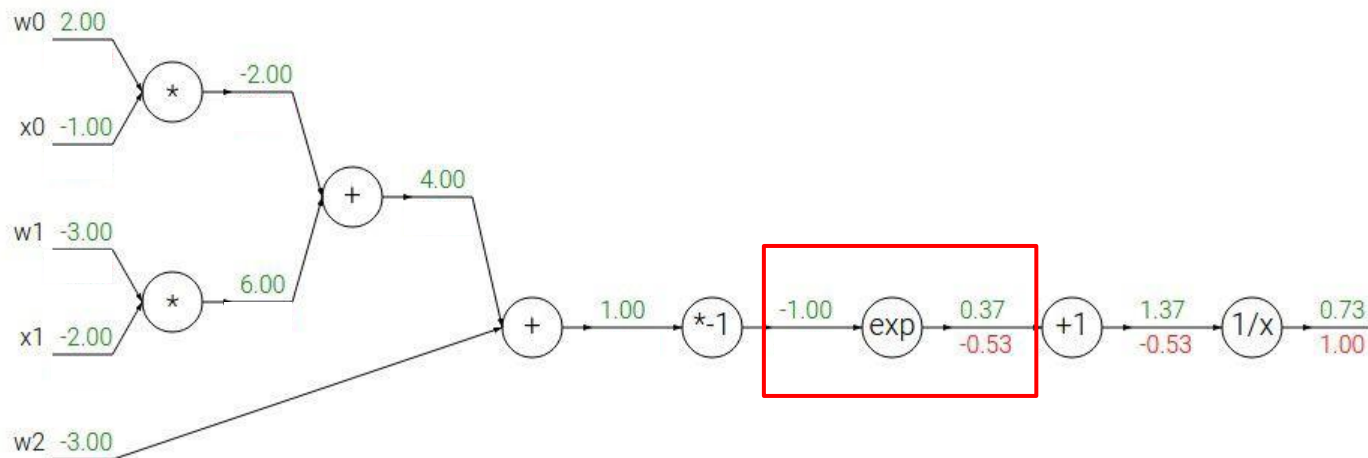
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



$f(x) = e^x$	\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	$\frac{df}{dx} = 1$

Another example:

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



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

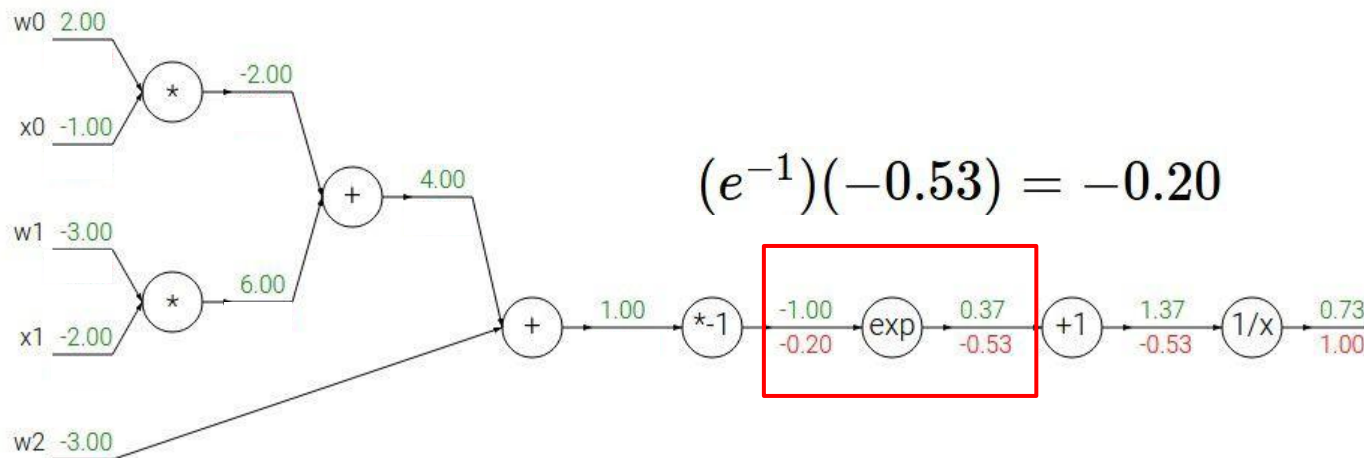
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



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

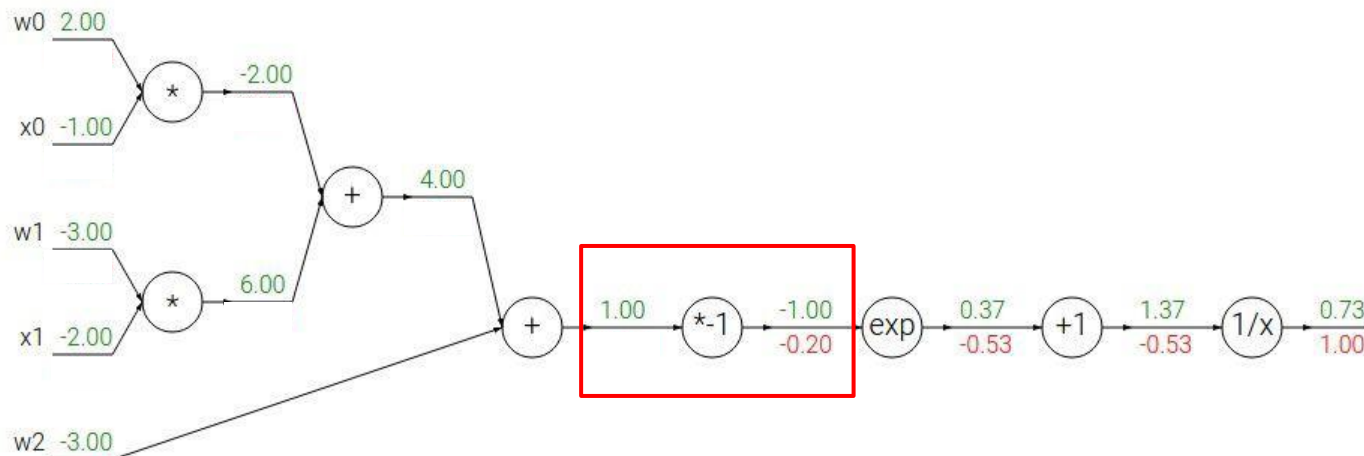
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



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

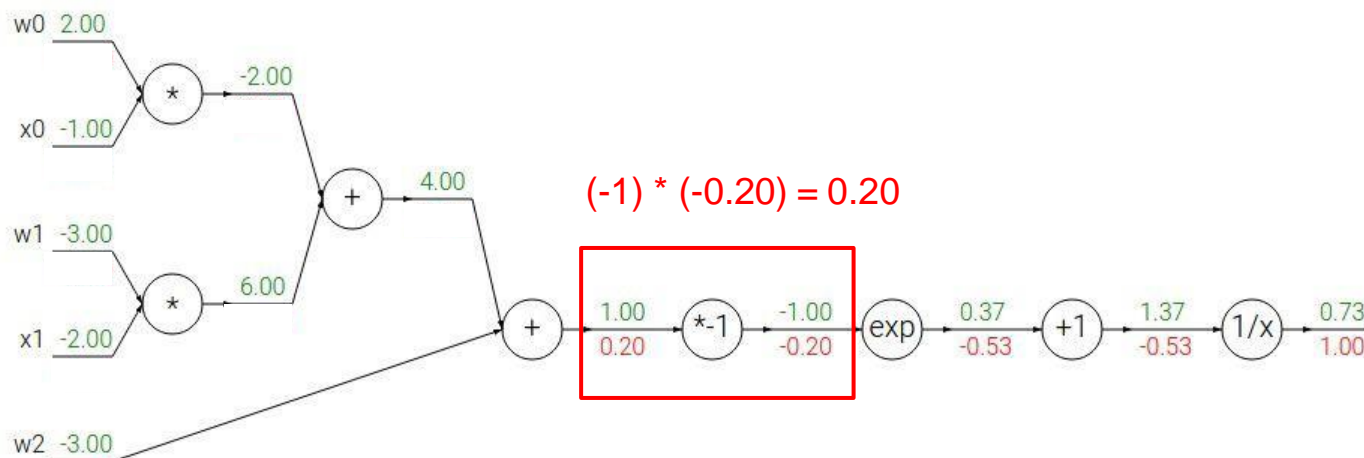
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

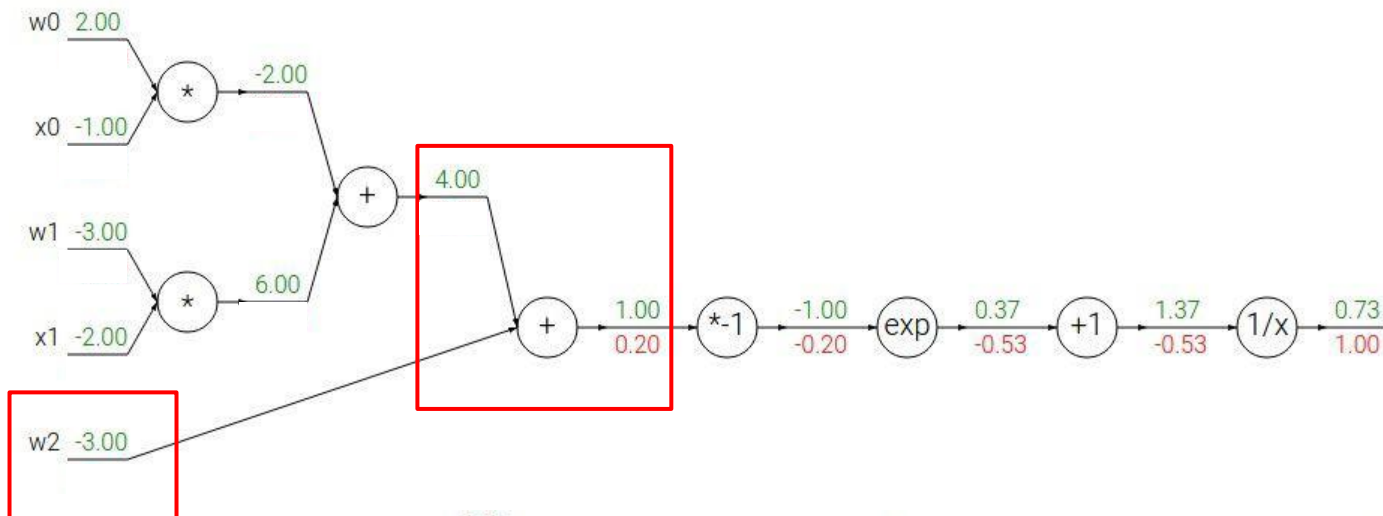
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



$f(x) = e^x$	\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	$\frac{df}{dx} = 1$

Another example:

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



$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

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

$$f(x) = \frac{1}{x}$$

→

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

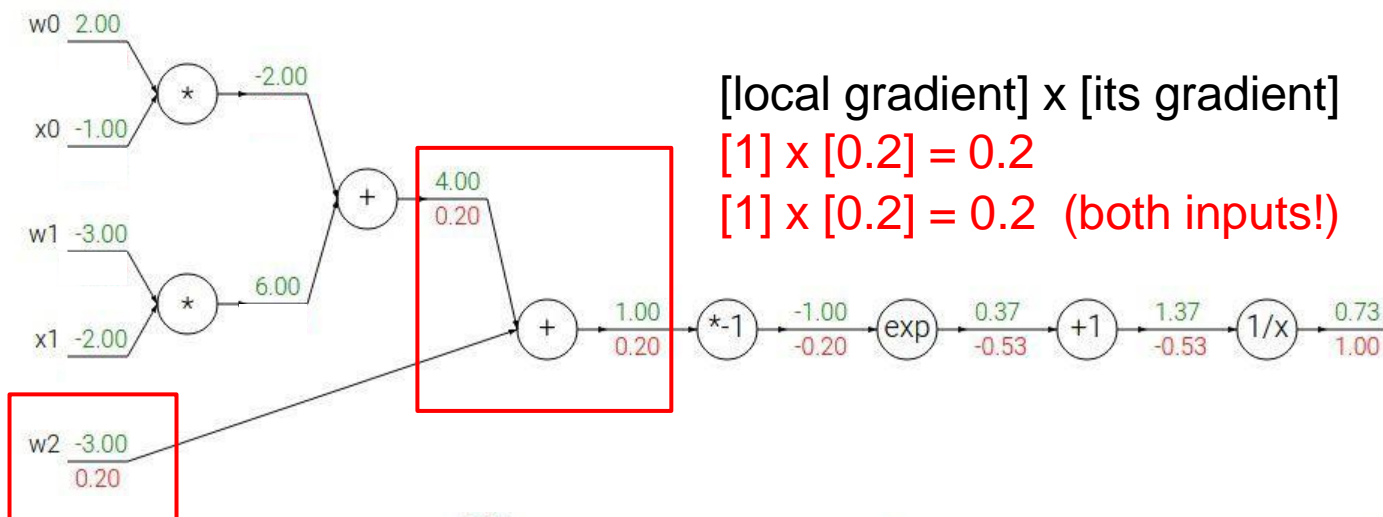
$$f_c(x) = c + x$$

→

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

Another example:

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



[local gradient] x [its gradient]

$$[1] \times [0.2] = 0.2$$

$$[1] \times [0.2] = 0.2 \text{ (both inputs!)}$$

$$f(x) = e^x$$

→

$$\frac{df}{dx} = e^x$$

$$f_a(x) = ax$$

→

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

$$f(x) = \frac{1}{x}$$

→

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

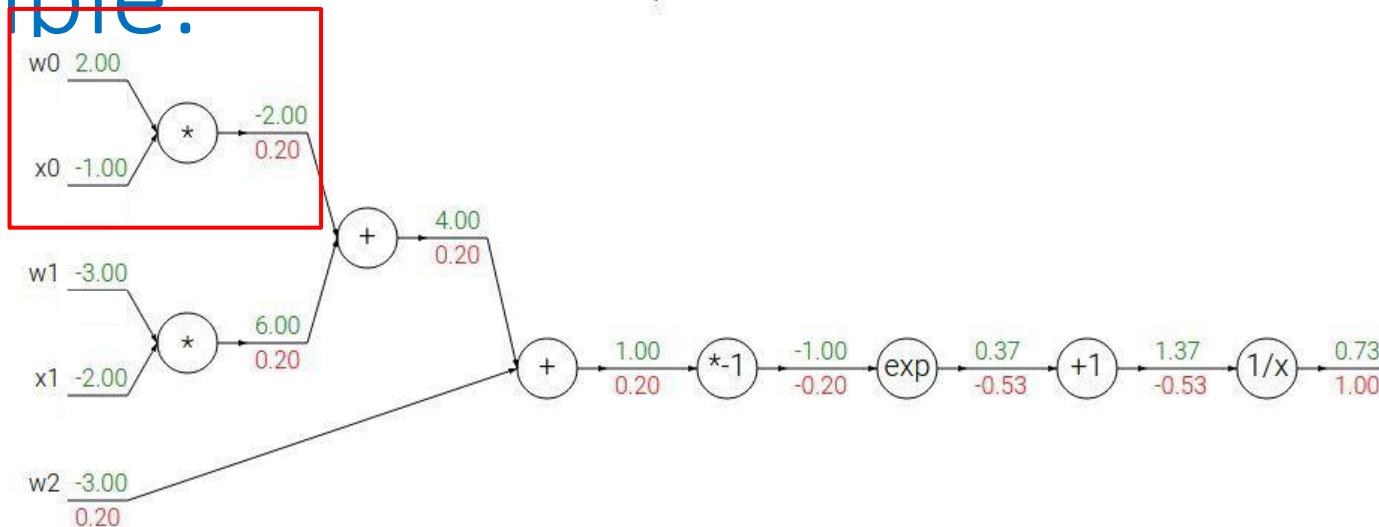
$$f_c(x) = c + x$$

→

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

Another example:

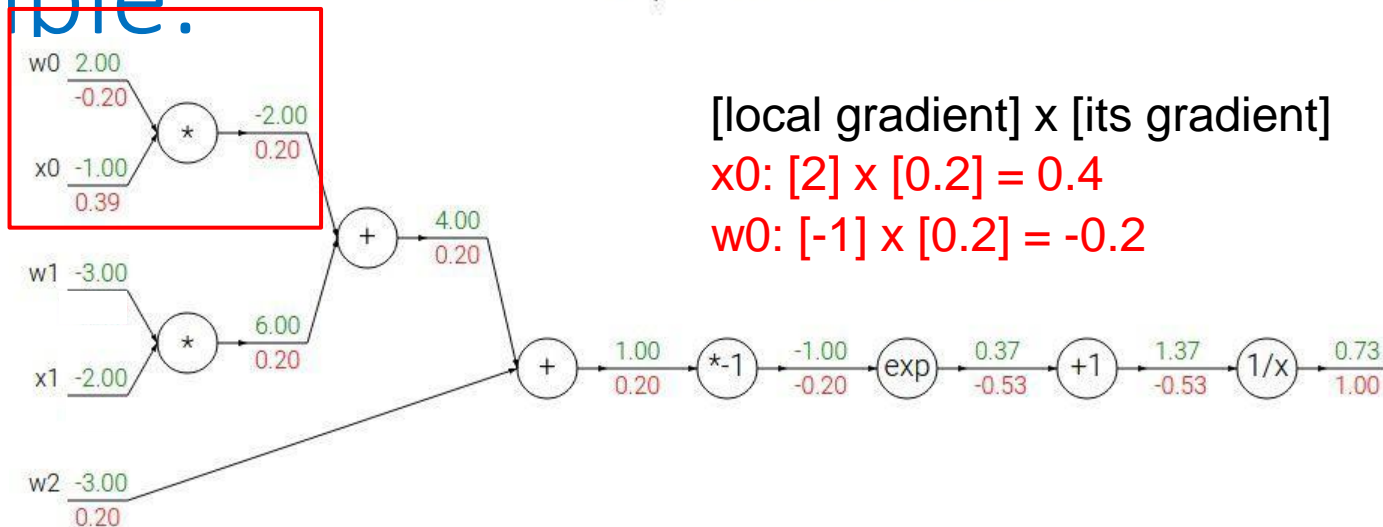
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



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

Another example:

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



[local gradient] x [its gradient]

$$x_0: [2] \times [0.2] = 0.4$$

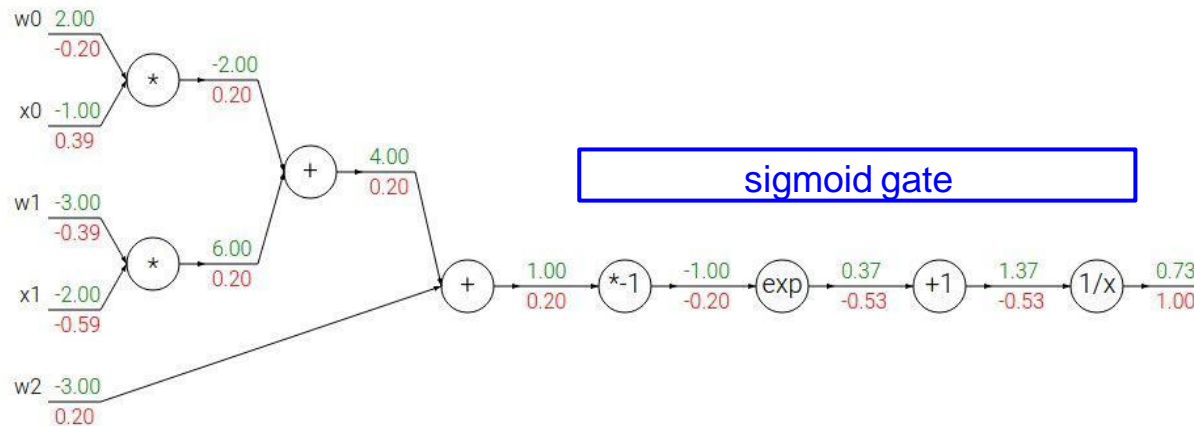
$$w_0: [-1] \times [0.2] = -0.2$$

$f(x) = e^x$	\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	$\frac{df}{dx} = 1$

$$f(w, x) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2 x_2)}}$$

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

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



$$f(w, x) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2 x_2)}}$$

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

sigmoid function

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

