Announcements

Reminder: self-grading forms for ps1 and ps2 due 10/5 at midnight (Boston)

- ps3 out today, due 10/8 (1 week)

- Midterm practice questions out next week

Today: Outline

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

Assignment Project Exam Help

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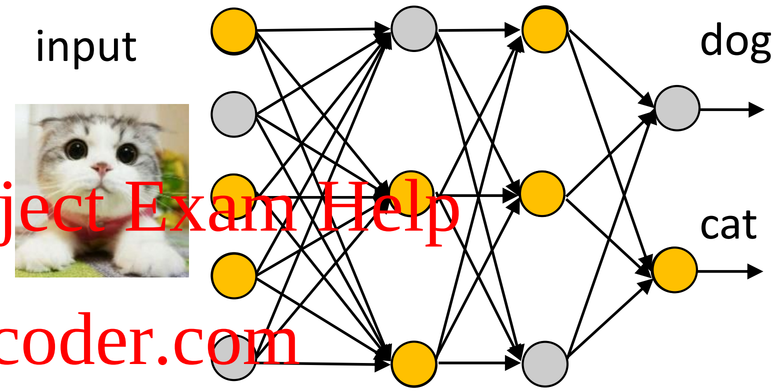
Neural Networks II

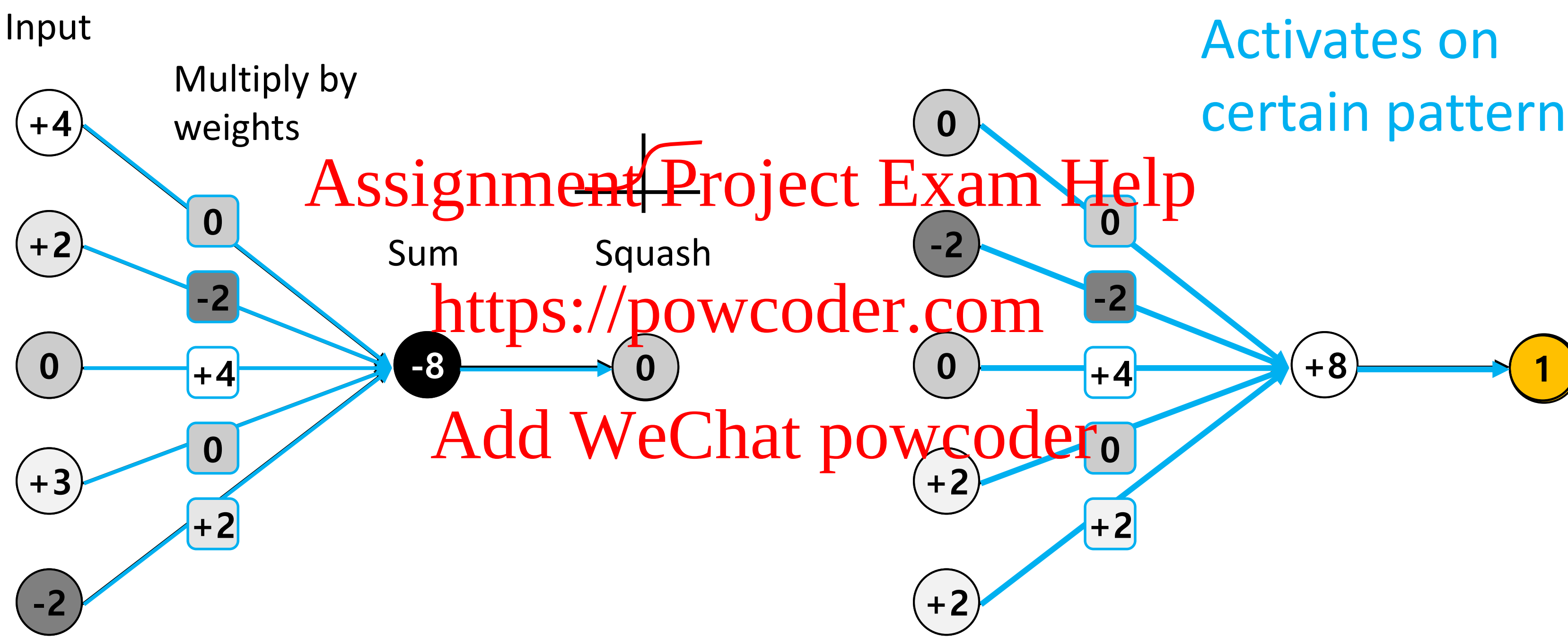
Learning

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)

Artificial Neuron: Activation

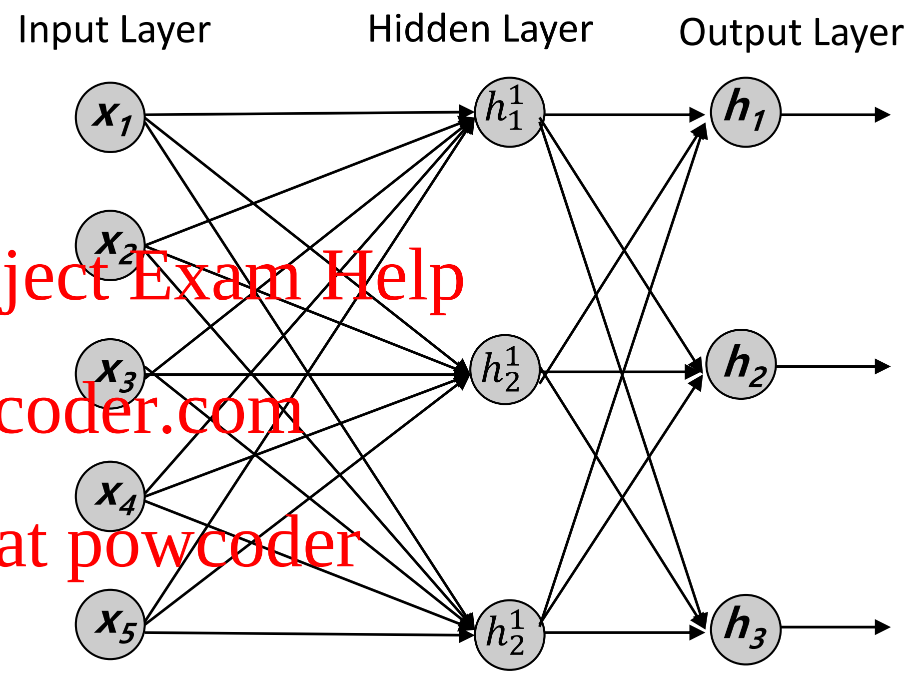


Activates on certain patterns

Artificial Neural Network: notation

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

hidden layer activations



Artificial Neural Network: notation

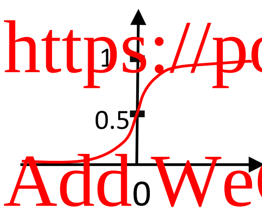
input

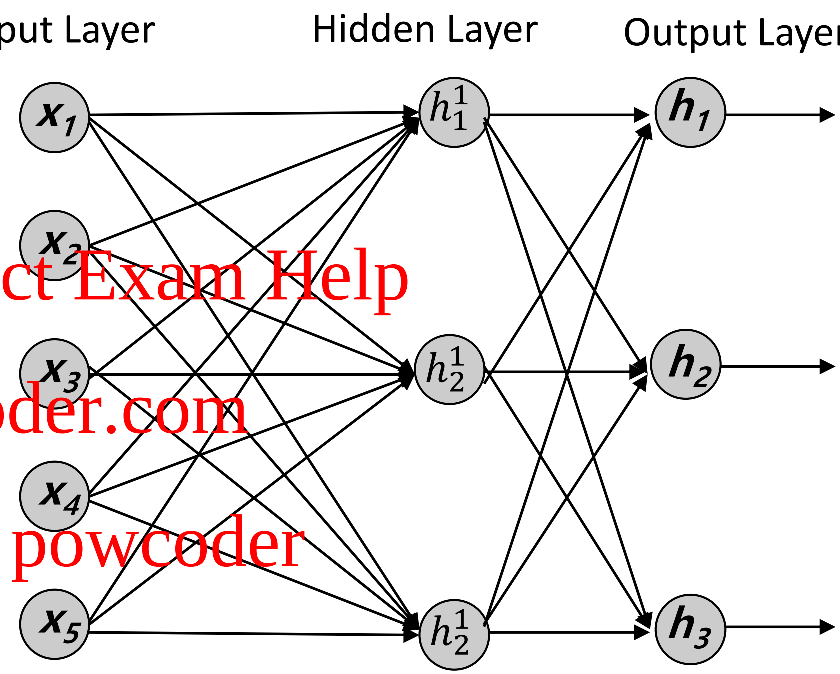
$$x = \begin{bmatrix} x_1 \\ \dots \\ x_5 \end{bmatrix}$$

hidden layer activations

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

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





output

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

weights

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

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

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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?

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

$$f(\theta) = f_1(f_2(f_3(\theta))) \qquad f'(\theta) =$$

- 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:

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

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

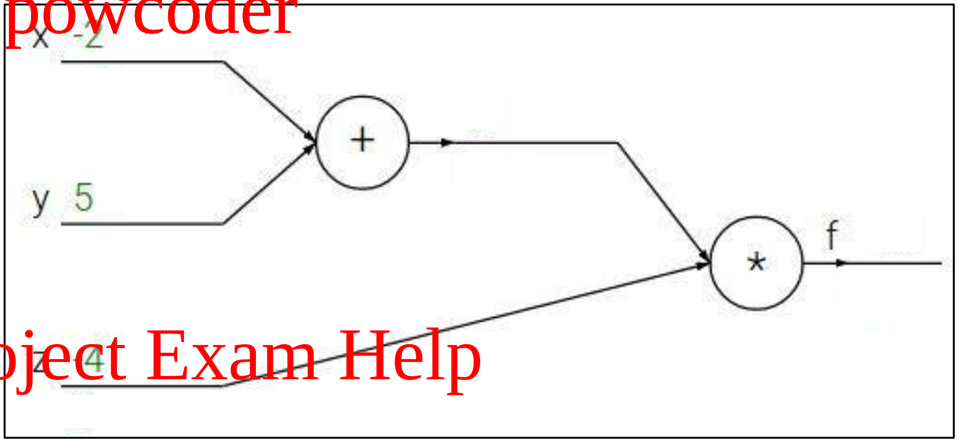
$$\frac{\partial f}{\partial \theta_3} = \frac{\partial f_1}{\partial f_2}\Big(f_2\big(f_3(\theta)\big)\Big) * \frac{\partial f_2}{\partial f_3}\big(f_3(\theta)\big) * \frac{\partial f_3}{\partial \theta_3}(\theta)$$

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

Chain Rule with a Computational Graph

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

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



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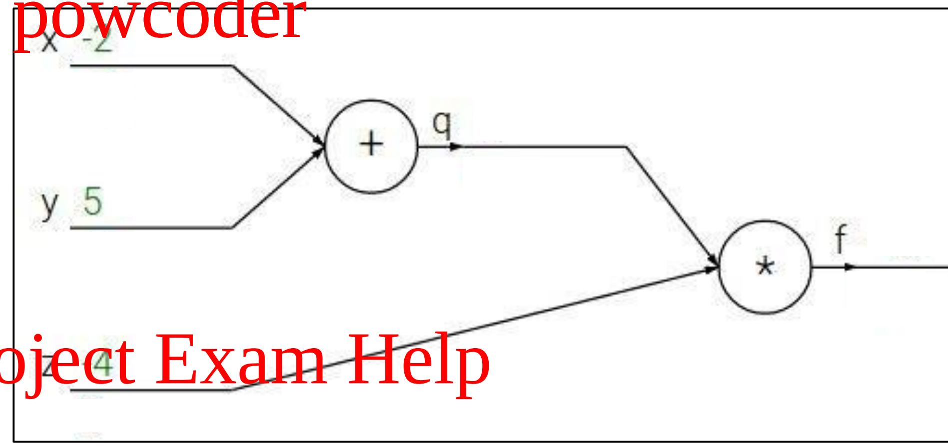

$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

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

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

Computation Graph: Forward

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

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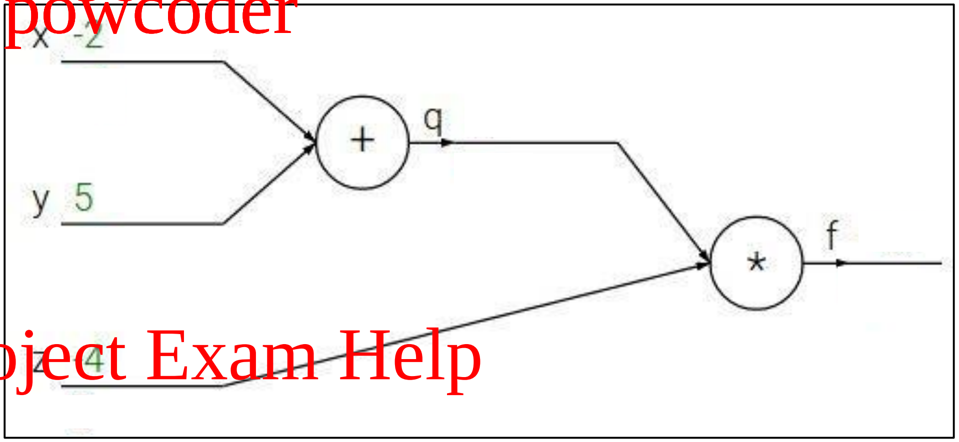


$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

compute values

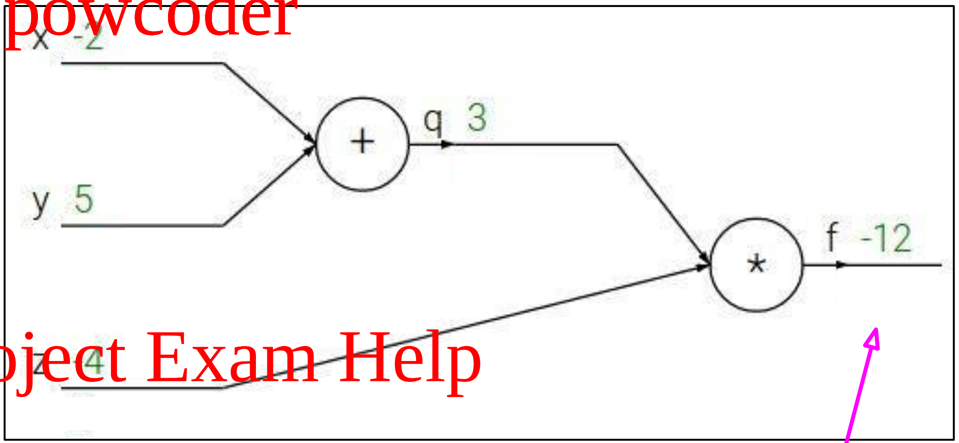
$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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

Computational Graph: Backward

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

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



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

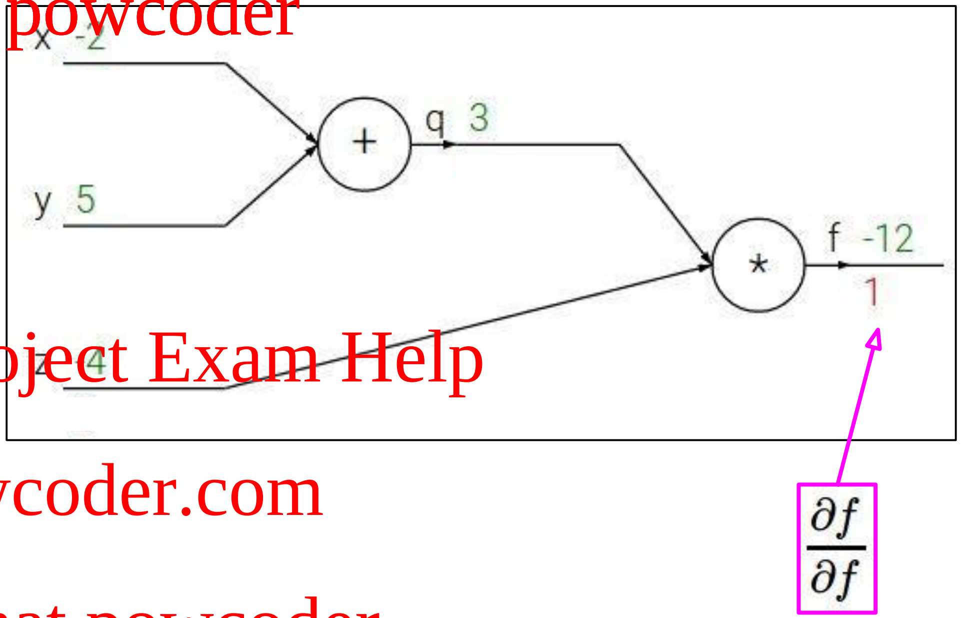
compute gradients

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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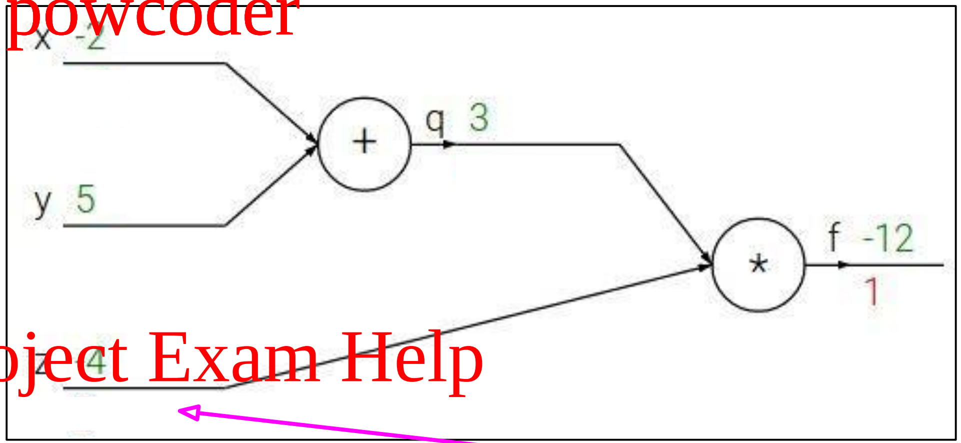

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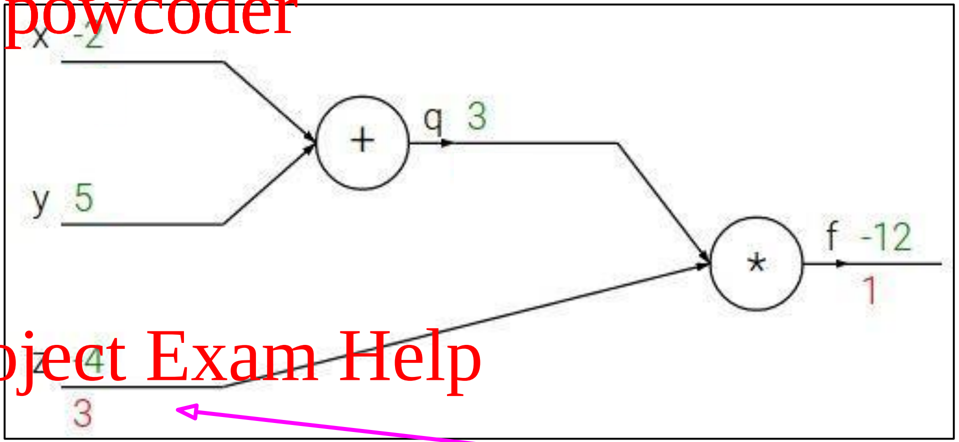

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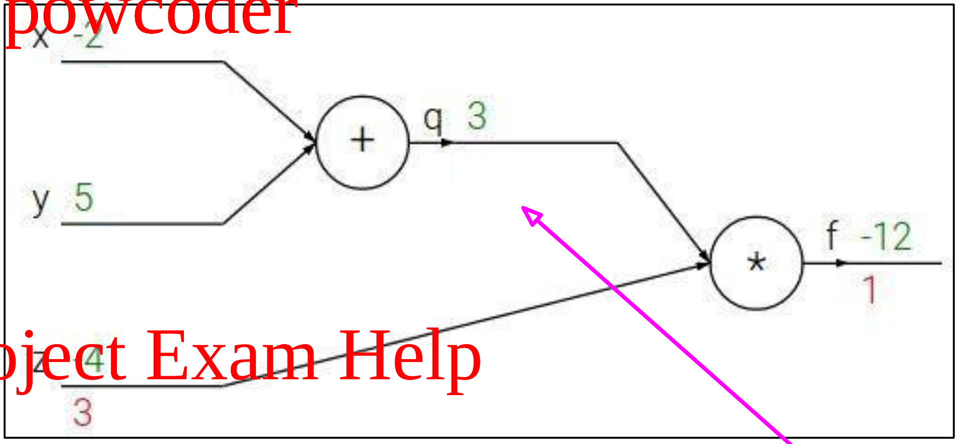

$$\frac{\partial f}{\partial q}$$

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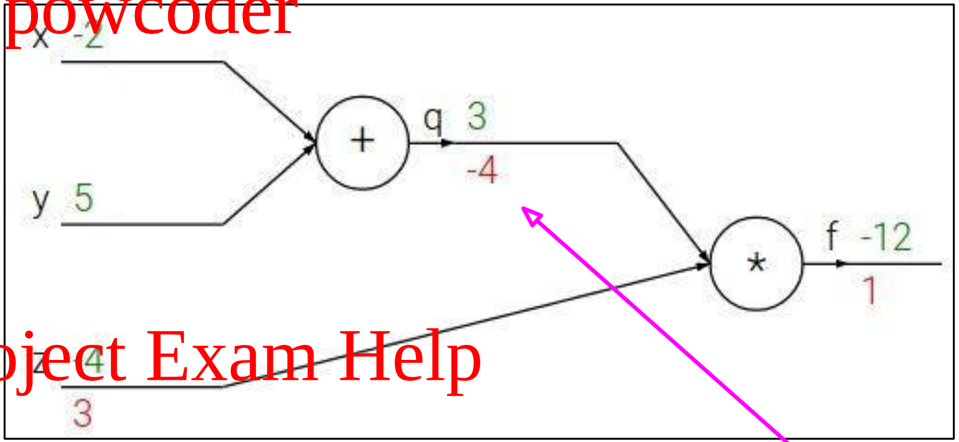

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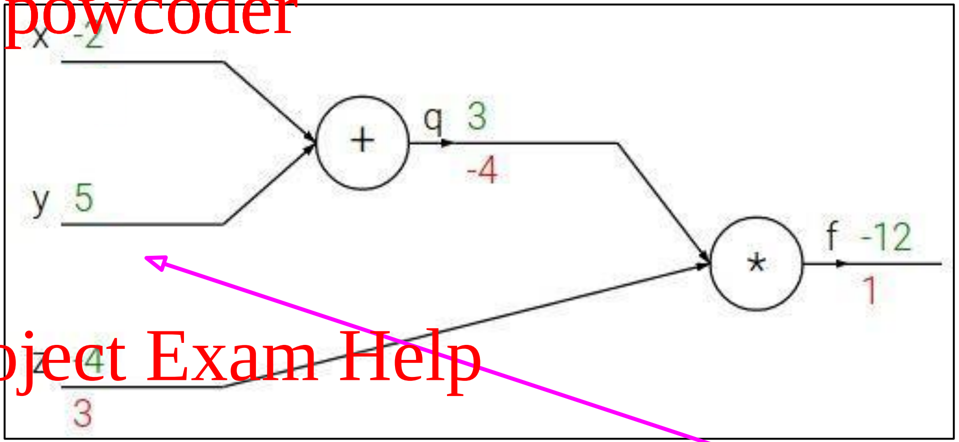

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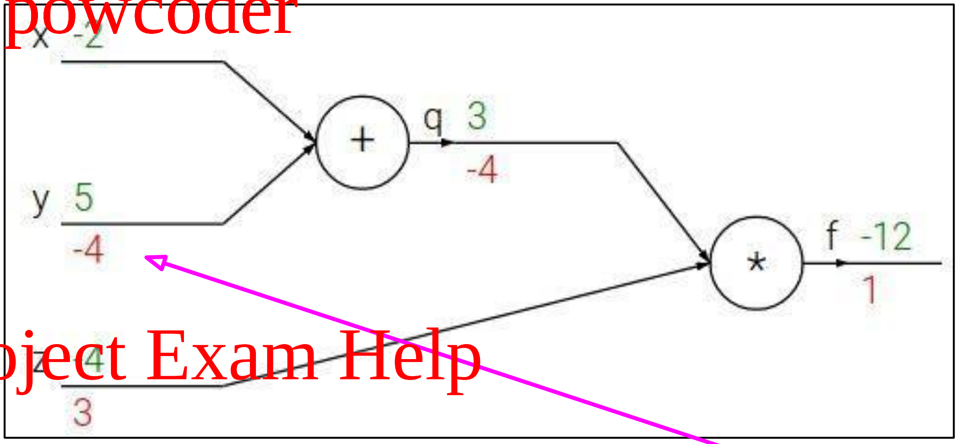

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$$\boxed{\frac{\partial f}{\partial y}}$$

Chain rule:

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

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

Computation Graph: Backward

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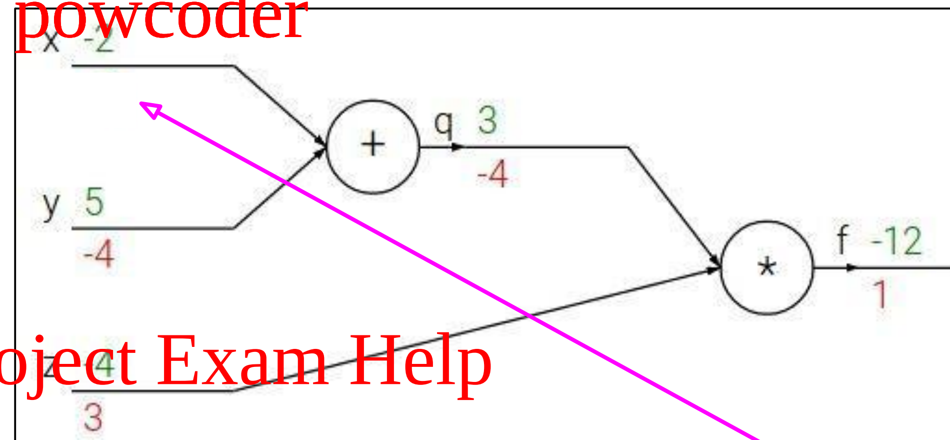

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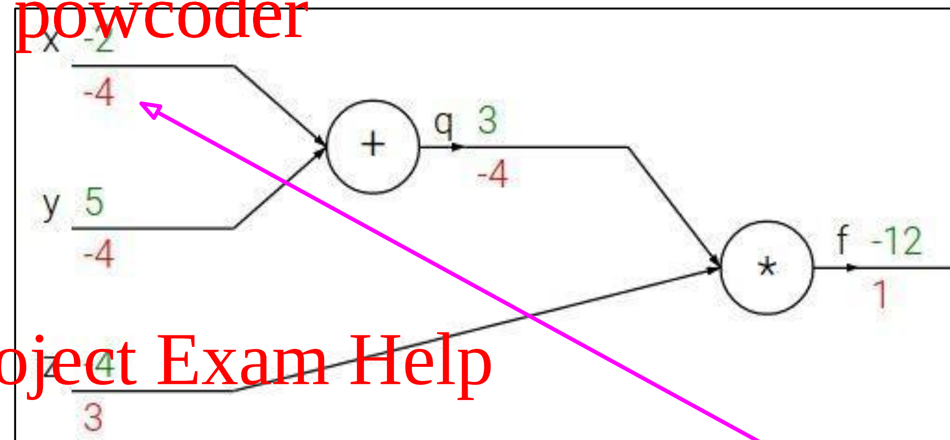

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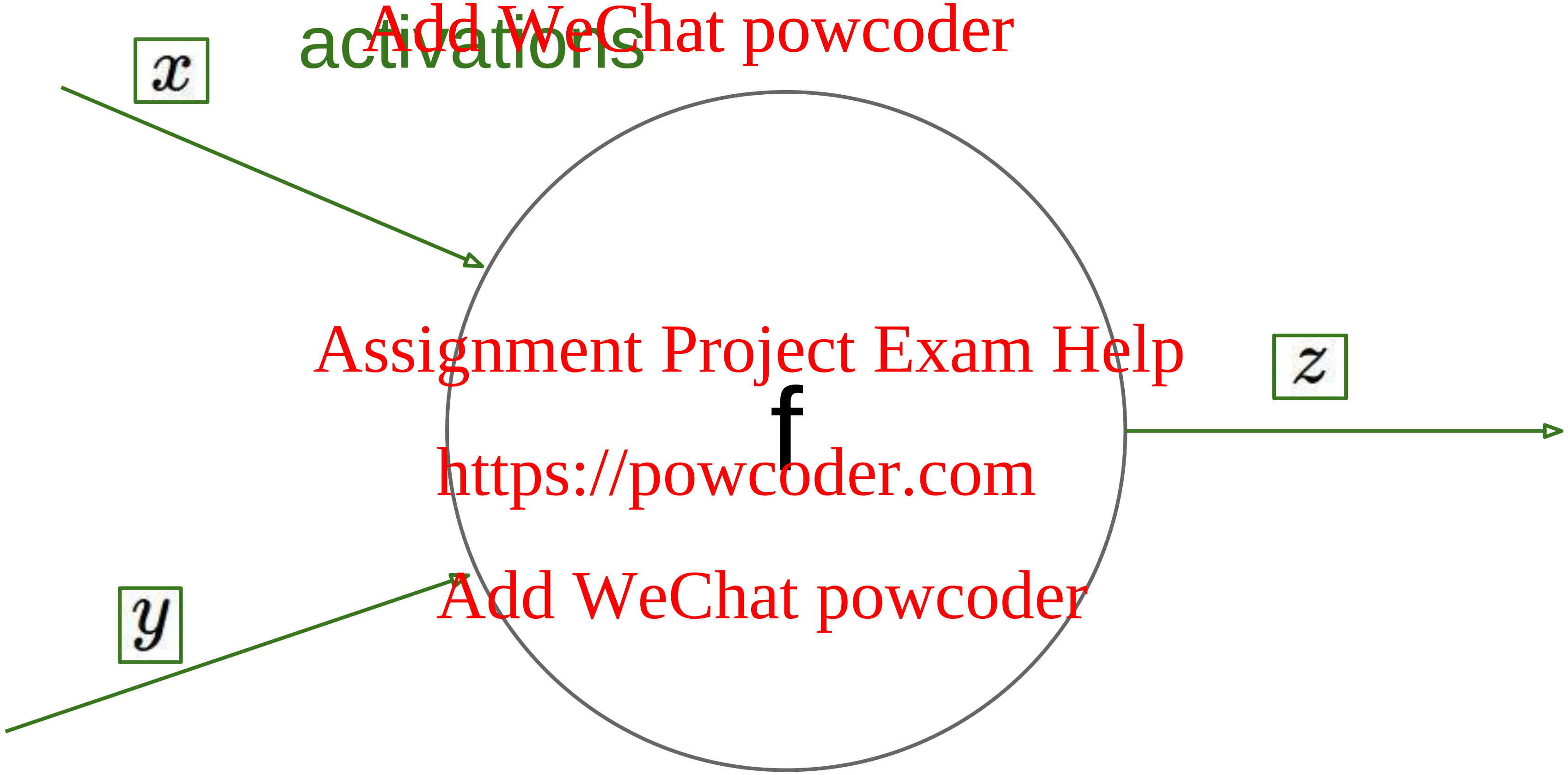
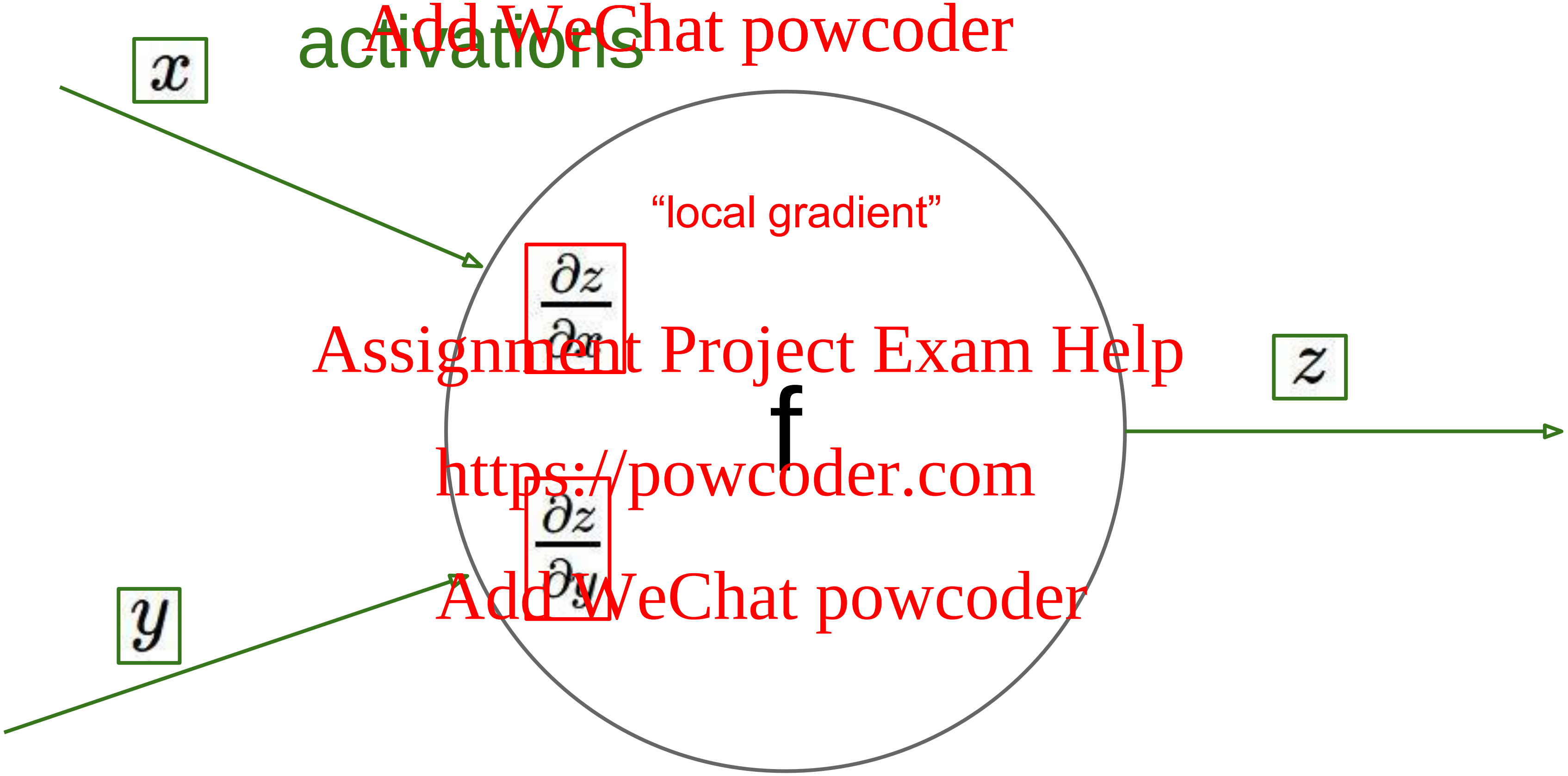

activations
x
y
z
f


activations
x
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z
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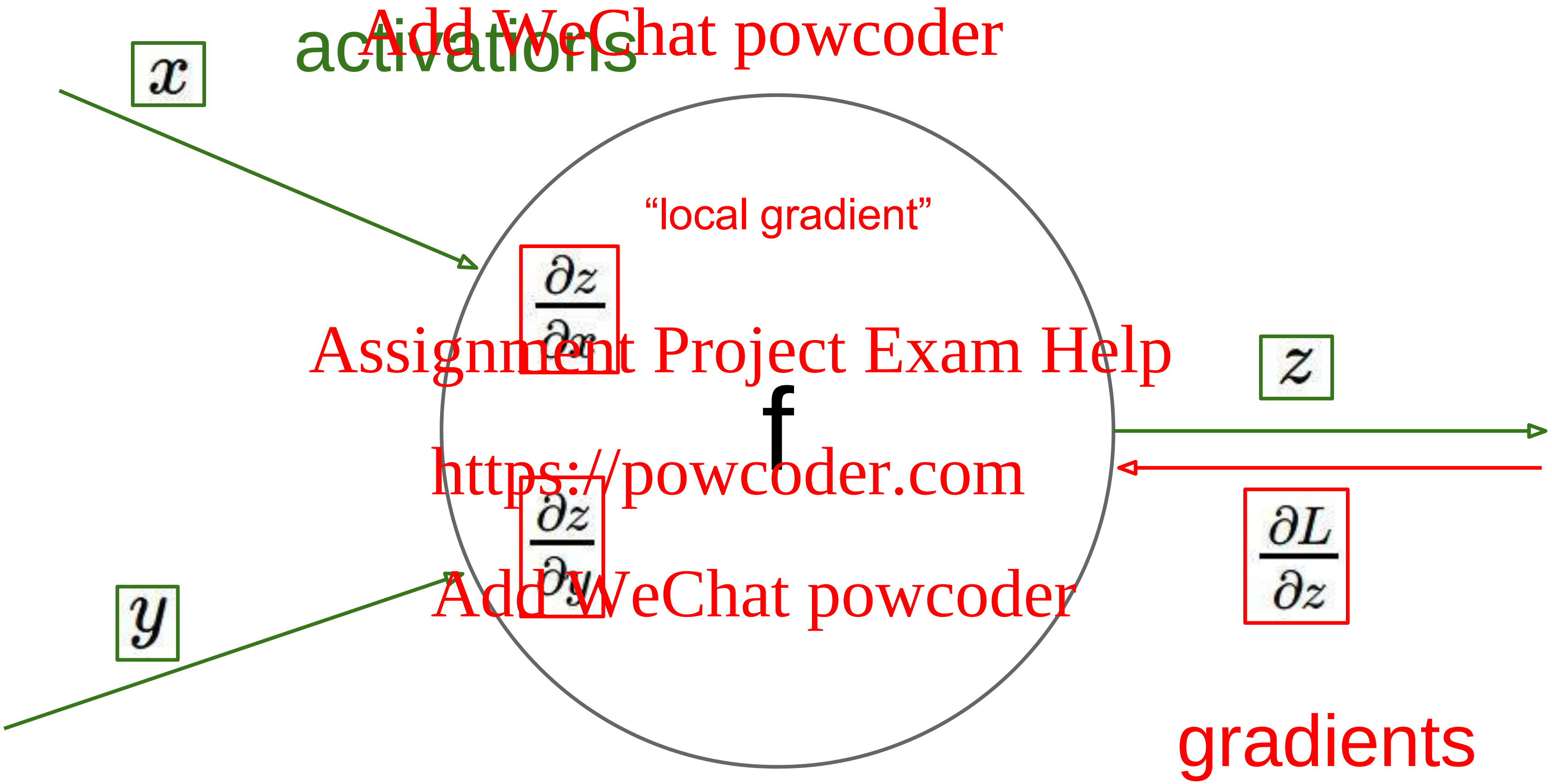
“local gradient”
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$



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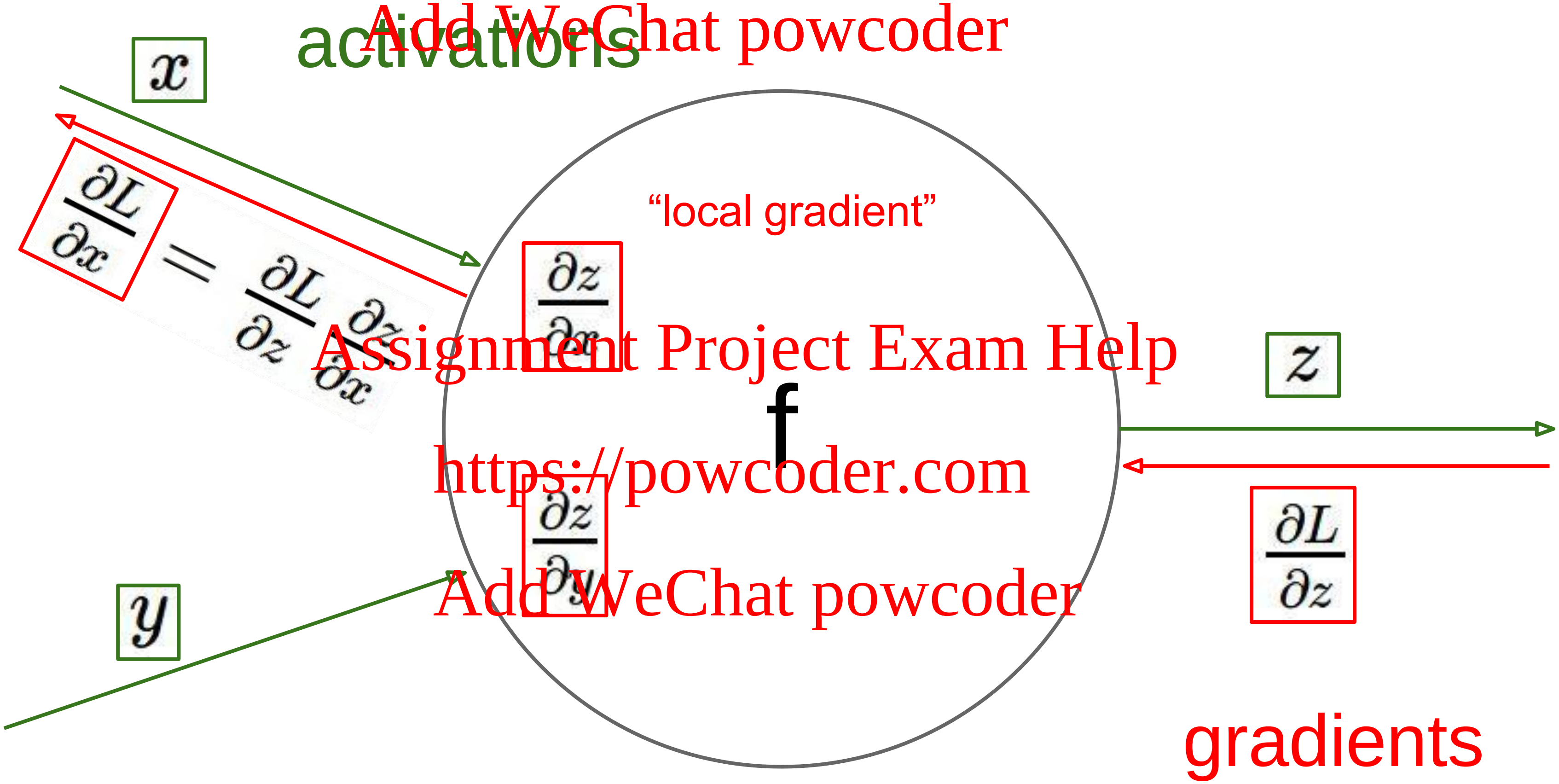
z
f
$\frac{\partial z}{\partial y}$
y
$\frac{\partial L}{\partial z}$
gradients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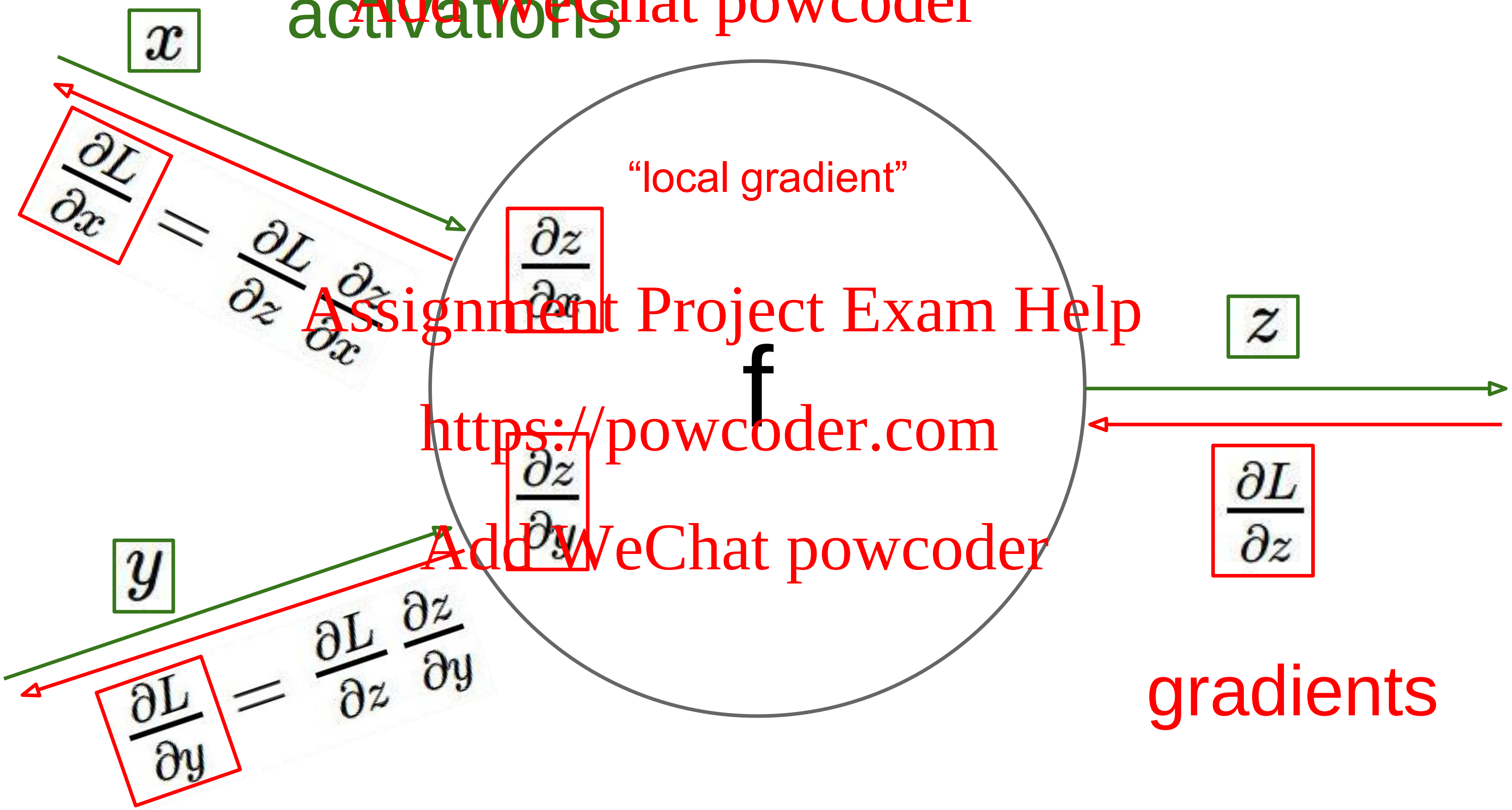
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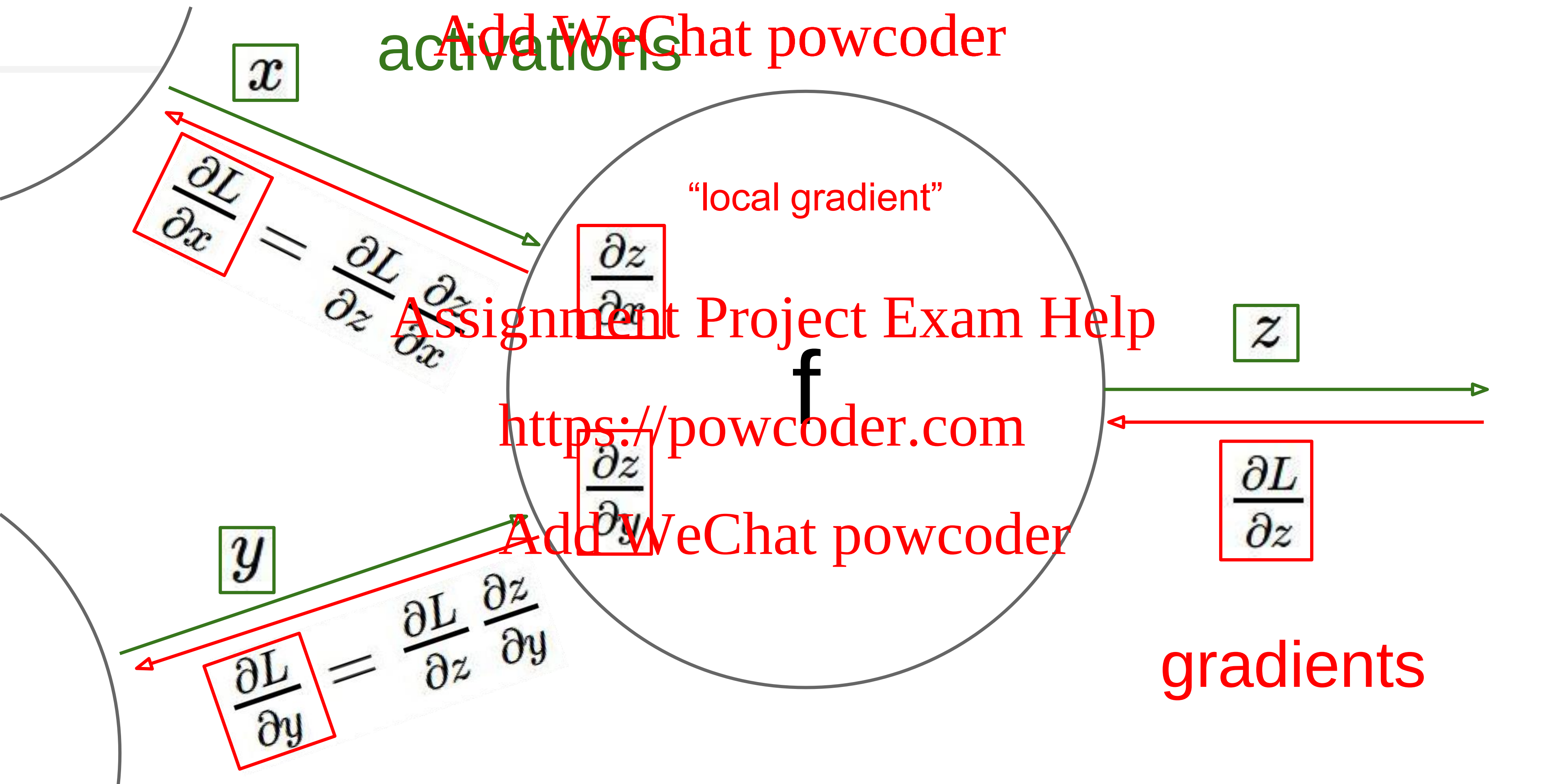
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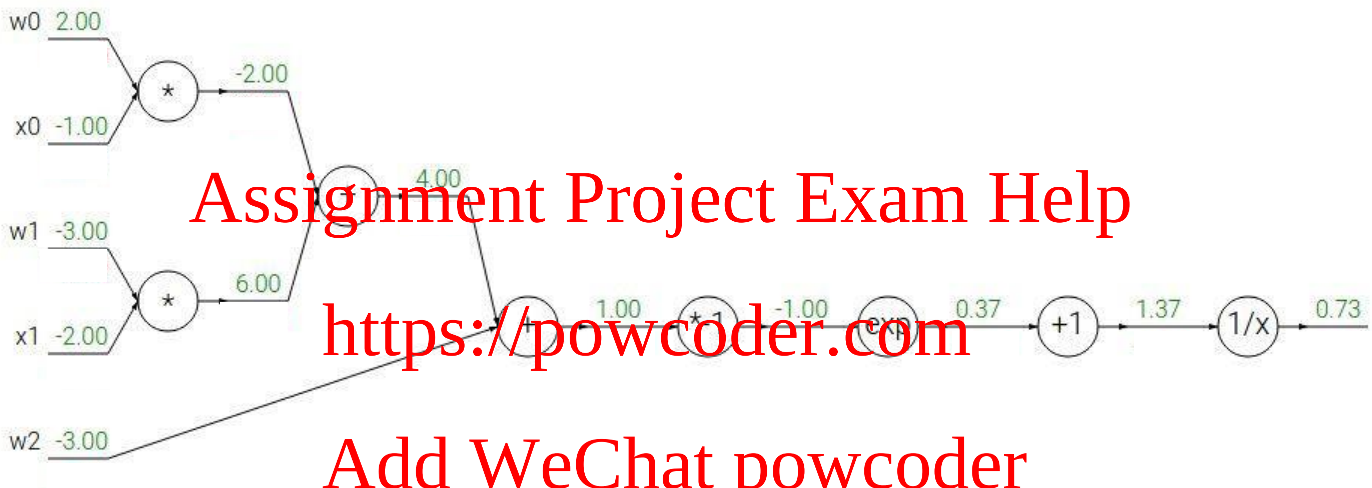
z
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients

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



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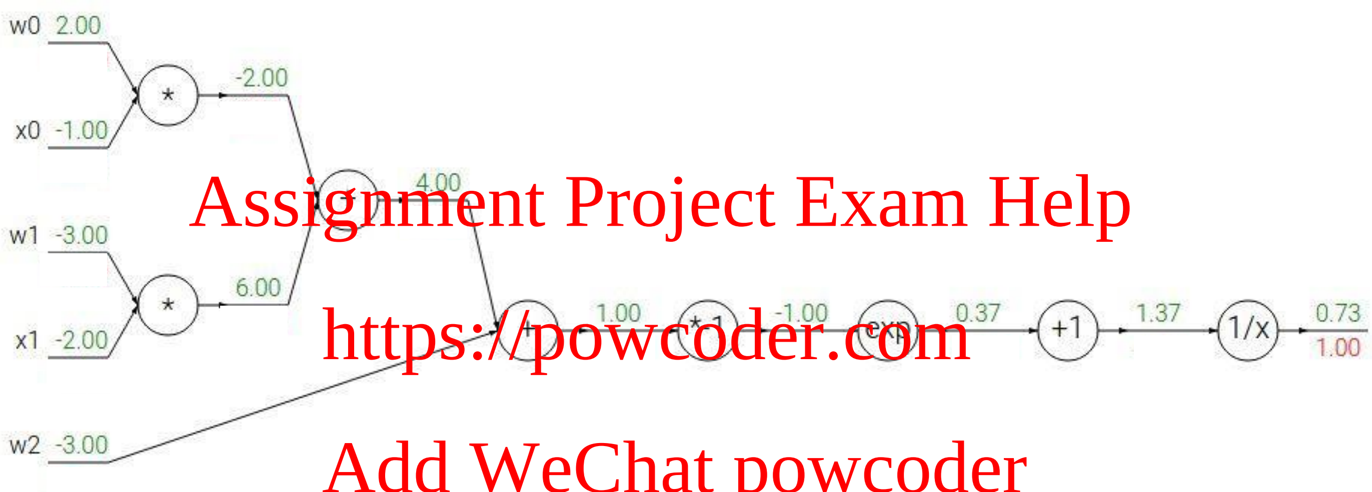

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x \qquad\qquad f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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

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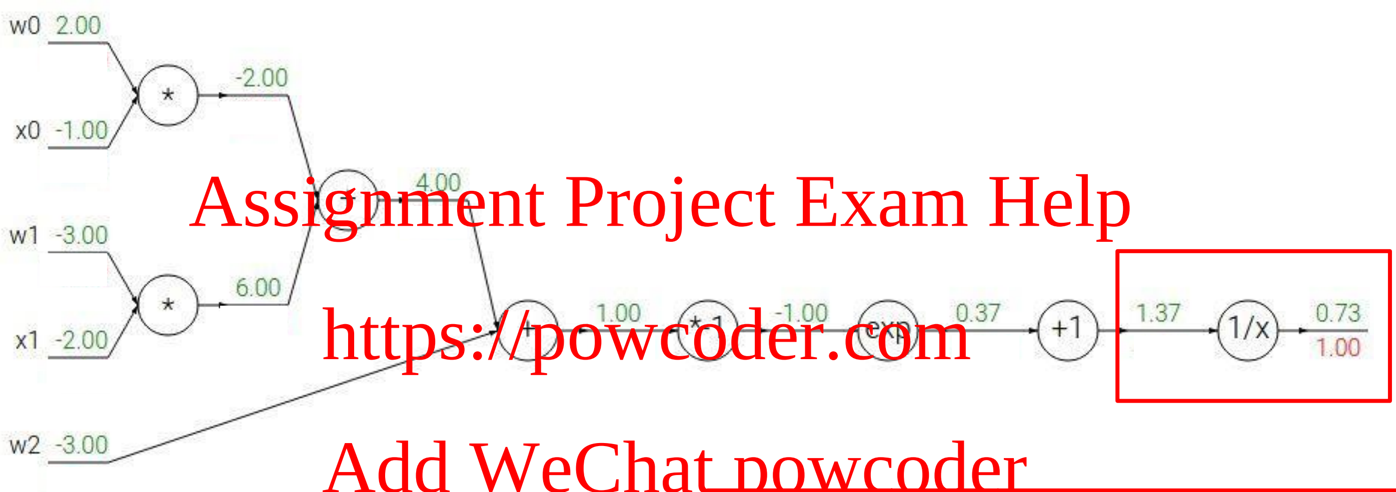

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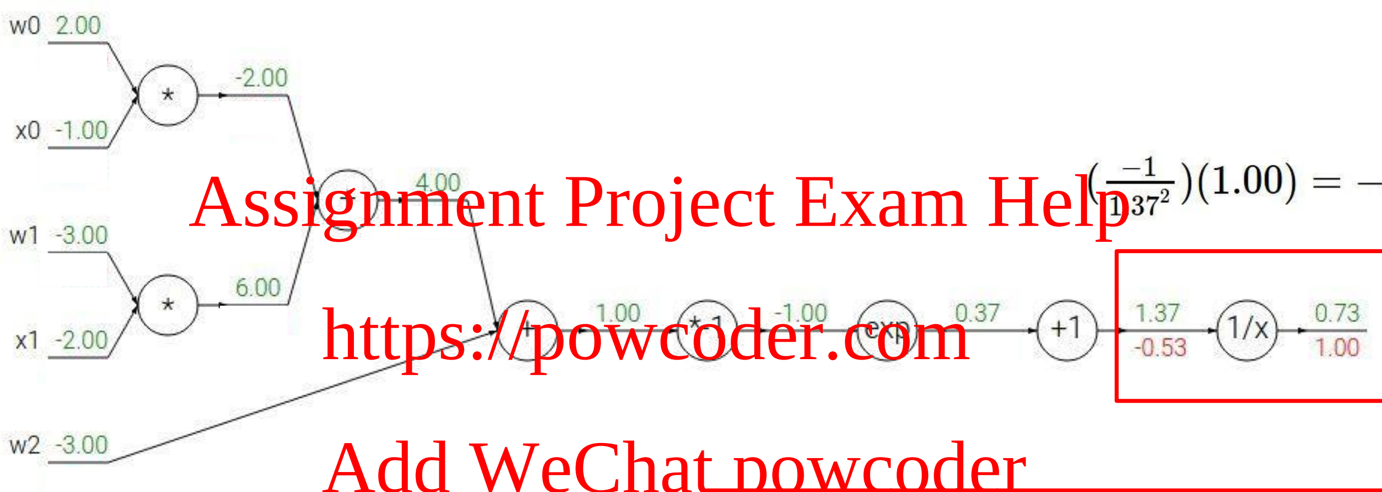
Another example: $f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$

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



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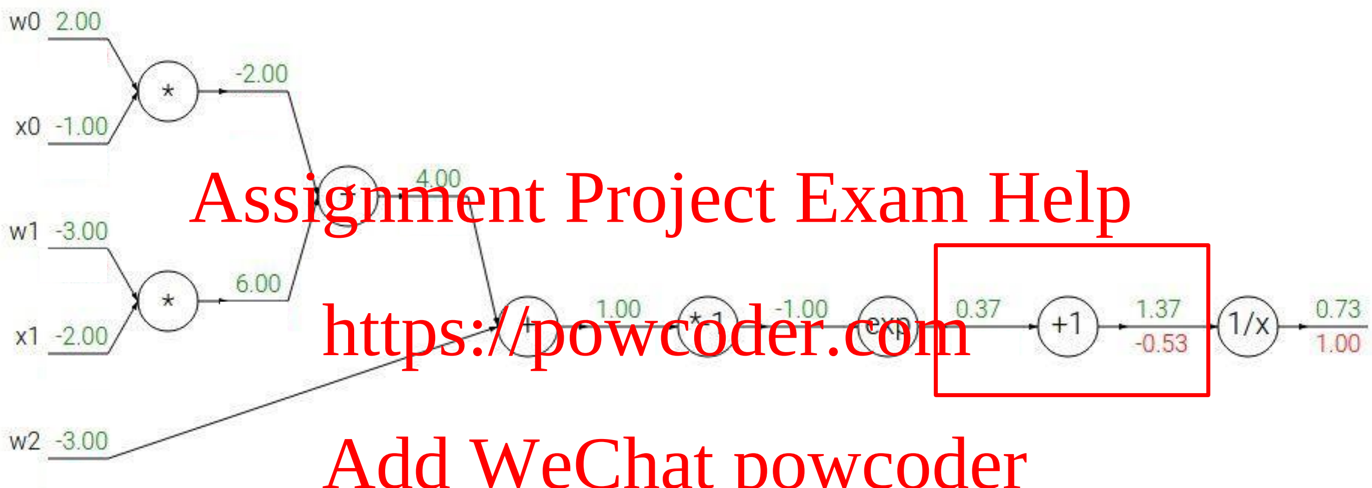

$f(x) = e^x \rightarrow \dfrac{df}{dx} = e^x$		$f(x) = \dfrac{1}{x} \rightarrow \dfrac{df}{dx} = -1/x^2$
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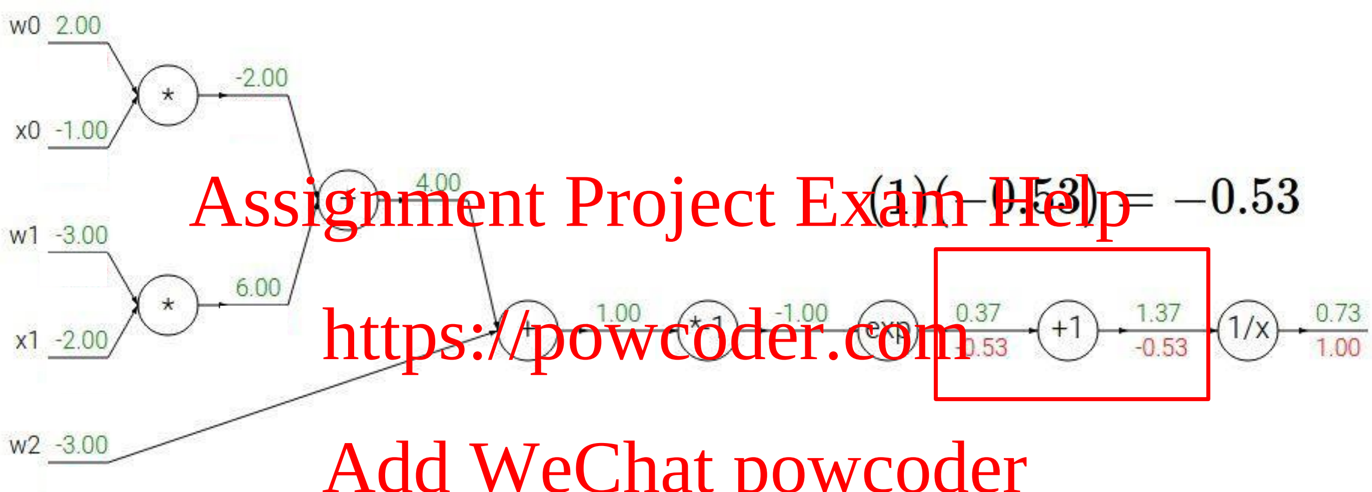

$$(1)(-0.53) = -0.53$$

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

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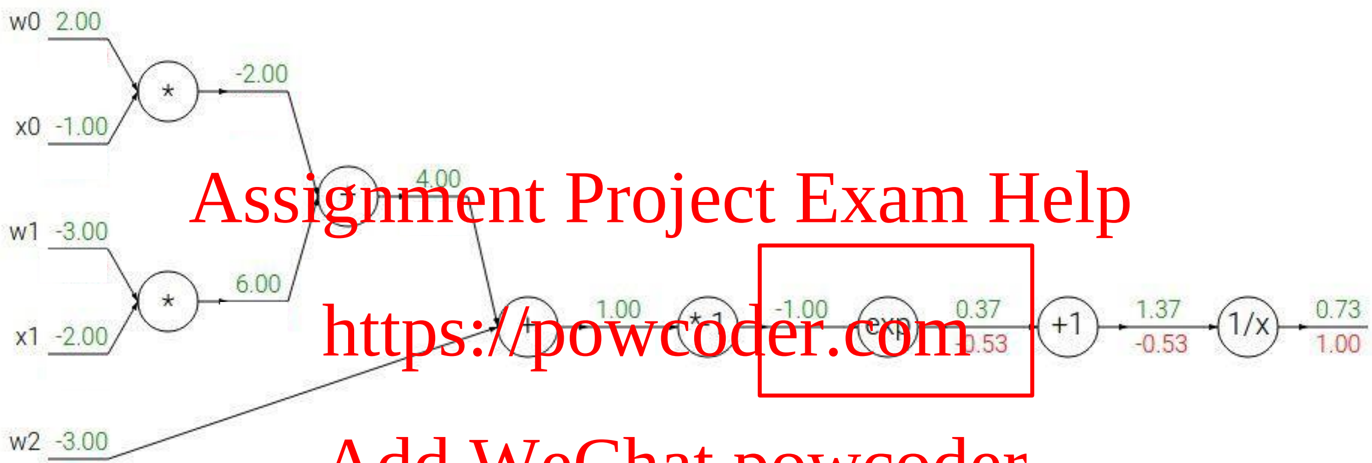

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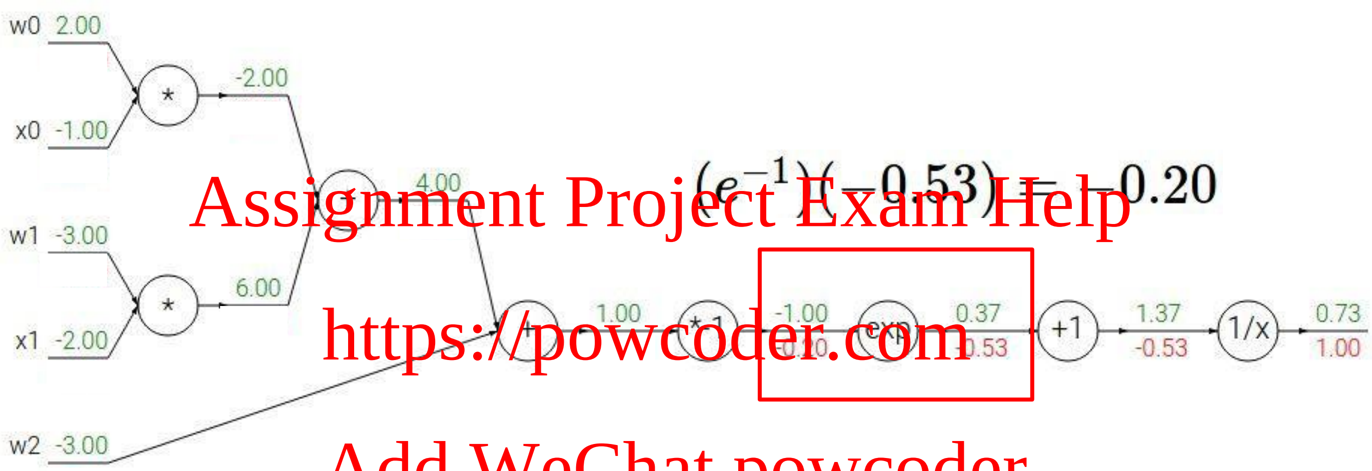
Another example: $f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$



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

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

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

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

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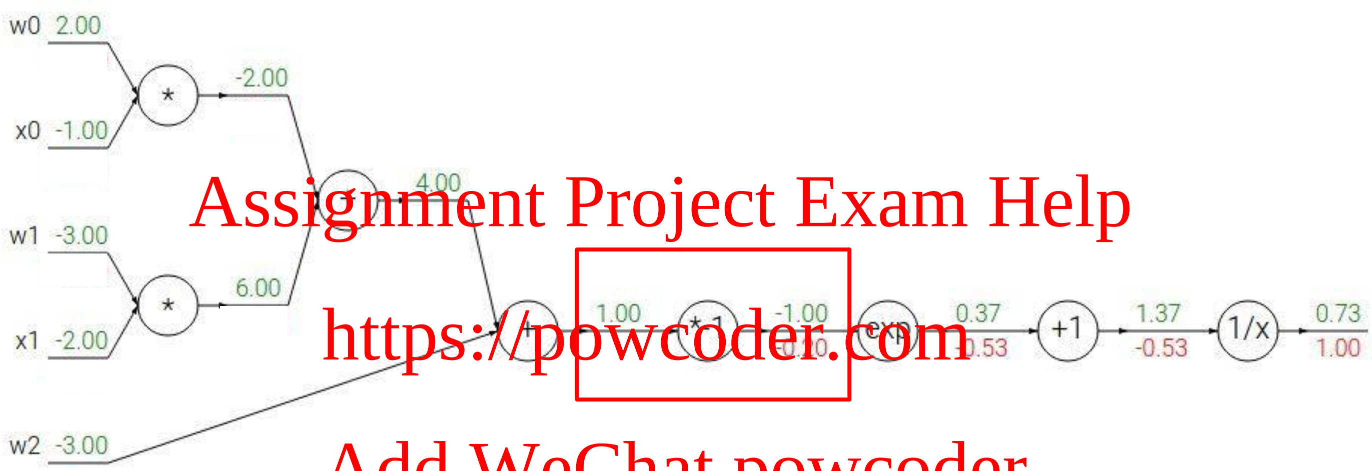

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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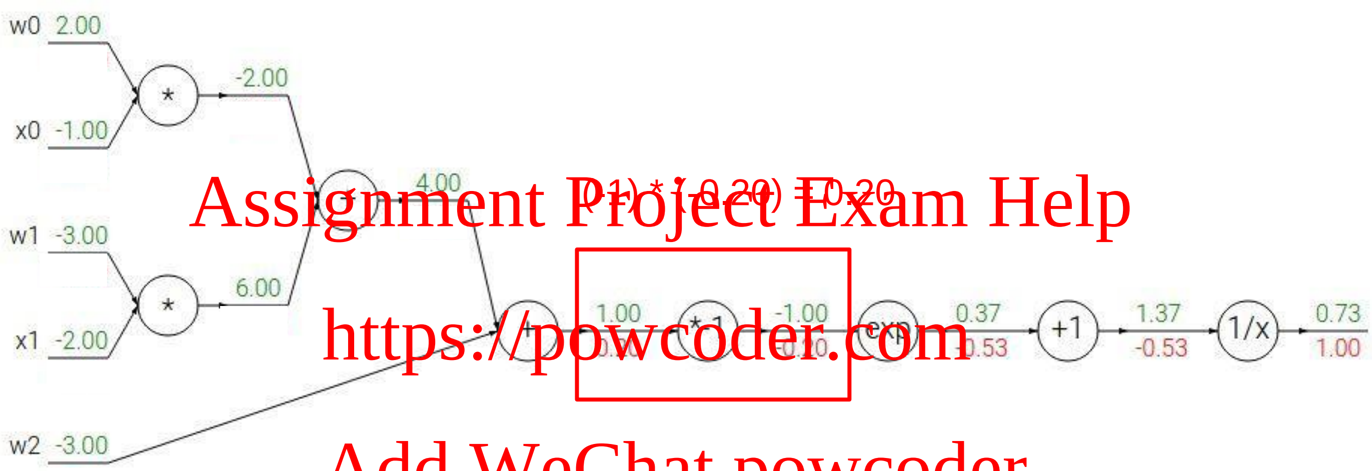

$f(x) = e^x \quad \rightarrow \quad \dfrac{df}{dx} = e^x$

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

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

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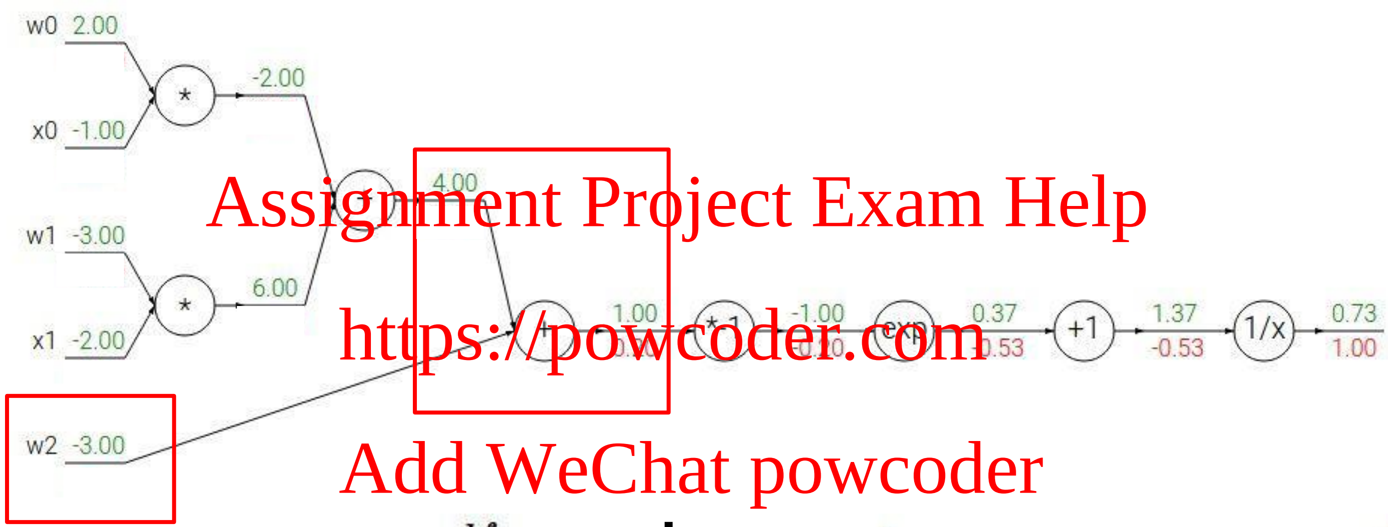
Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



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

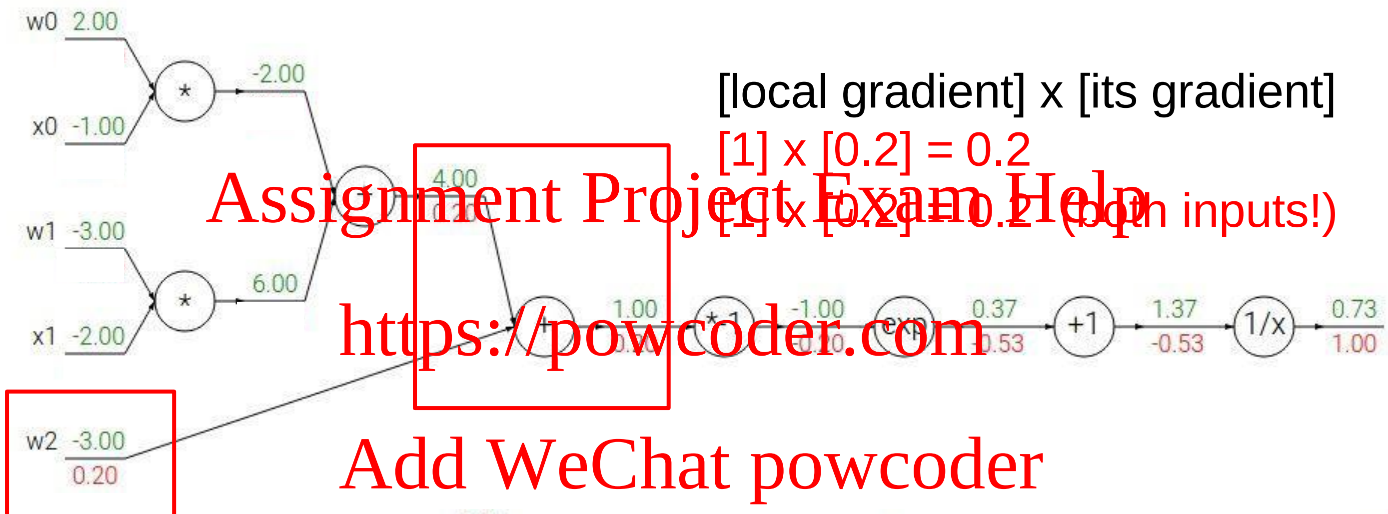
$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a \qquad\qquad f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

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

[local gradient] x [its gradient]

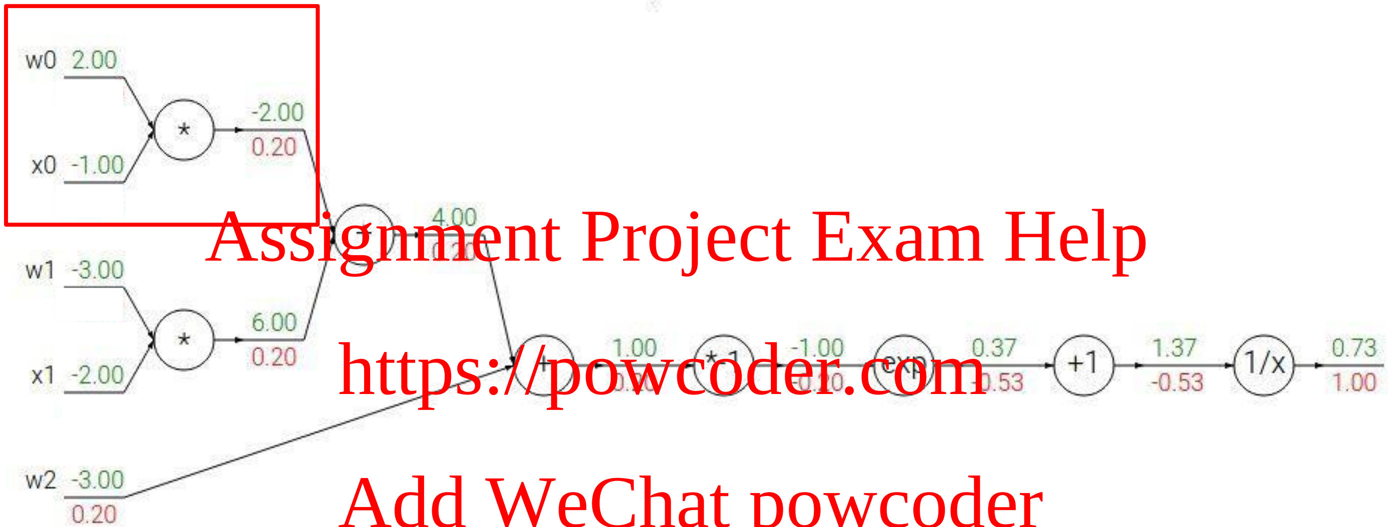
[1] x [0.2] = 0.2

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



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

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



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

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

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

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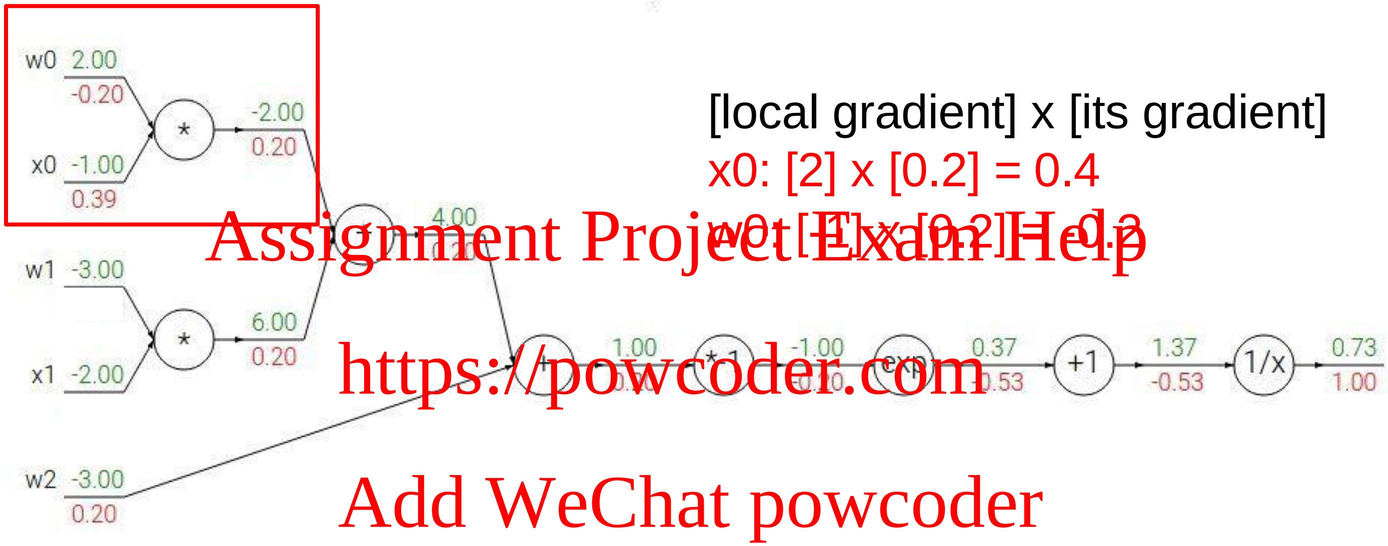
Another example: $f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$



[local gradient] x [its gradient]
x0: [2] x [0.2] = 0.4
w0: [-1] x [0.2] = -0.2

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

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

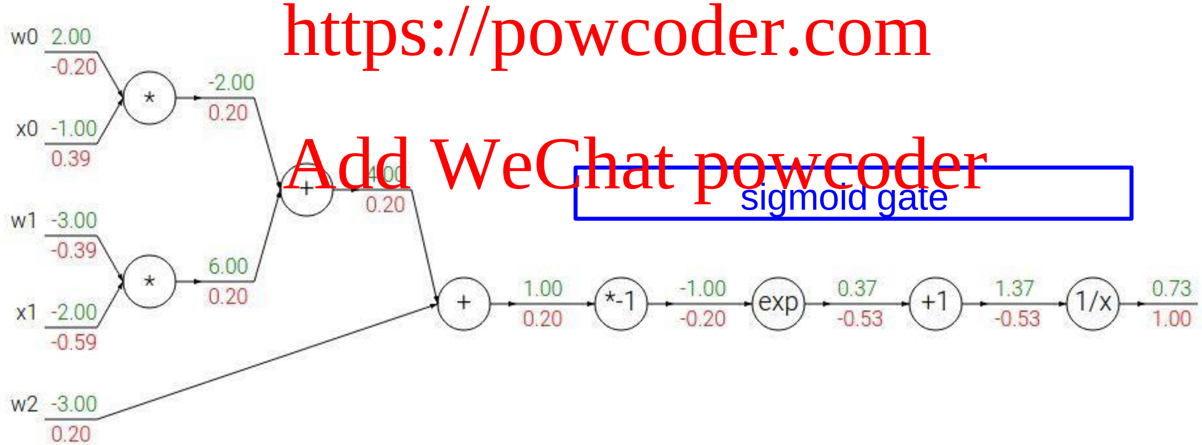
$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$

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

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

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

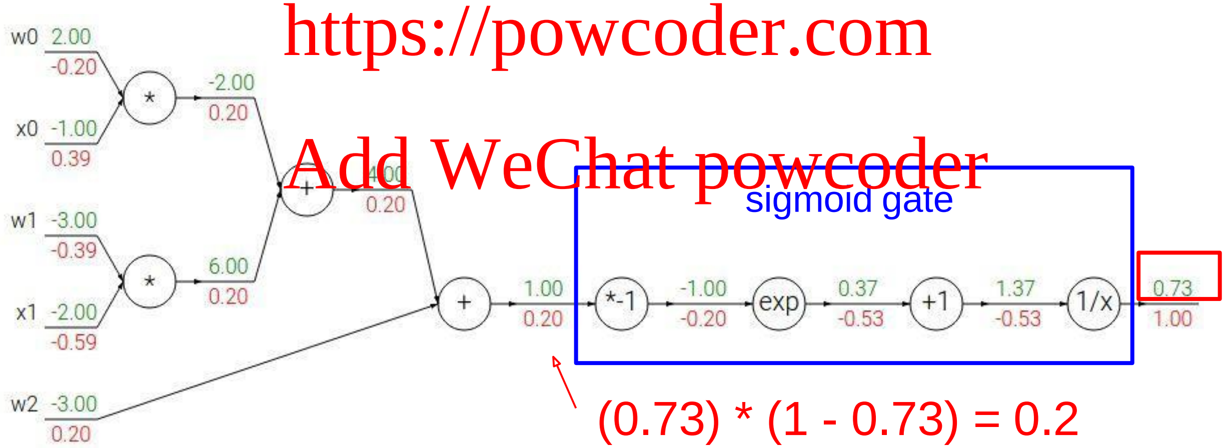
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\,\sigma(x)$$



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

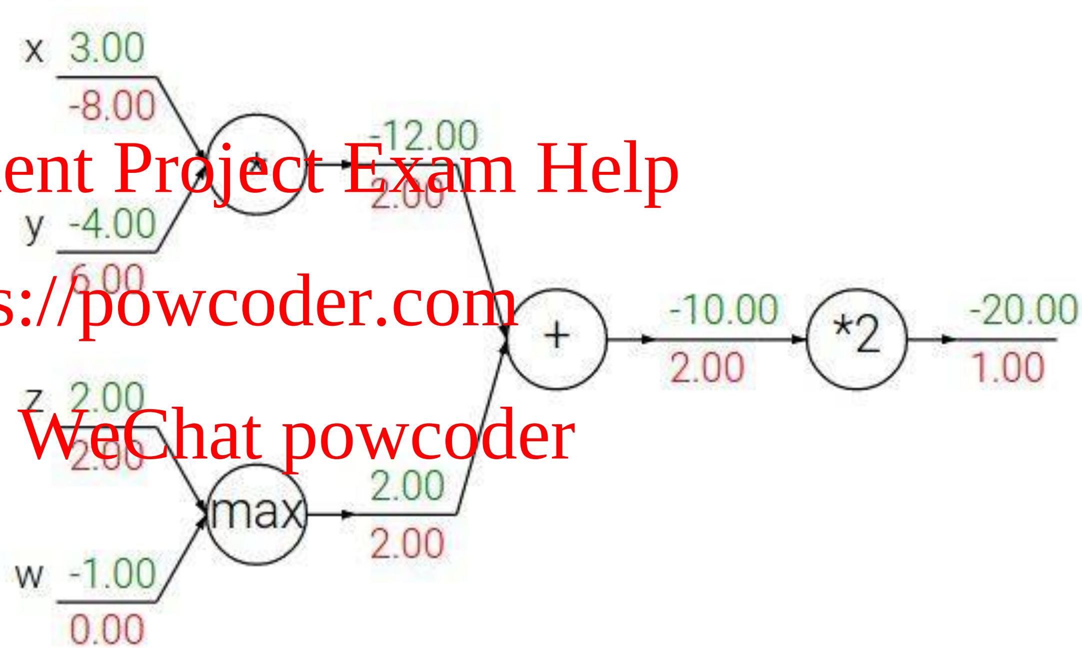
$$\boxed{\sigma(x) = \frac{1}{1+e^{-x}}}$$ sigmoid function

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



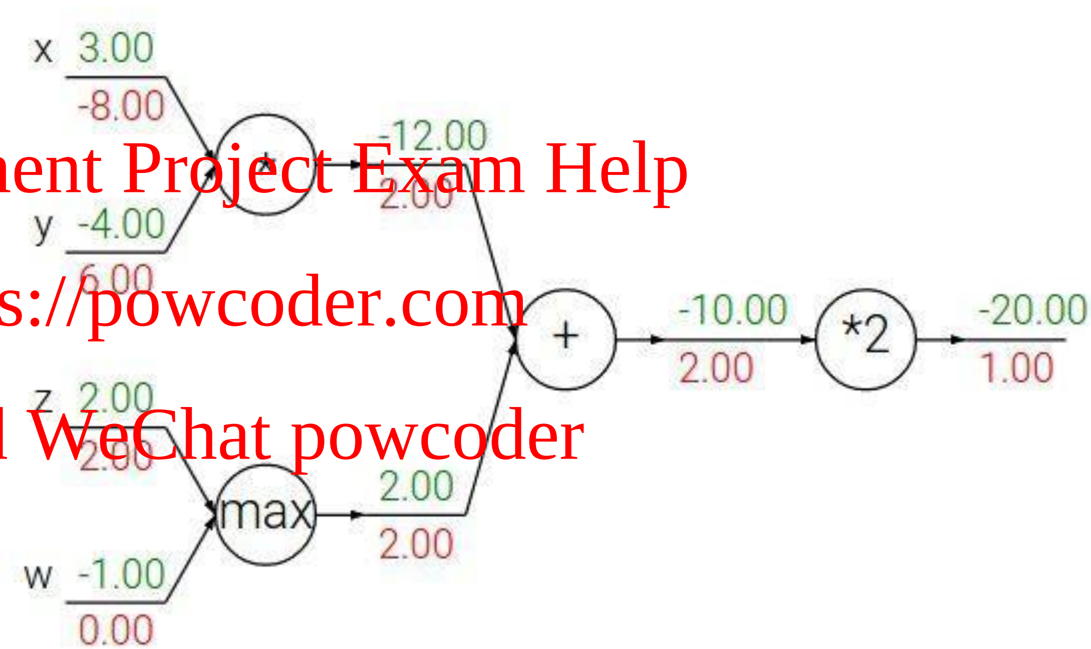
(0.73) * (1 - 0.73) = 0.2

Patterns in backward flow



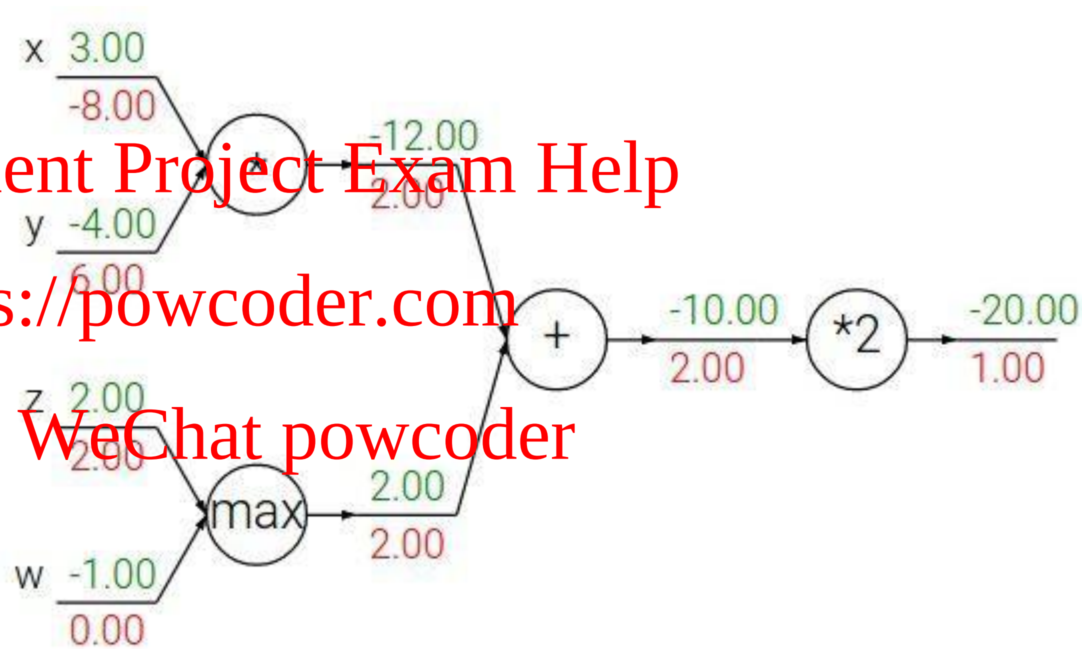
Patterns in backward flow

add gate: gradient distributor



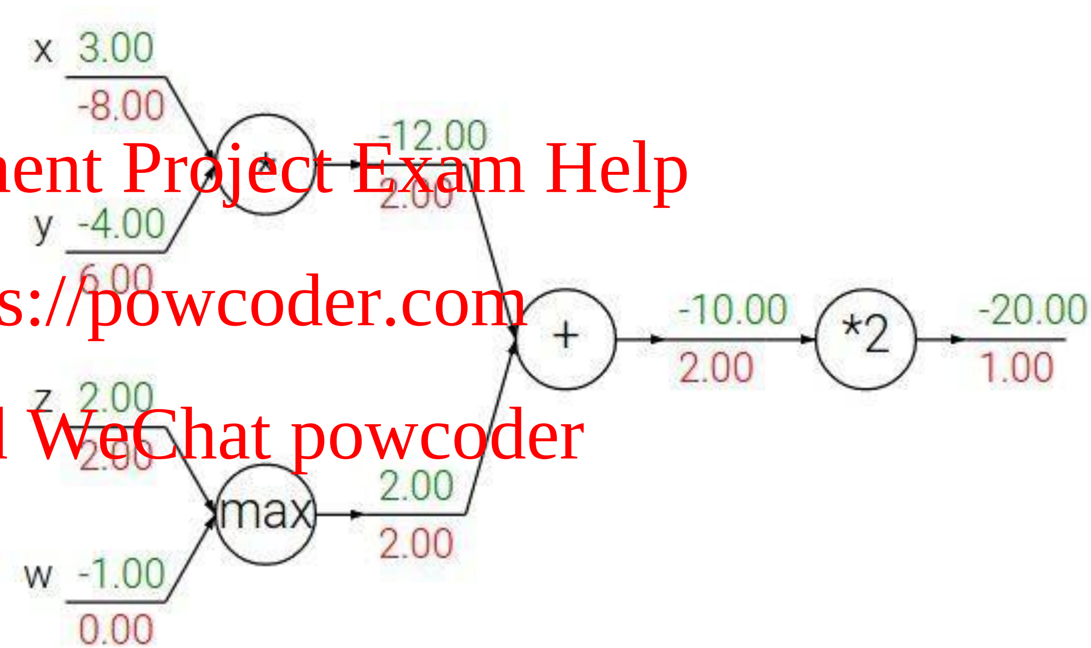
Patterns in backward flow

add gate: gradient distributor
max gate: gradient router

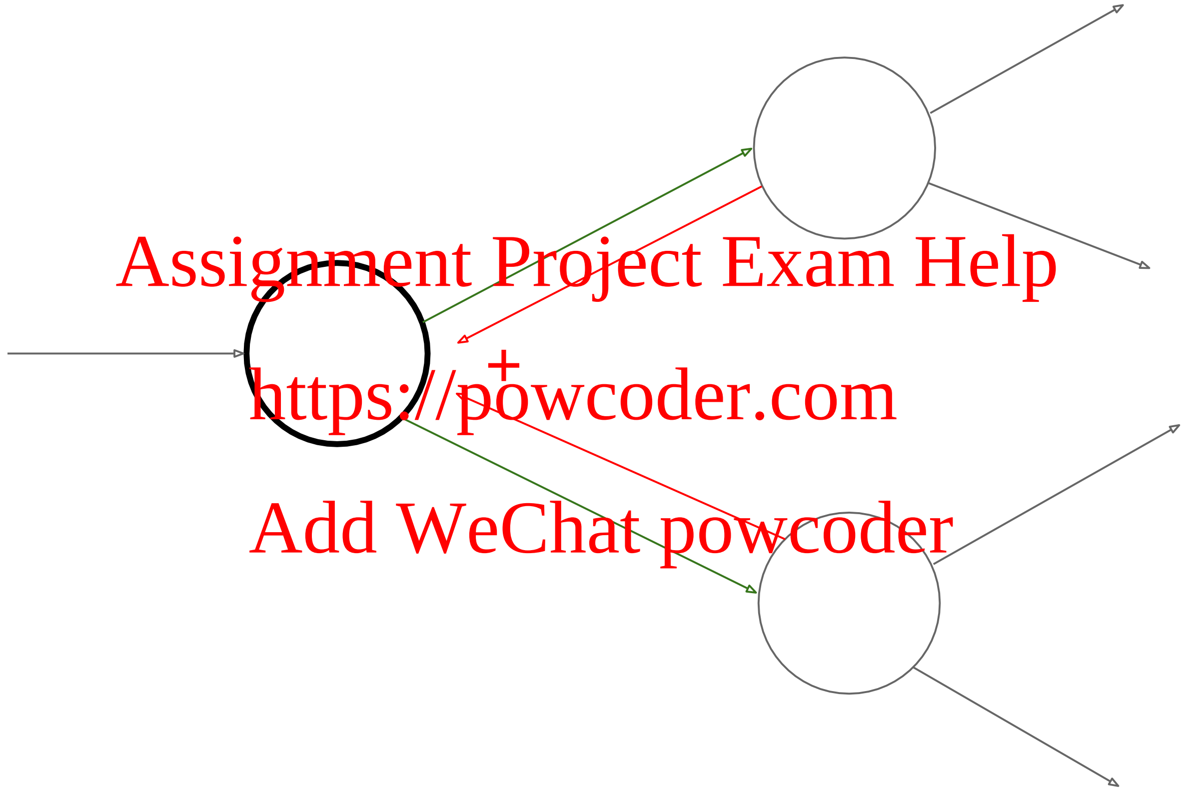


Patterns in backward flow

add gate: gradient distributor
max gate: gradient router
mul gate: gradient… "switcher"?



Gradients add at branches



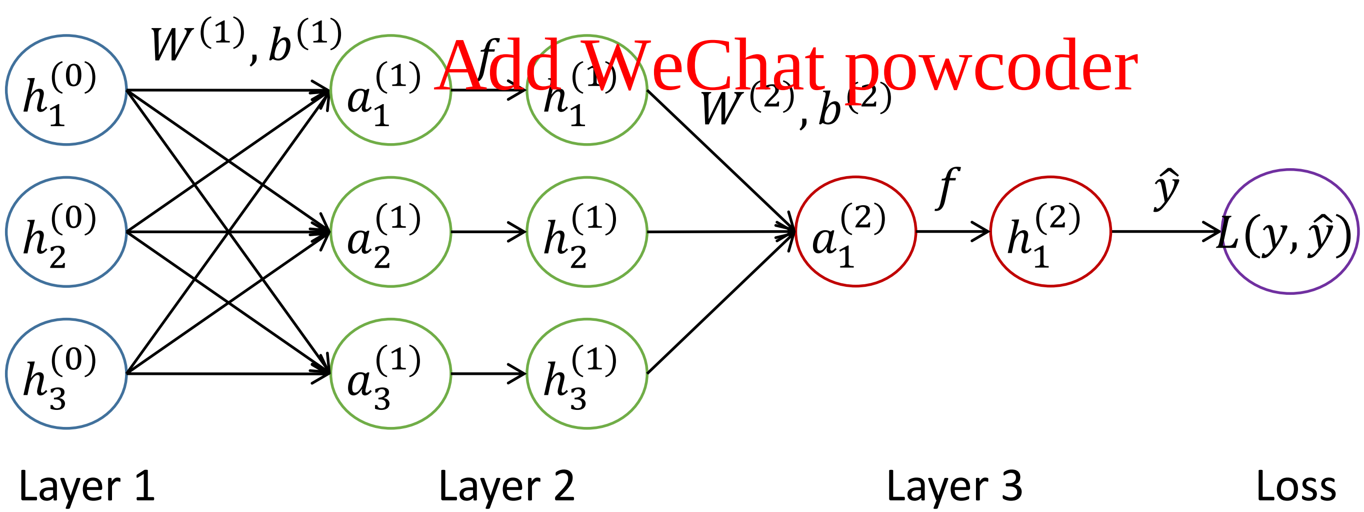
Neural Networks II

Vectorized Backpropagation

Forward Pass

Require: Network depth, l
Require: $\boldsymbol{W}^{(i)}, i \in \{1, \dots, l\}$, the weight matrices of the model
Require: $\boldsymbol{b}^{(i)}, i \in \{1, \dots, l\}$, the bias parameters of the model
Require: $\boldsymbol{x}$, the input to process
Require: $\boldsymbol{y}$, the target output

$\boldsymbol{h}^{(0)} = \boldsymbol{x}$
for $k = 1, \dots, l$ **do**
  $\boldsymbol{a}^{(k)} = \boldsymbol{b}^{(k)} + \boldsymbol{W}^{(k)} \boldsymbol{h}^{(k-1)}$
  $\boldsymbol{h}^{(k)} = f(\boldsymbol{a}^{(k)})$
end for
$\hat{\boldsymbol{y}} = \boldsymbol{h}^{(l)}$
$J = L(\hat{\boldsymbol{y}}, \boldsymbol{y}) + \lambda \Omega(\theta)$



Backward Pass

After the forward computation, compute the gradient on the output layer:

$\boldsymbol{g} \leftarrow \nabla_{\hat{\boldsymbol{y}}} J = \nabla_{\hat{\boldsymbol{y}}} L(\hat{\boldsymbol{y}}, \boldsymbol{y})$

for $k = l, l-1, \ldots, 1$ **do**

Convert the gradient on the layer's output into a gradient into the pre-nonlinearity activation (element-wise multiplication if f is element-wise):

$\boldsymbol{g} \leftarrow \nabla_{\boldsymbol{a}^{(k)}} J = \boldsymbol{g} \odot f'(\boldsymbol{a}^{(k)})$

Compute gradients on weights and biases (including the regularization term, where needed):

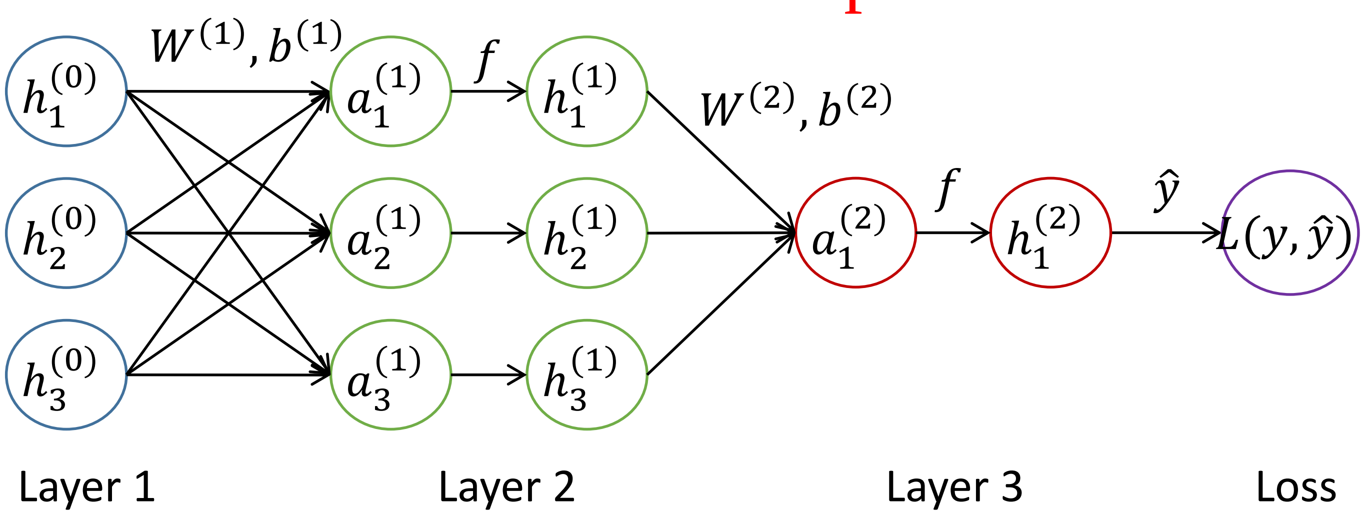
$\nabla_{\boldsymbol{b}^{(k)}} J = \boldsymbol{g} + \lambda \nabla_{\boldsymbol{b}^{(k)}} \Omega(\theta)$

$\nabla_{\boldsymbol{W}^{(k)}} J = \boldsymbol{g}\, \boldsymbol{h}^{(k-1)\top} + \lambda \nabla_{\boldsymbol{W}^{(k)}} \Omega(\theta)$

Propagate the gradients w.r.t. the next lower-level hidden layer's activations:

$\boldsymbol{g} \leftarrow \nabla_{\boldsymbol{h}^{(k-1)}} J = \boldsymbol{W}^{(k)\top} \boldsymbol{g}$

end for



Backpropagation example with vectorized gradients:

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

Next Class

Neural Networks III: Convolutional Nets:

Convolutional networks.

Reading: Bishop Ch 5.5