

Announcements

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

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- ps3 out today, due 10/8 (1 week)
- Midterm practice questions out next week

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Today: Outline

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

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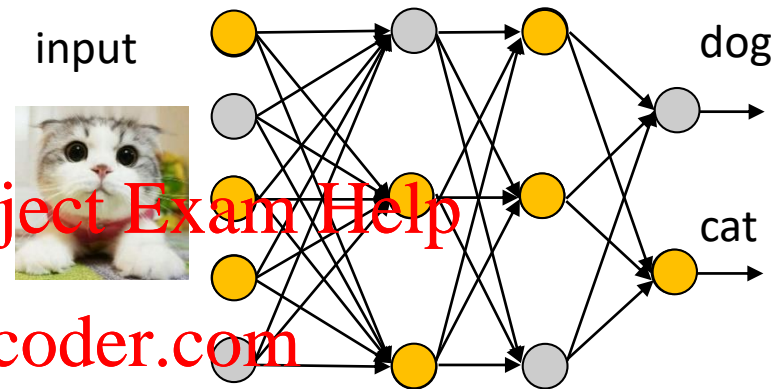
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Neural Networks II

Learning

Artificial Neural Network



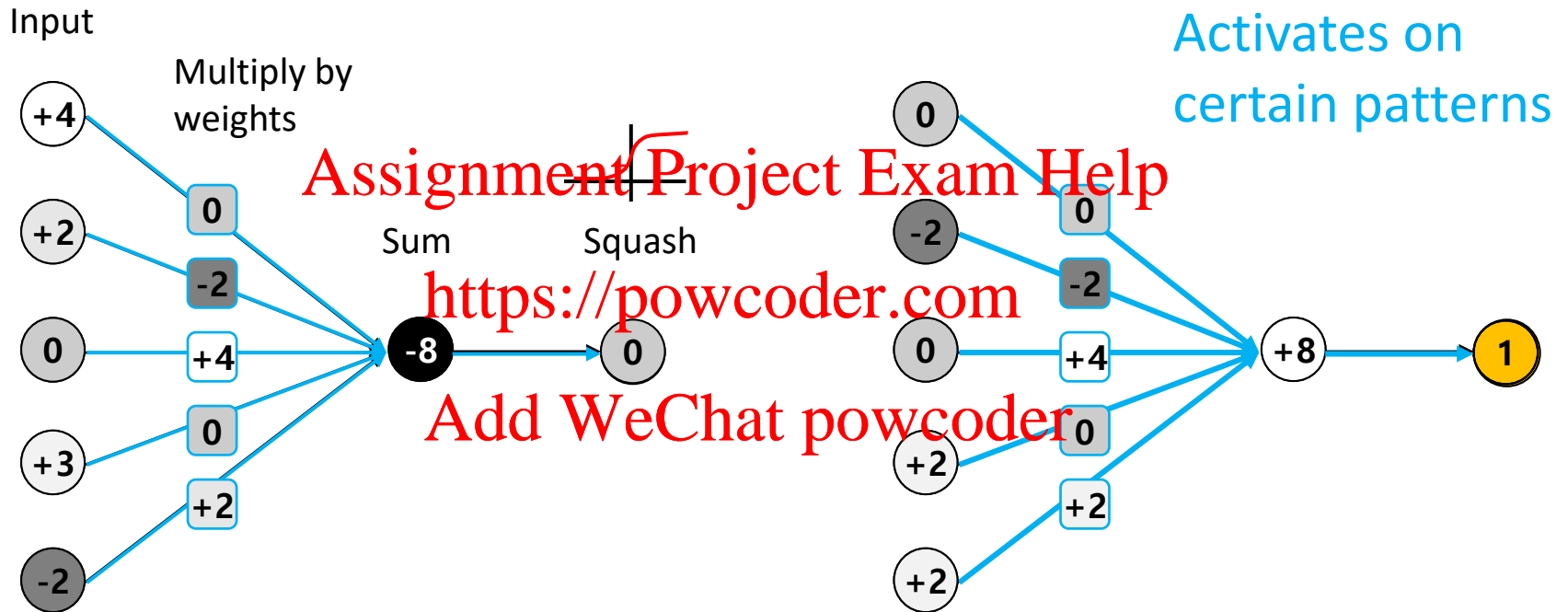
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- **Artificial neural networks:** consist of many inter-connected neurons organized in layers
- **Neurons:** each neuron receives inputs from neurons in previous layer, passes its output to next layer
- **Activation:** neuron's output between 1 (excited)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

Artificial Neuron: Activation



Artificial Neural Network: notation

input

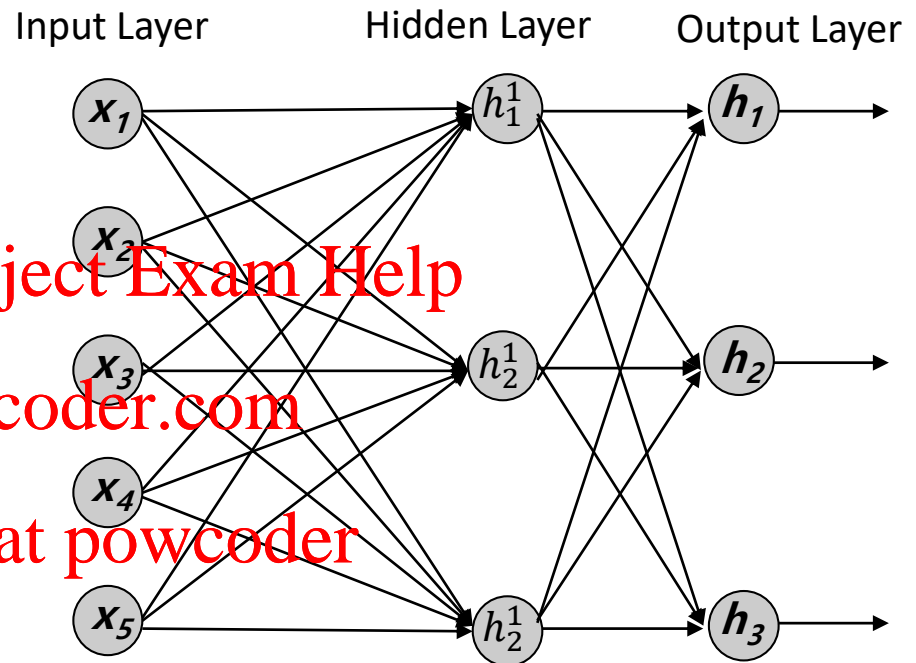
$$x = \begin{bmatrix} x_1 \\ \dots \\ x_5 \end{bmatrix}$$

hidden layer activations

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Artificial Neural Network: notation

input

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

hidden layer activations

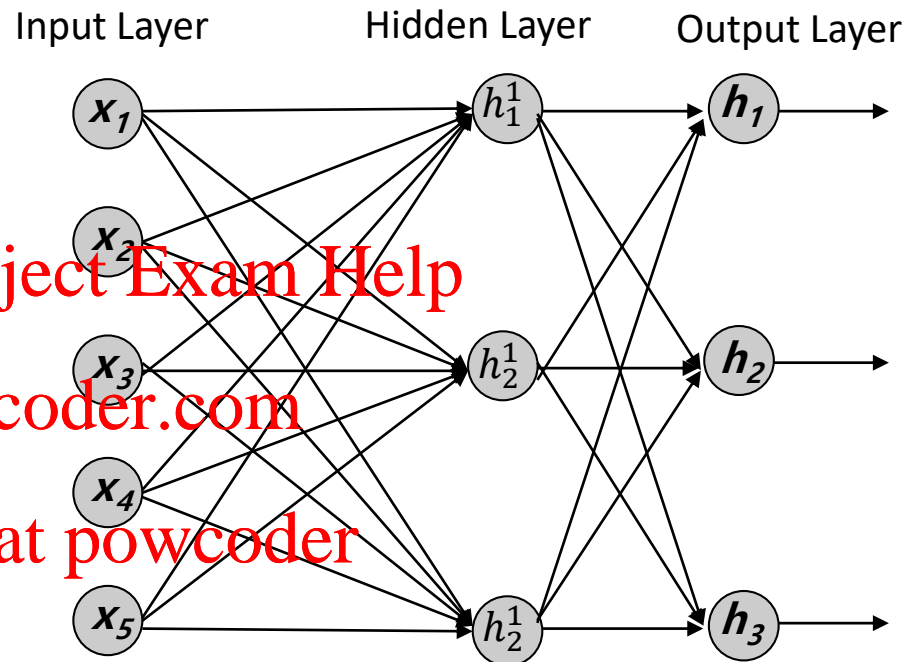
$$h^i = g(\Theta^{(i)}x)$$

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

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output

$$h_{\Theta}(x) = g(\Theta^{(2)}h^i) \quad \text{weights} \quad \Theta^{(1)} = \begin{pmatrix} \theta_{11} & \dots & \theta_{15} \\ \vdots & \ddots & \vdots \\ \theta_{31} & \dots & \theta_{35} \end{pmatrix} \quad \Theta^{(2)} = \begin{pmatrix} \theta_{11} & \dots & \theta_{13} \\ \vdots & \ddots & \vdots \\ \theta_{31} & \dots & \theta_{33} \end{pmatrix}$$



Cost function

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

Assignment Project Exam Help training error

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

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

regularization

Gradient computation

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

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

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Use “Backpropagation algorithm”

Need code to compute:

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

- 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

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

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

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

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

- 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:

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

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

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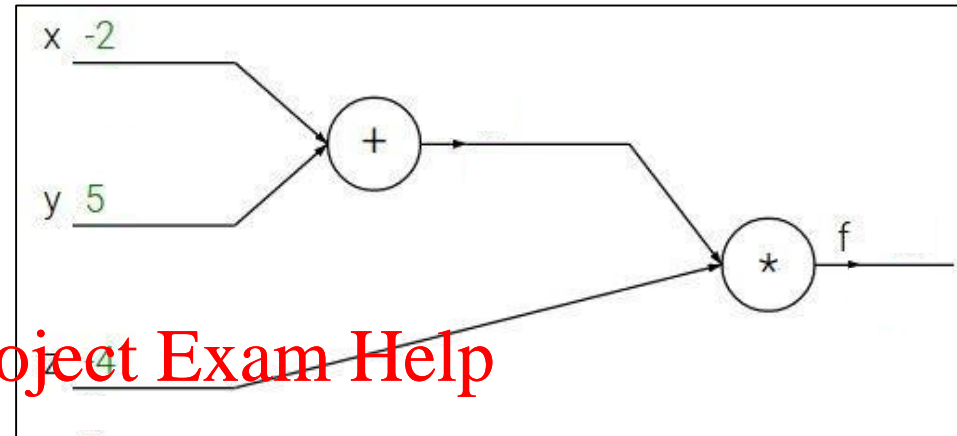
$$\frac{\partial f}{\partial \theta_3} = \frac{\partial f_1}{\partial f_2} (f_2(f_3(\theta))) * \frac{\partial f_2}{\partial f_3} (f_3(\theta)) * \frac{\partial f_3}{\partial \theta_3} (\theta)$$

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

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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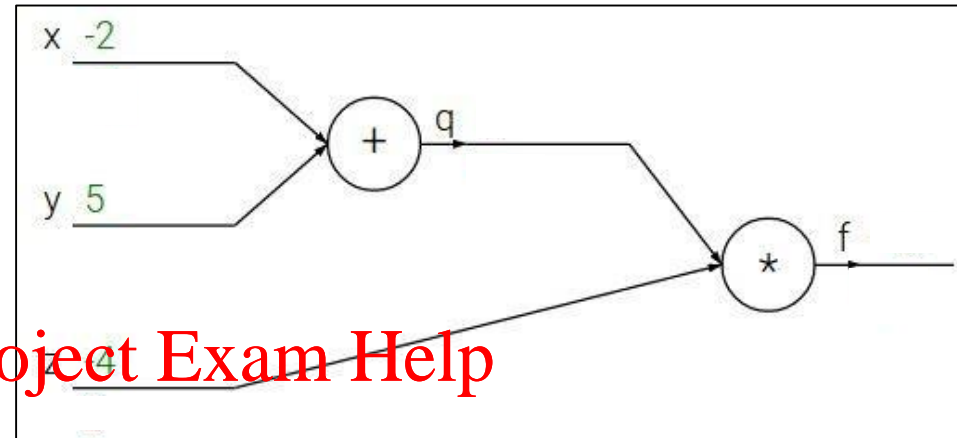
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Chain Rule with a Computational Graph

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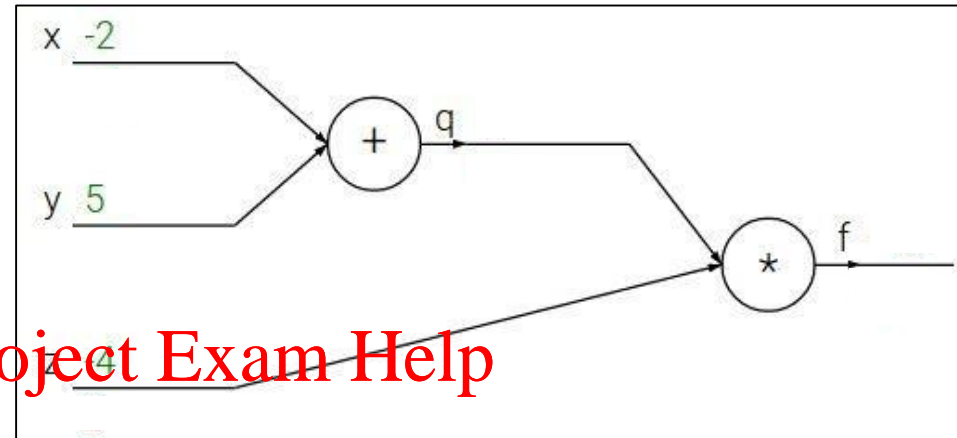
$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

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

Computation Graph: Forward

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

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



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<https://powcoder.com> compute values

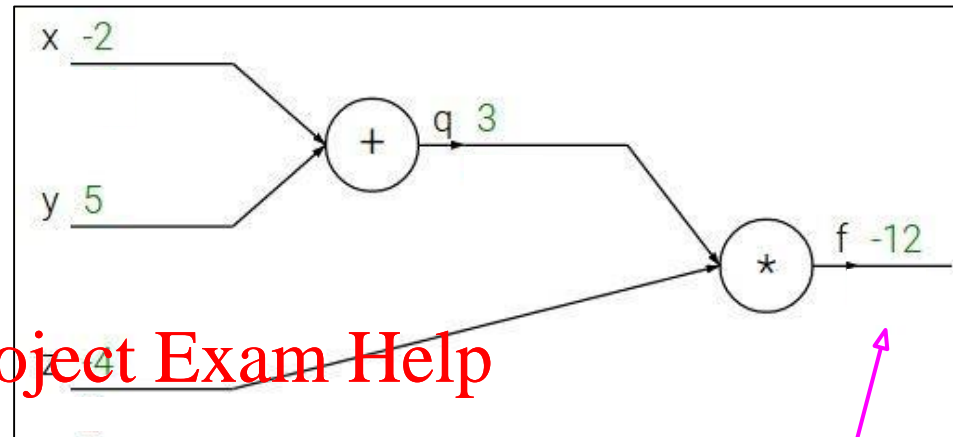
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

Computation Graph: Backward

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

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



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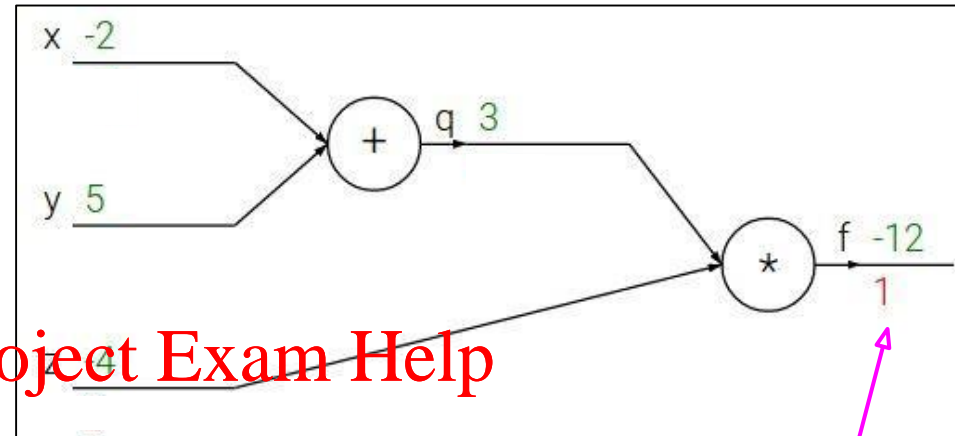
compute gradients

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

Computation Graph: Backward

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

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



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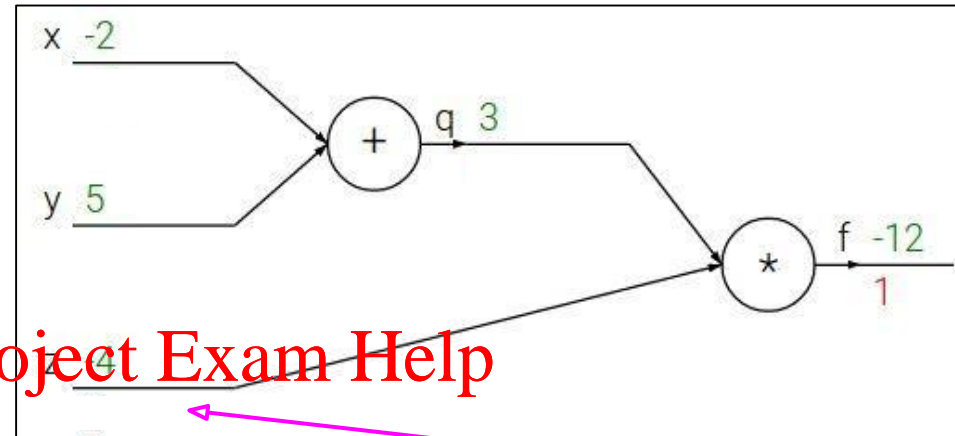
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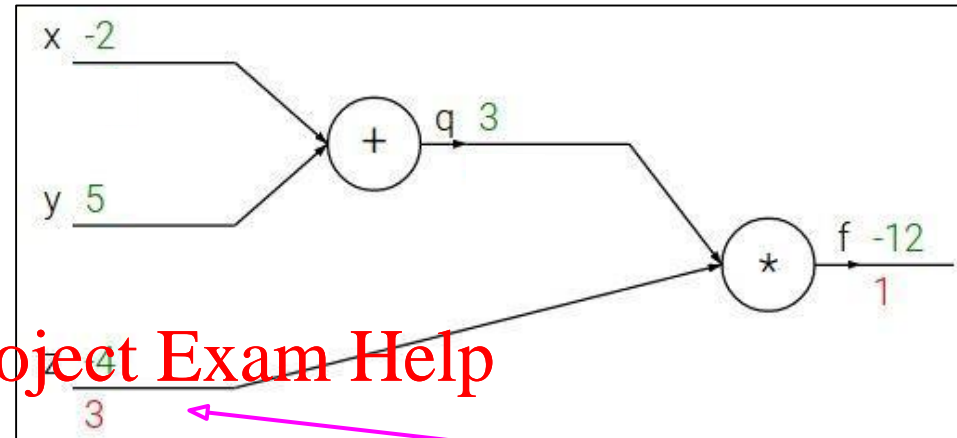
$$\frac{\partial f}{\partial z}$$

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

Computation Graph: Backward

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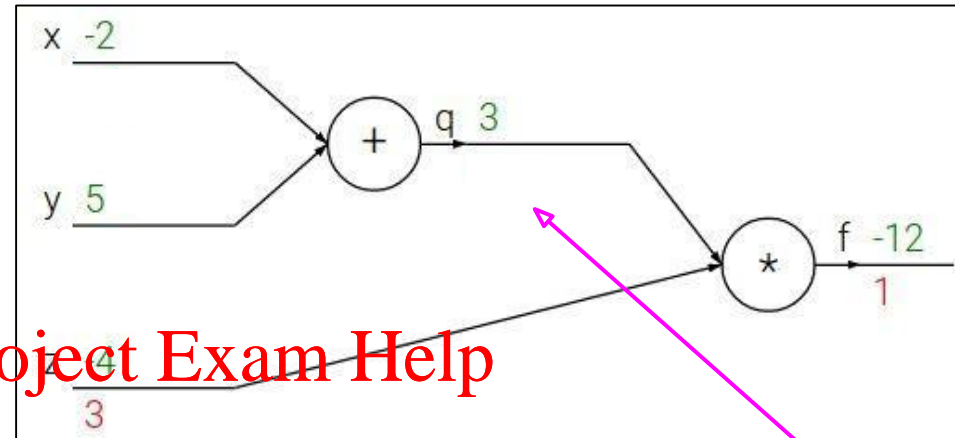
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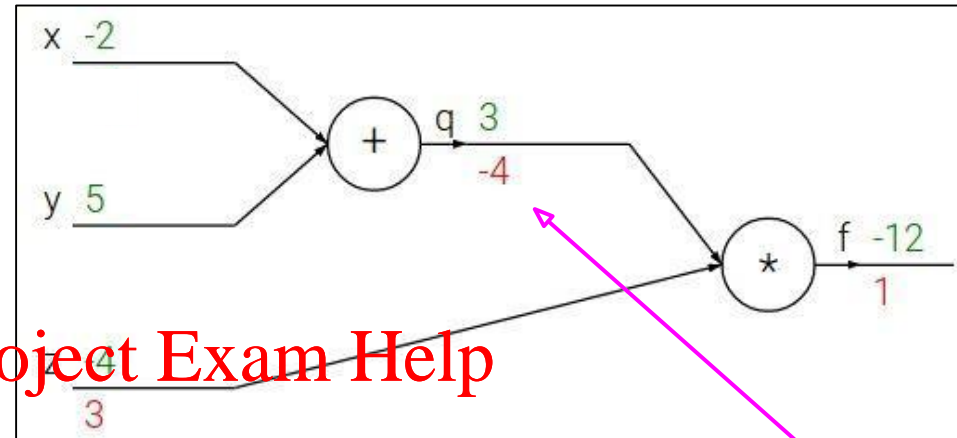
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$$\frac{\partial f}{\partial q}$$

Computation Graph: Backward

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

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



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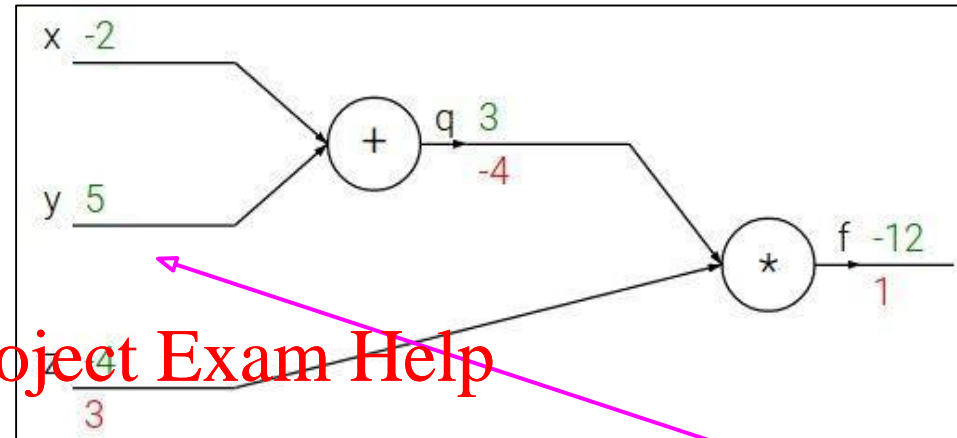
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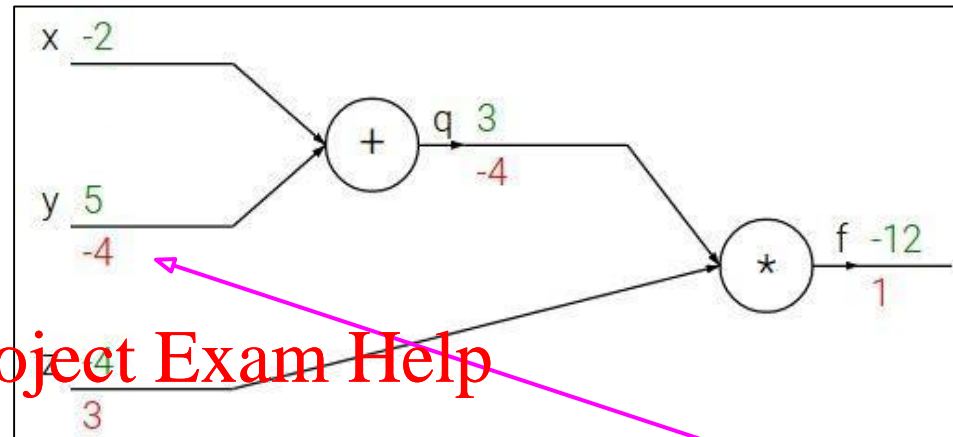
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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

Computation Graph: Backward

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Chain rule:

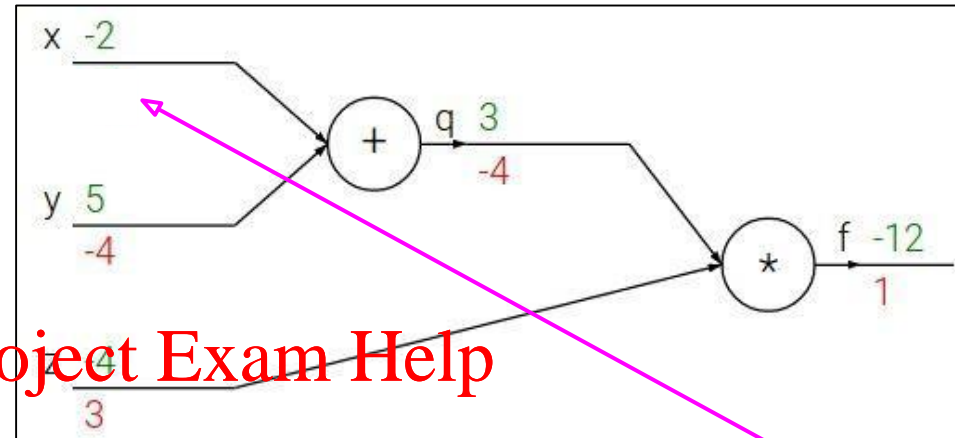
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial y}$$

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

Computation Graph: Backward

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

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



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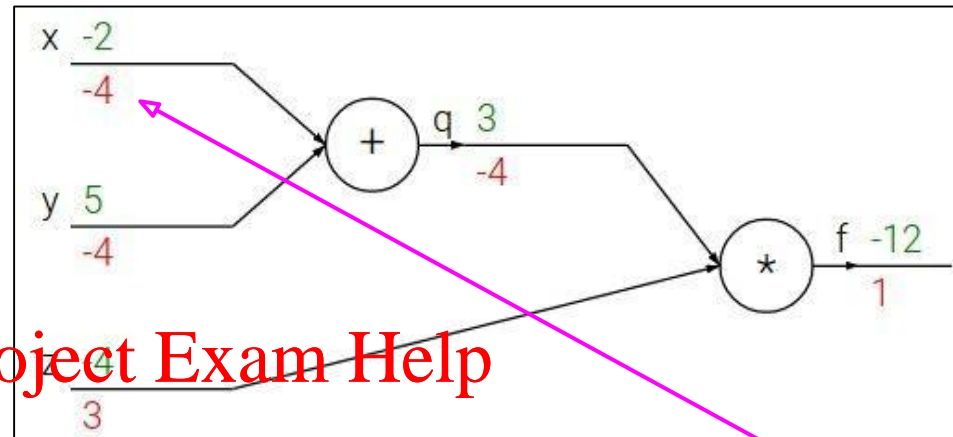
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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

Computation Graph: Backward

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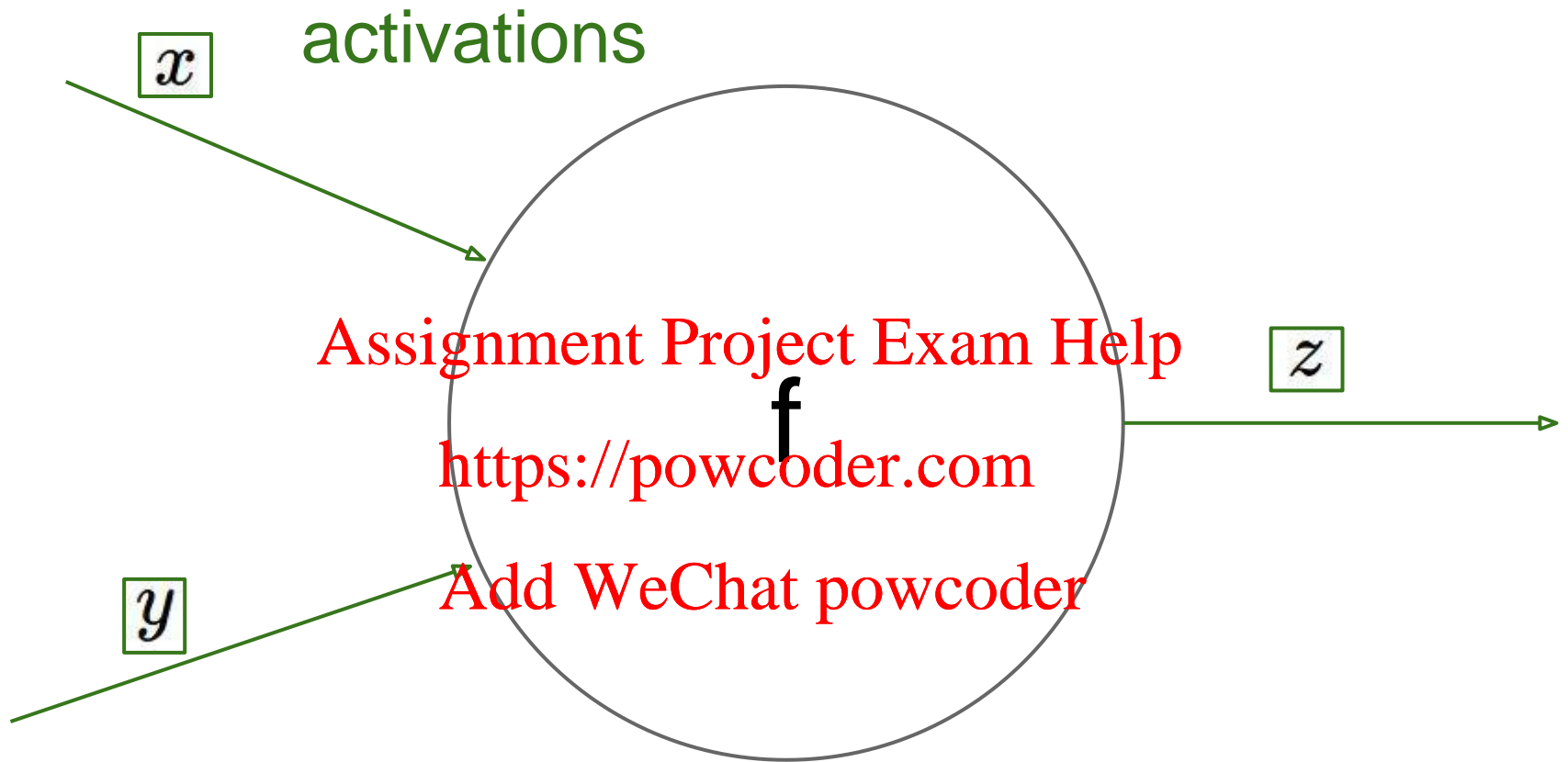
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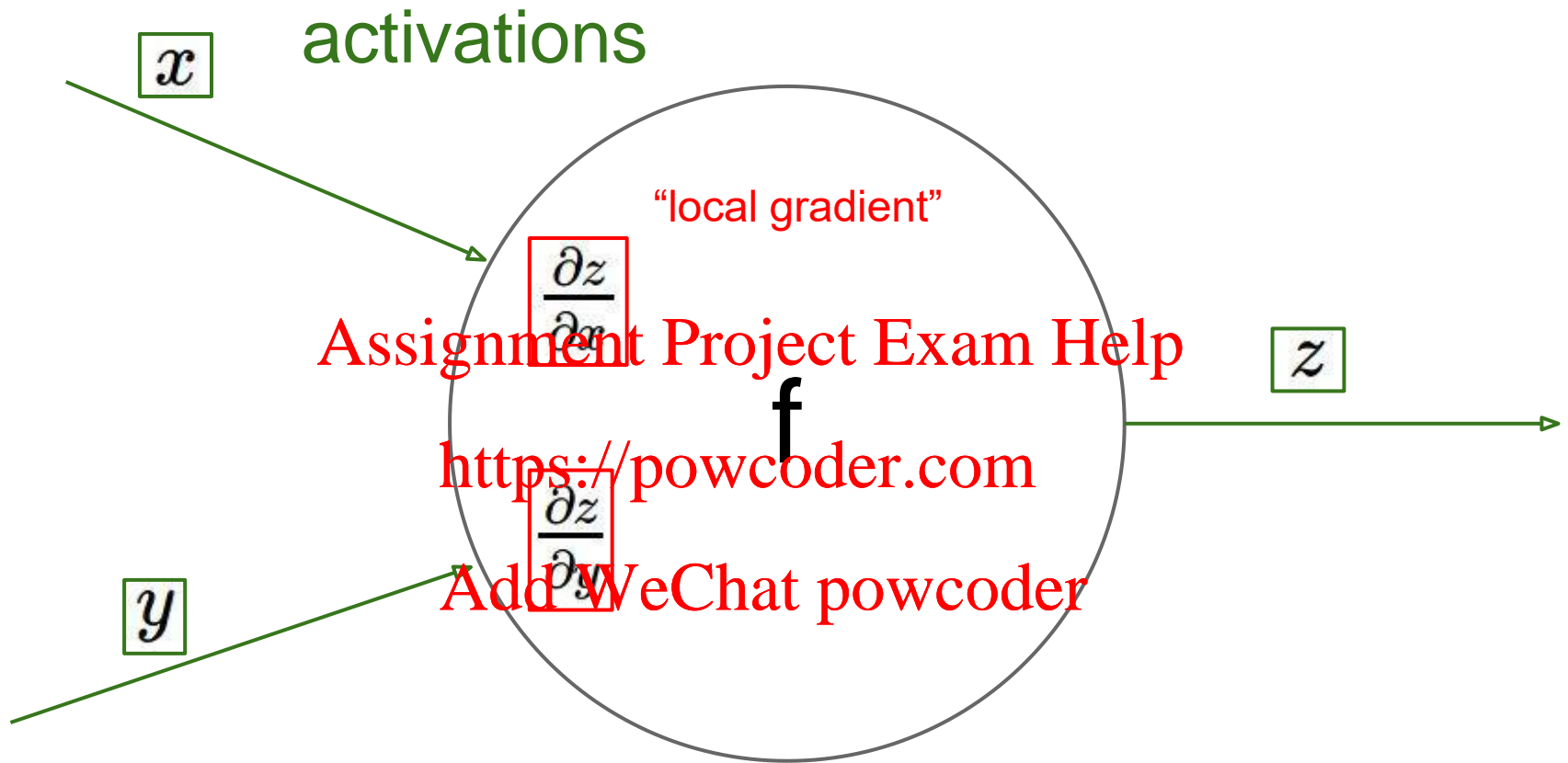
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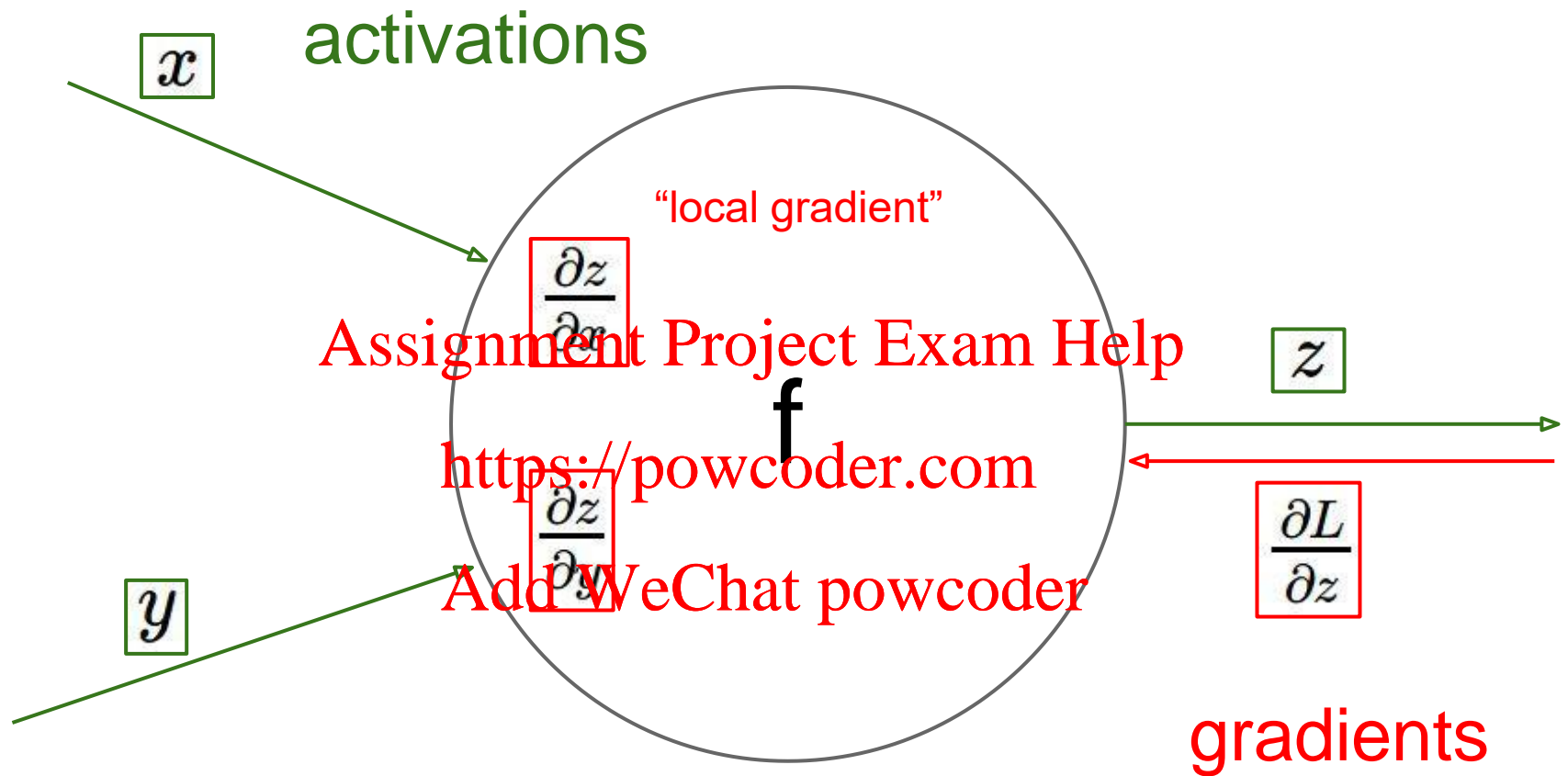
Chain rule:

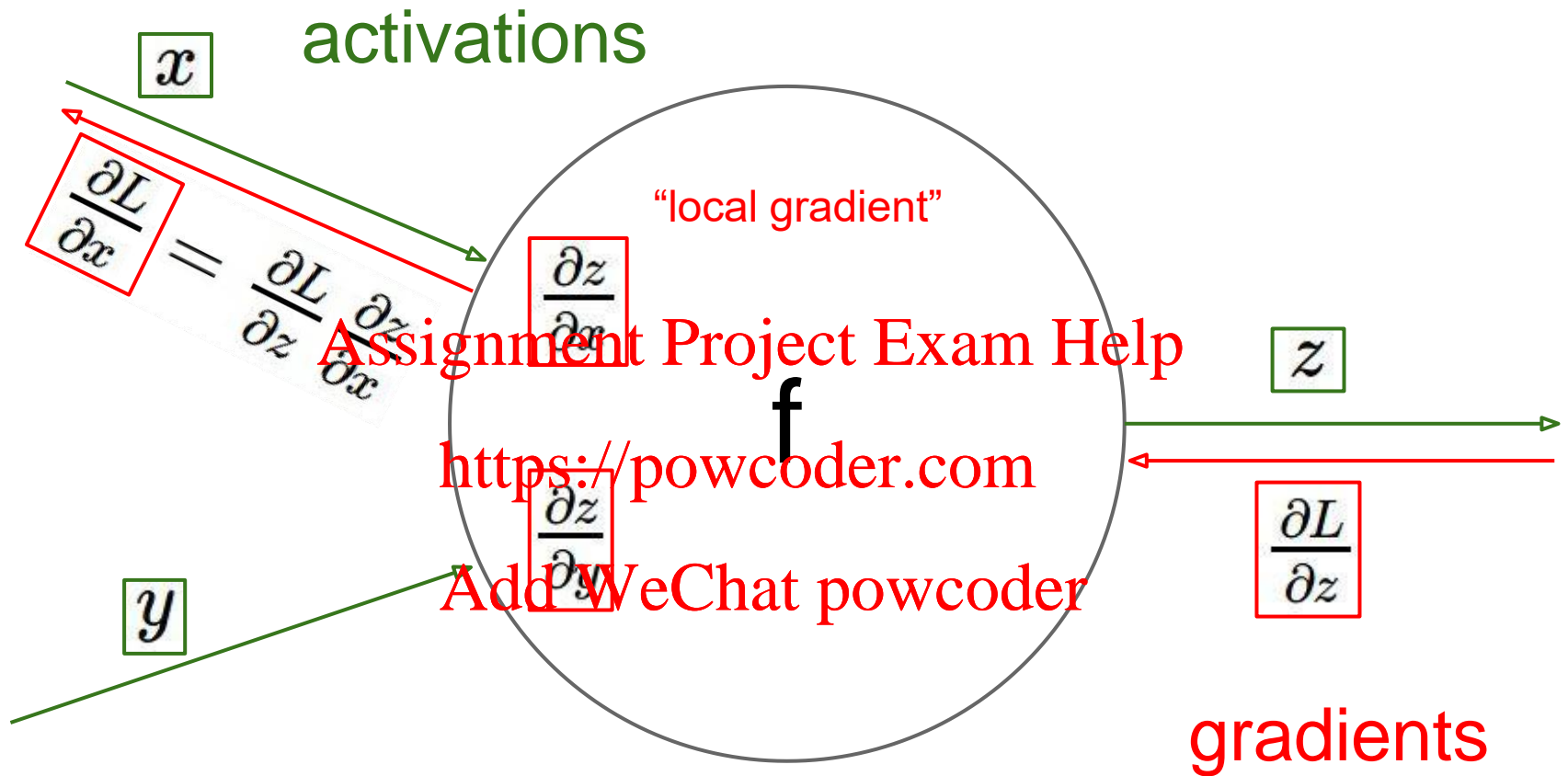
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

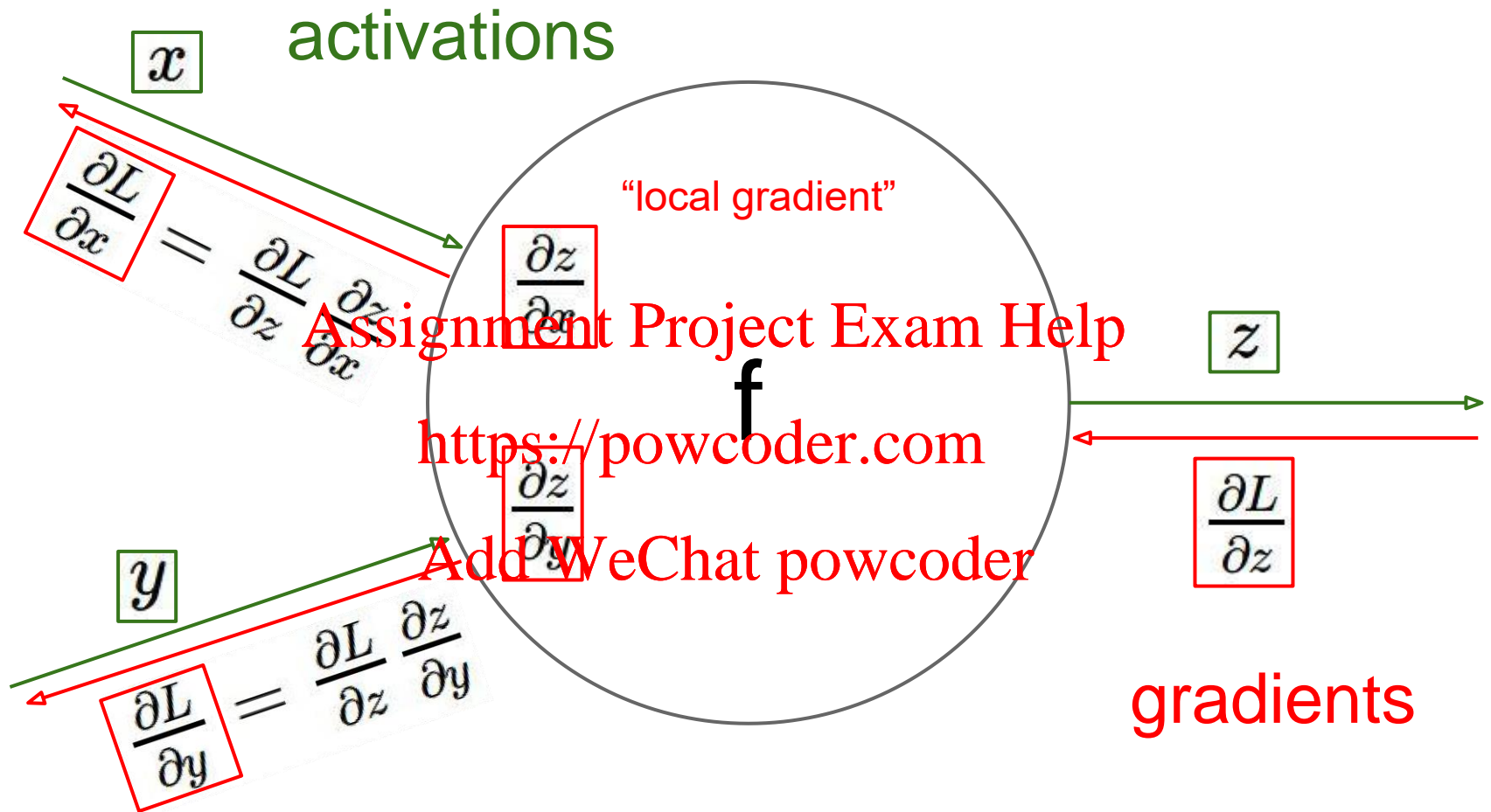
$$\frac{\partial f}{\partial x}$$

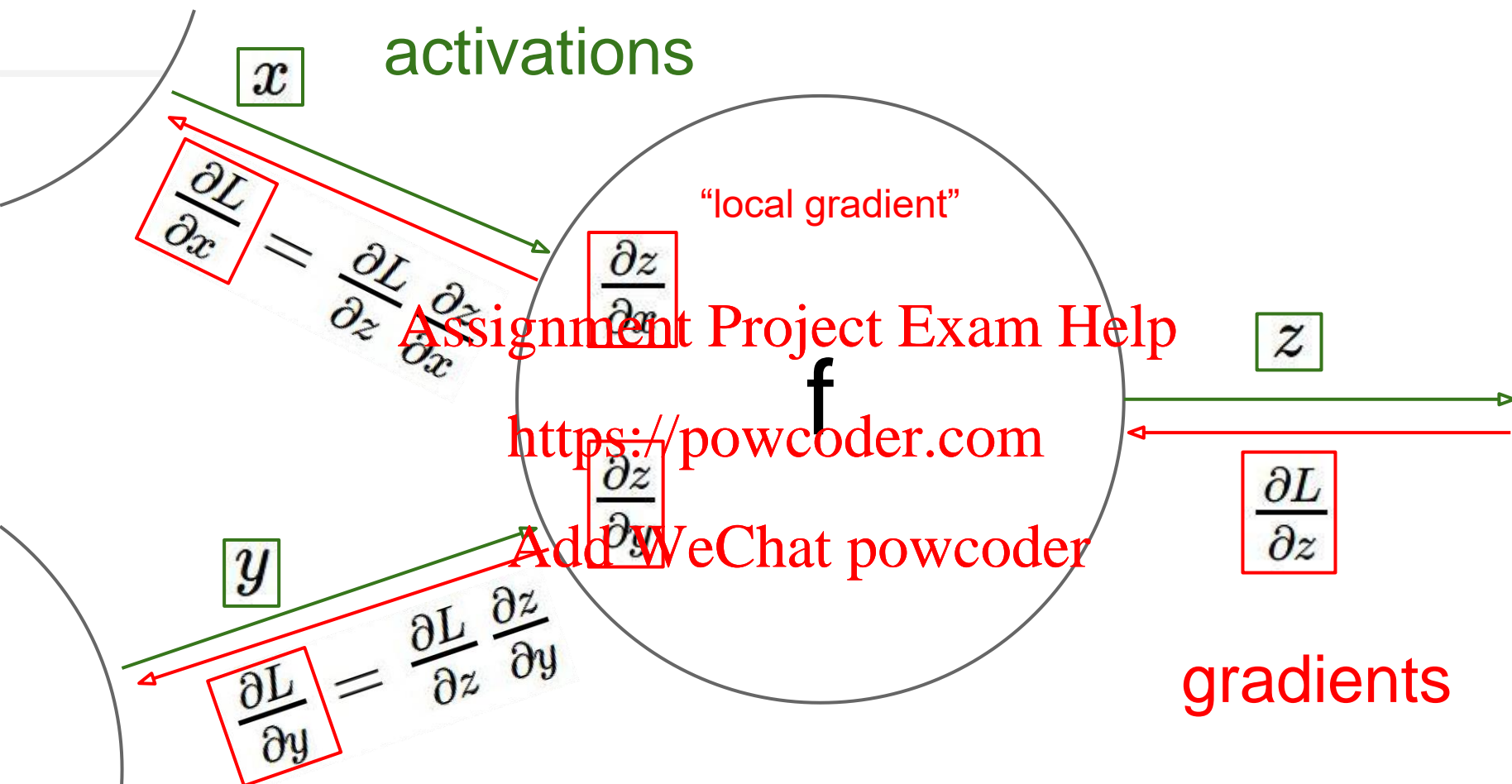






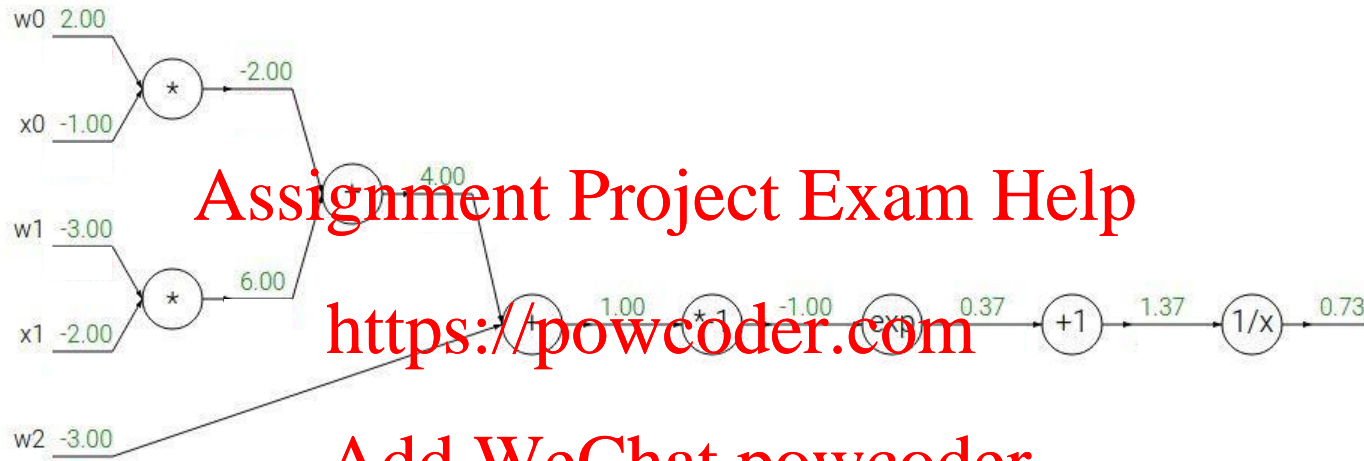






Another example:

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



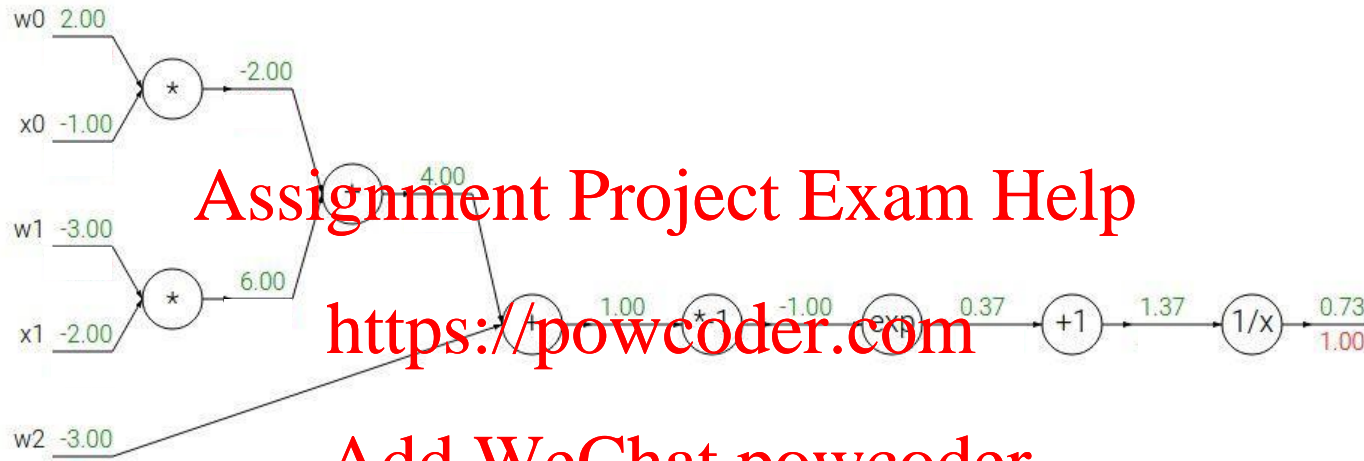
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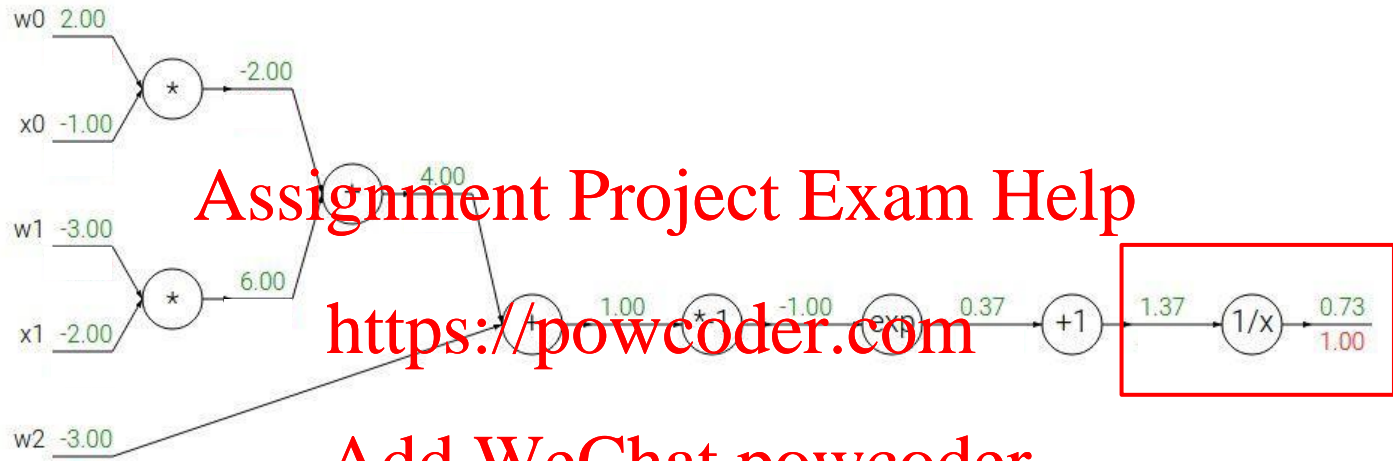
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$f(x) = e^x$	\rightarrow	$\frac{df}{dx} = e^x$		$f(x) = \frac{1}{x}$	\rightarrow	$\frac{df}{dx} = -1/x^2$
$f_a(x) = ax$	\rightarrow	$\frac{df}{dx} = a$		$f_c(x) = c + x$	\rightarrow	$\frac{df}{dx} = 1$

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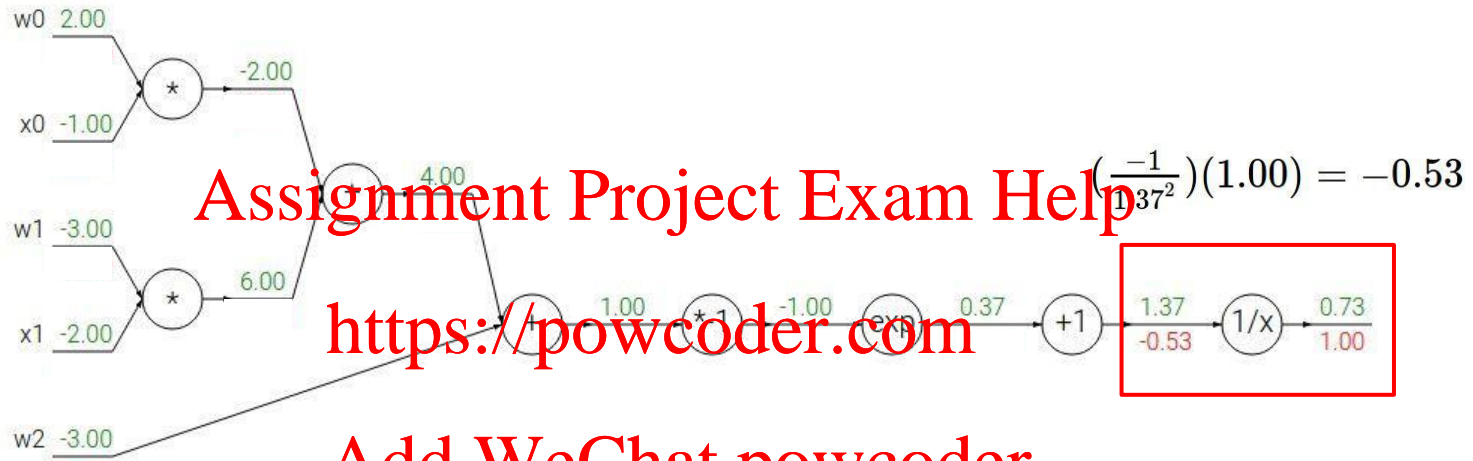
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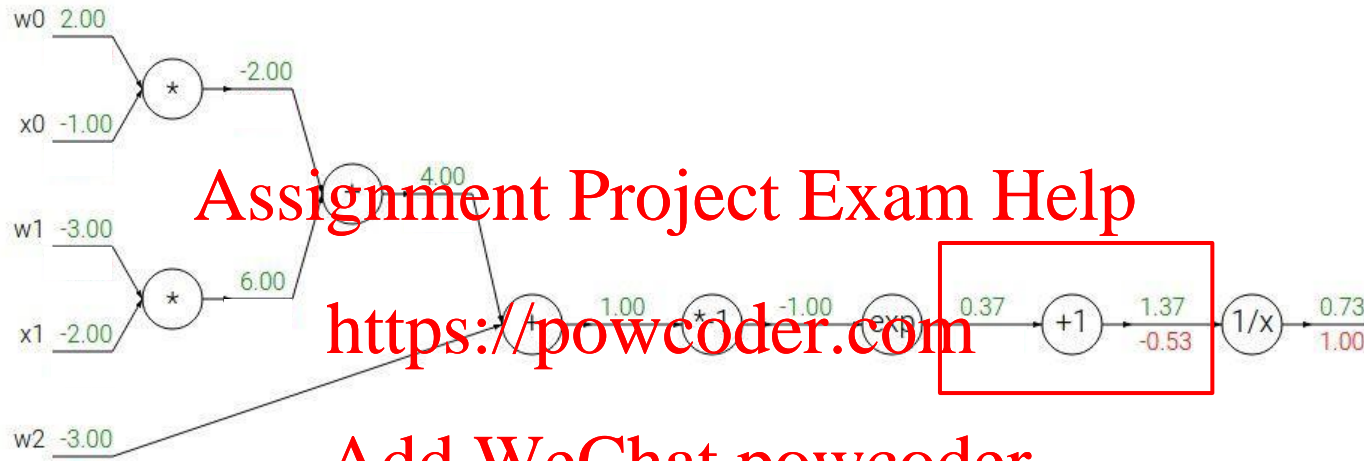
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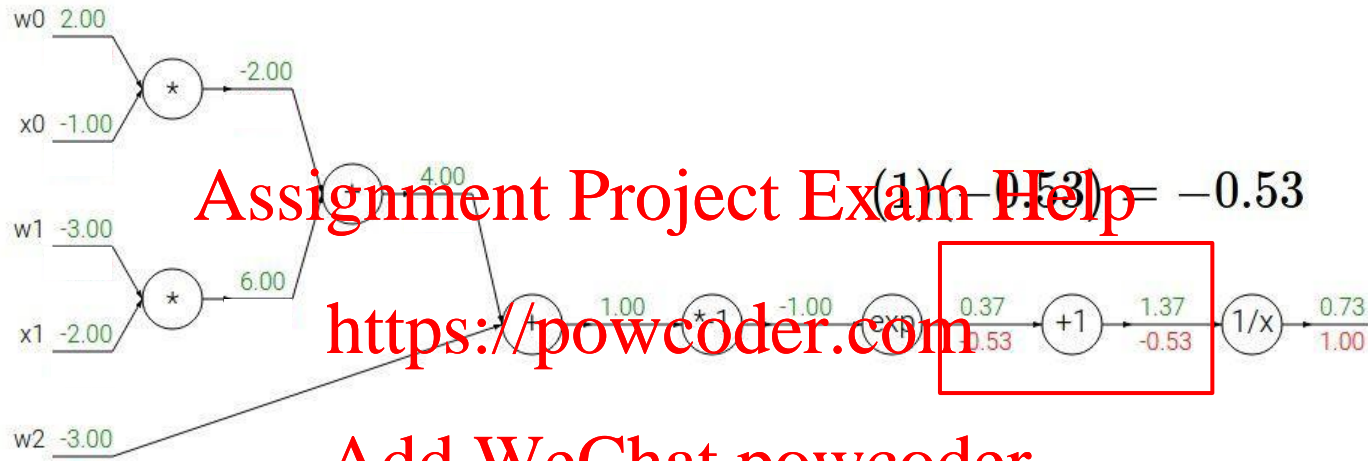
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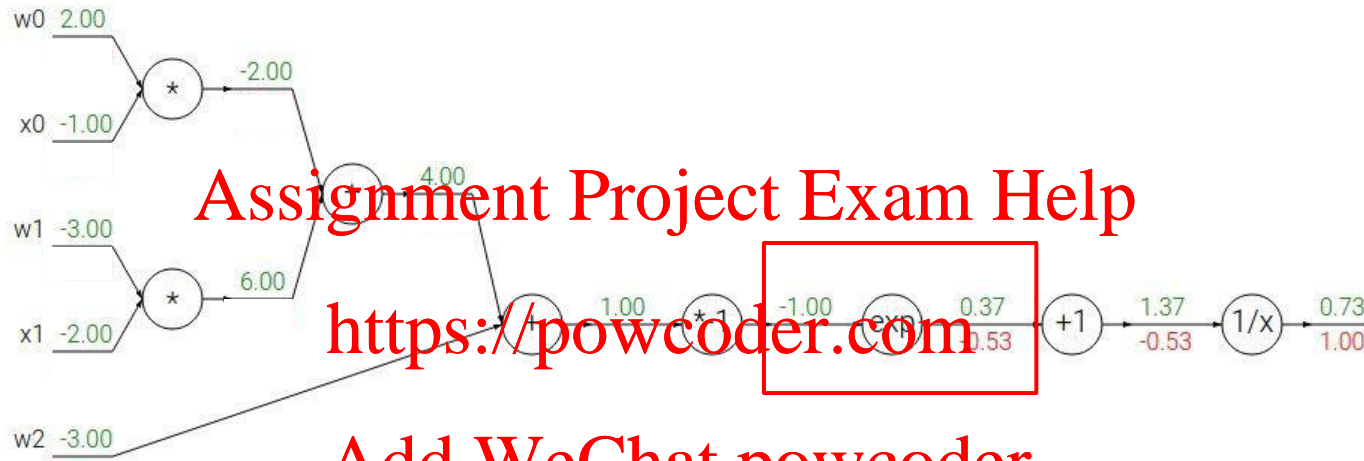
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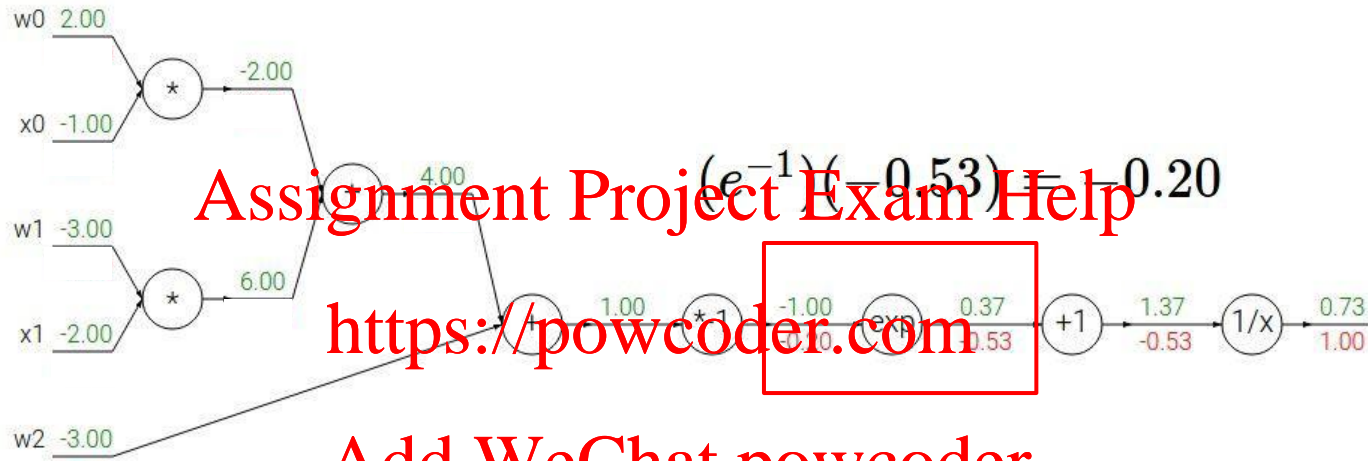
$$f_a(x) = ax \rightarrow \frac{df}{dx} = a$$

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

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

Another example:

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



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

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

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

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

\rightarrow

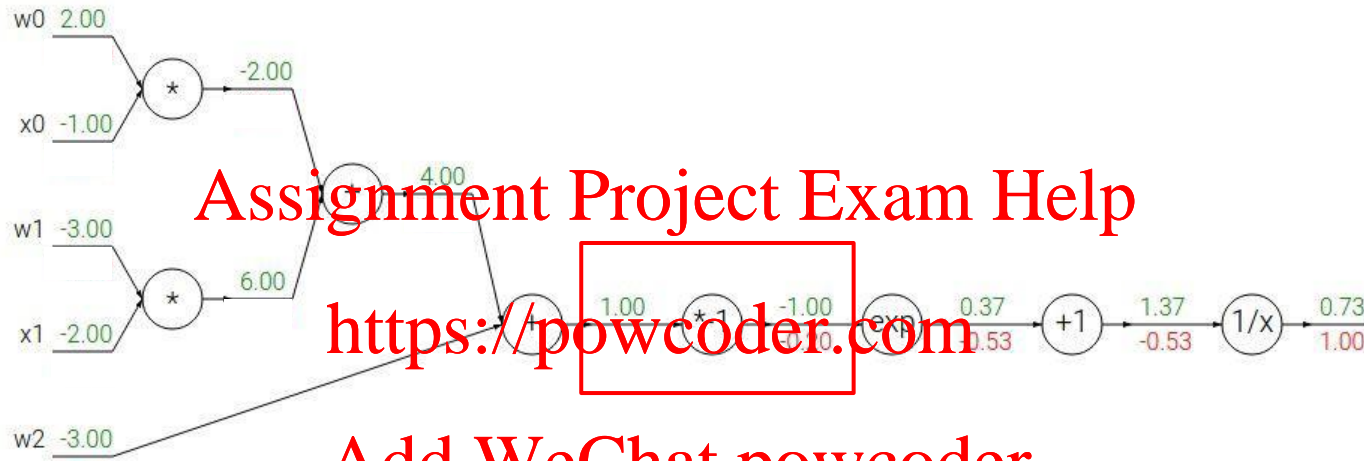
$$\frac{df}{dx} = -1/x^2$$

\rightarrow

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

Another example:

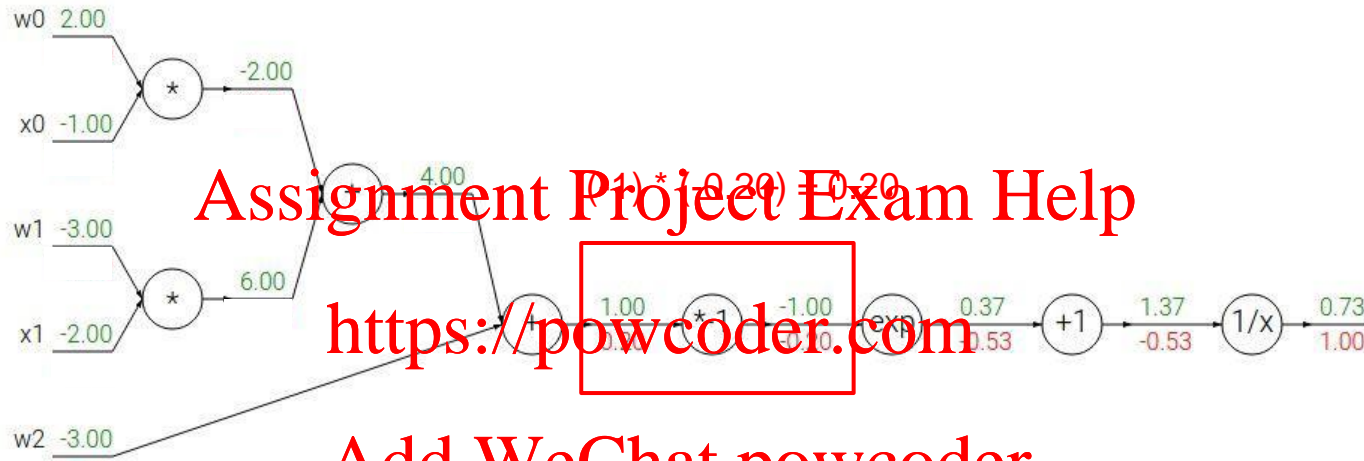
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$$f(x) = e^x$$

→

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

$$f_a(x) = ax$$

→

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

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

→

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

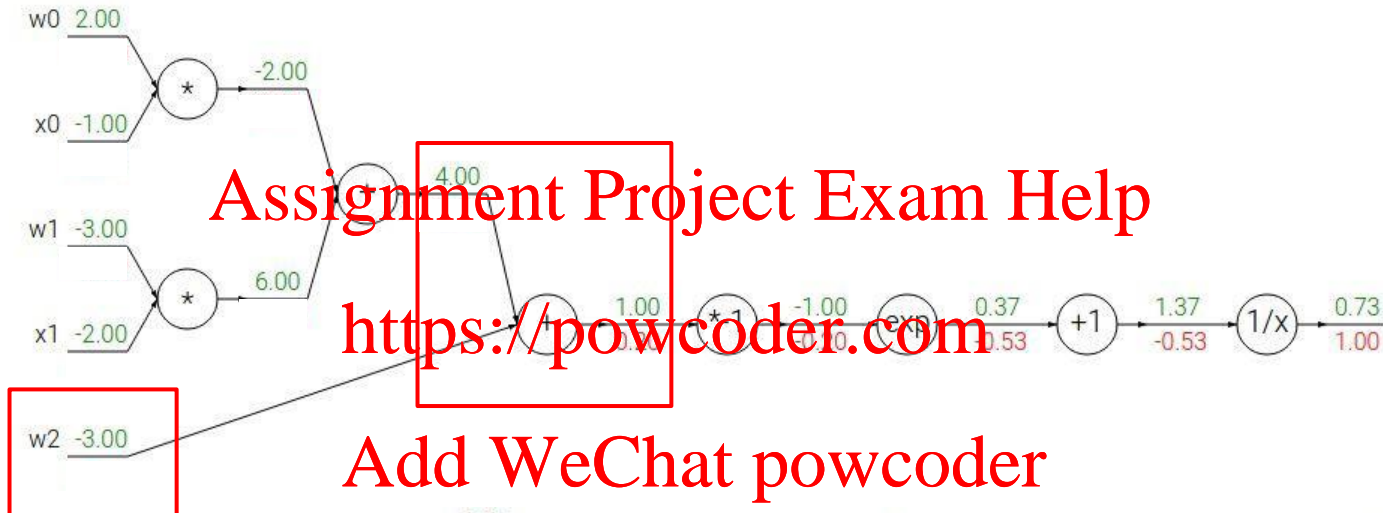
$$f_c(x) = c + x$$

→

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

Another example:

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



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

→

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

$$f_a(x) = ax$$

→

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

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

→

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

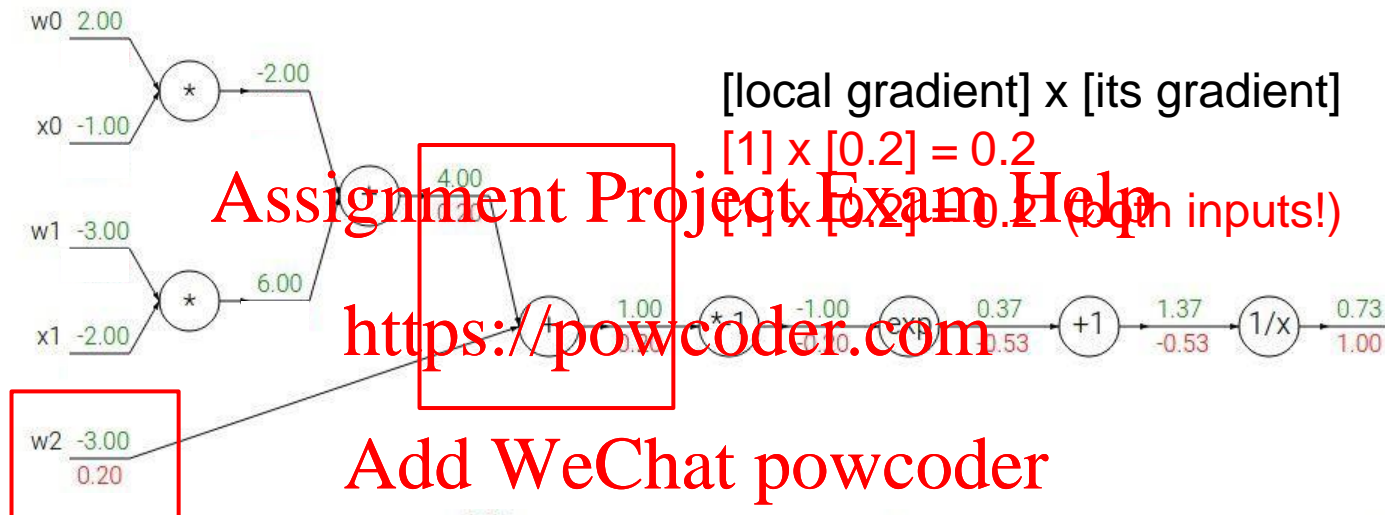
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→

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

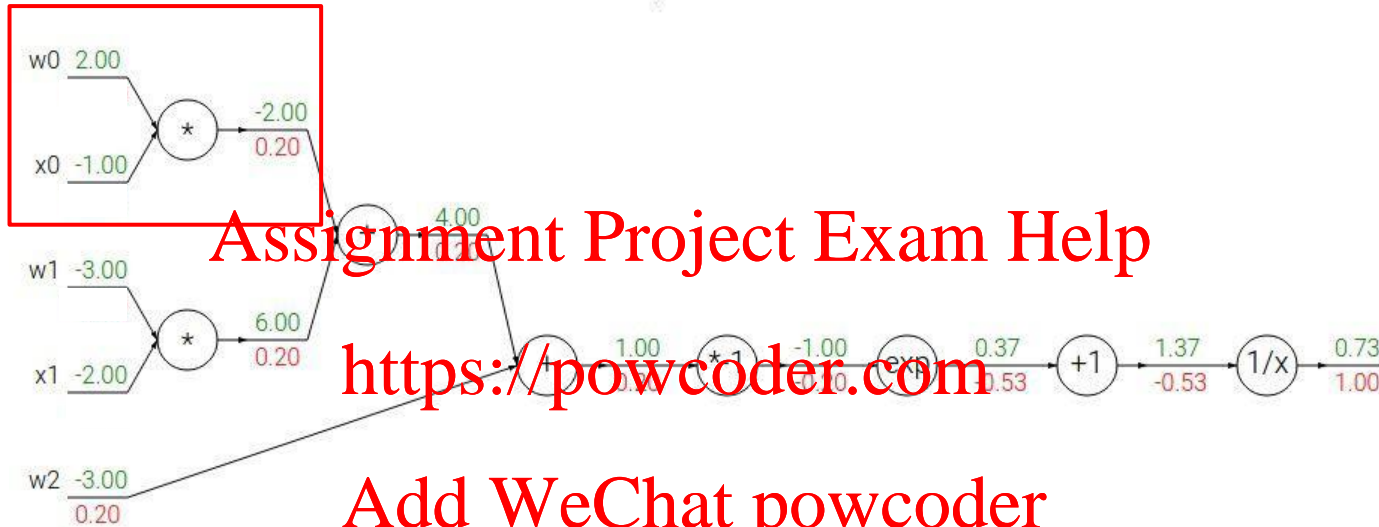
$$f_c(x) = c + x$$

→

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

Another example:

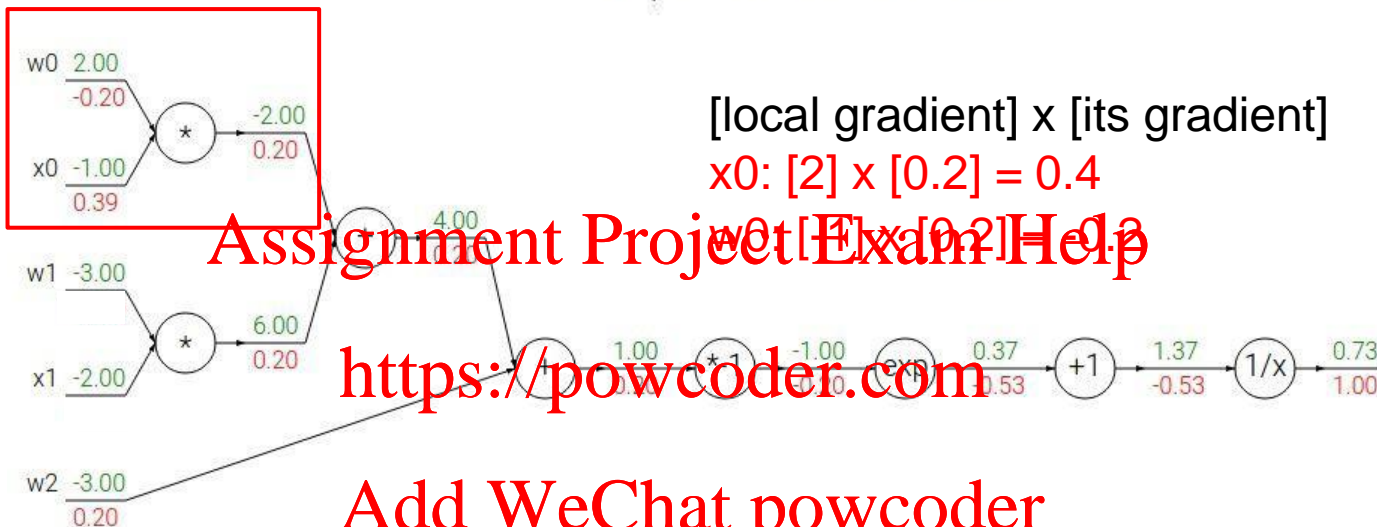
$$f(w, x) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$$



$$\begin{array}{lcl}
 f(x) = e^x & \rightarrow & \frac{df}{dx} = e^x \\
 f_a(x) = ax & \rightarrow & \frac{df}{dx} = a
 \end{array}
 \quad \Bigg| \quad
 \begin{array}{lcl}
 f(x) = \frac{1}{x} & \rightarrow & \frac{df}{dx} = -1/x^2 \\
 f_c(x) = c + x & \rightarrow & \frac{df}{dx} = 1
 \end{array}$$

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

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

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

sigmoid function

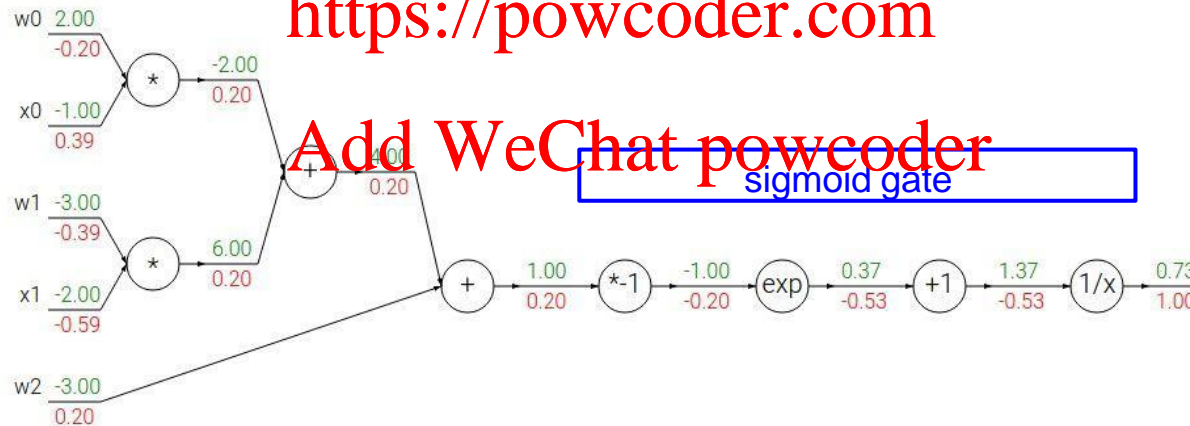
$$\frac{d\sigma(x)}{dx} = \frac{e^{-x}}{(1 + e^{-x})^2} = \left(\frac{1 + e^{-x} - 1}{1 + e^{-x}} \right) \left(\frac{1}{1 + e^{-x}} \right) = (1 - \sigma(x)) \sigma(x)$$

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sigmoid gate



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

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

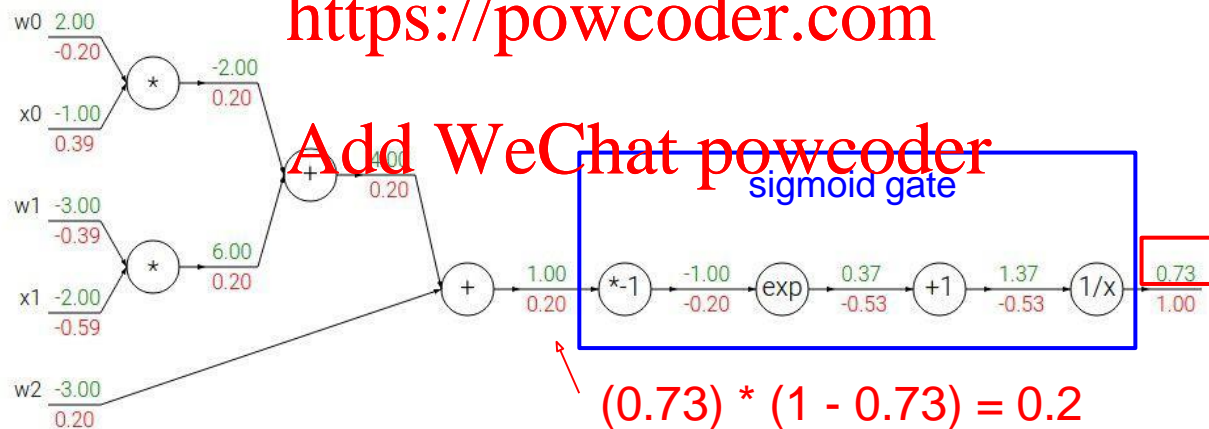
sigmoid function

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

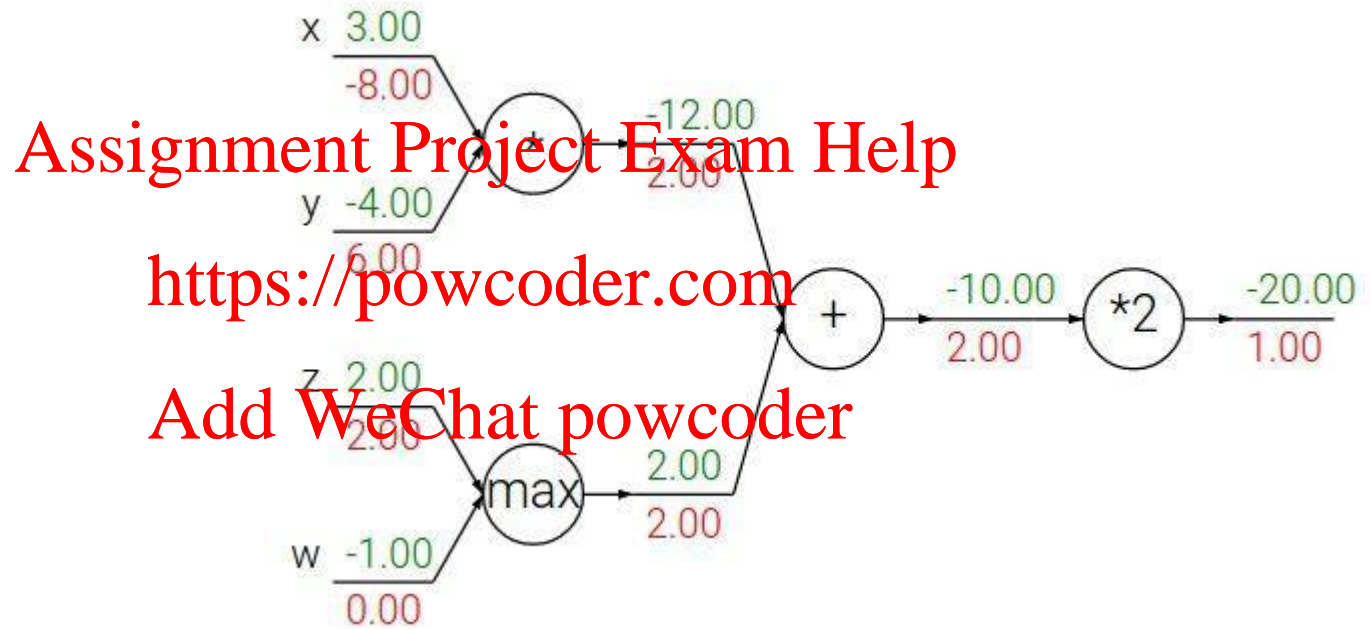
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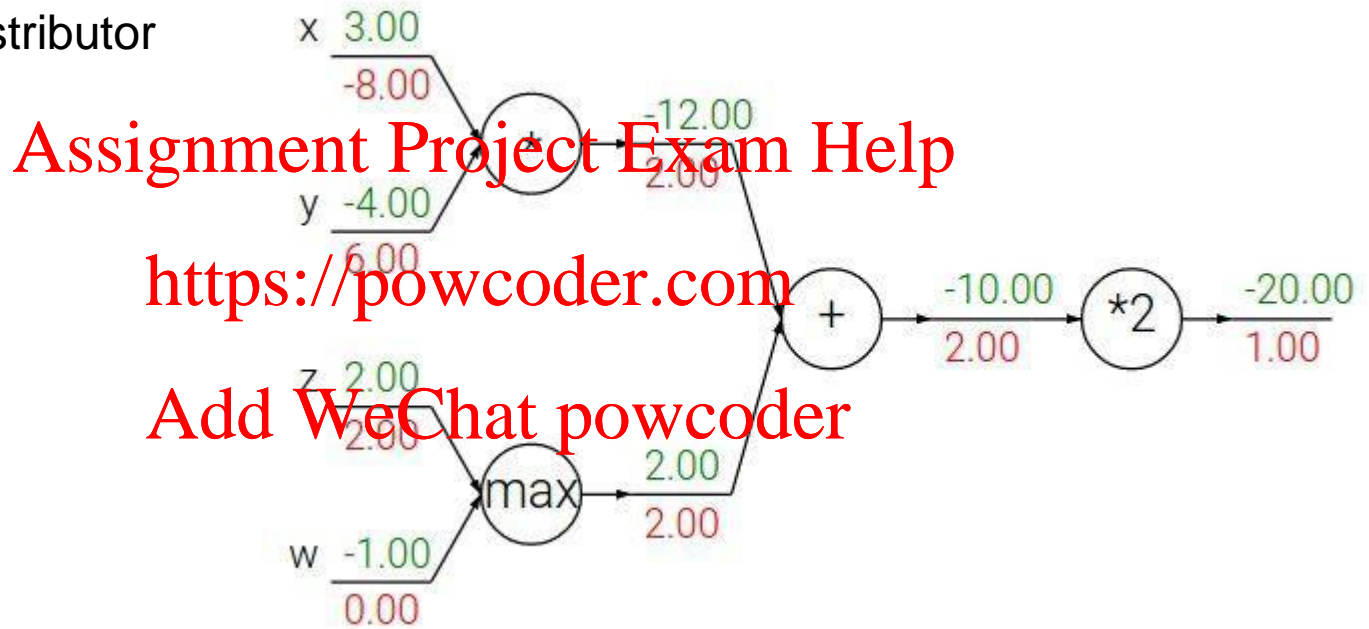


Patterns in backward flow



Patterns in backward flow

add gate: gradient distributor



Patterns in backward flow

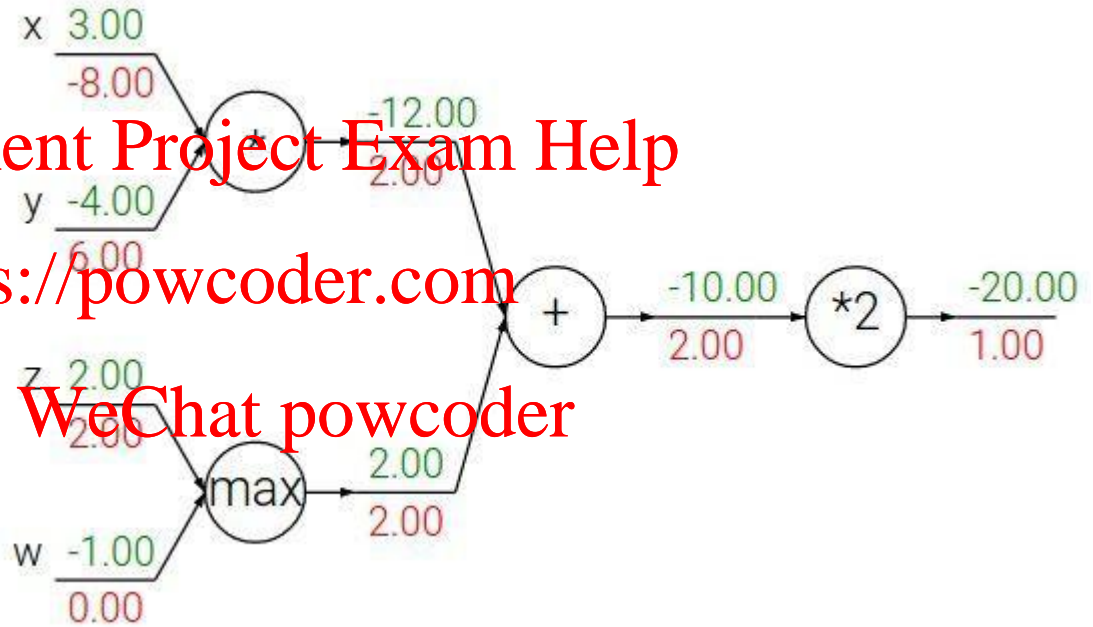
add gate: gradient distributor

max gate: gradient router

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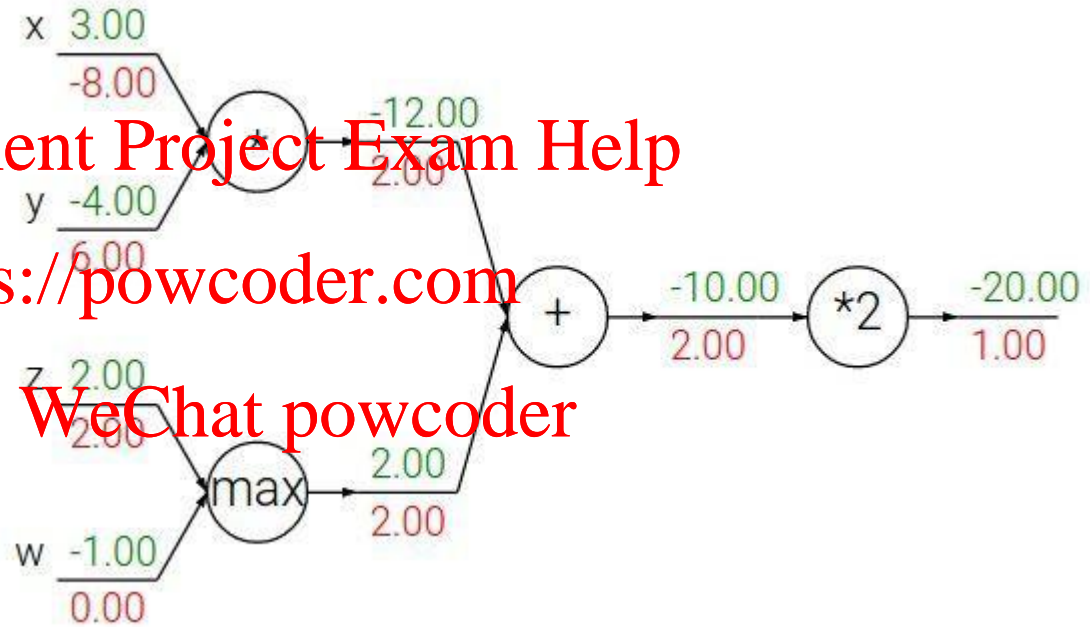


Patterns in backward flow

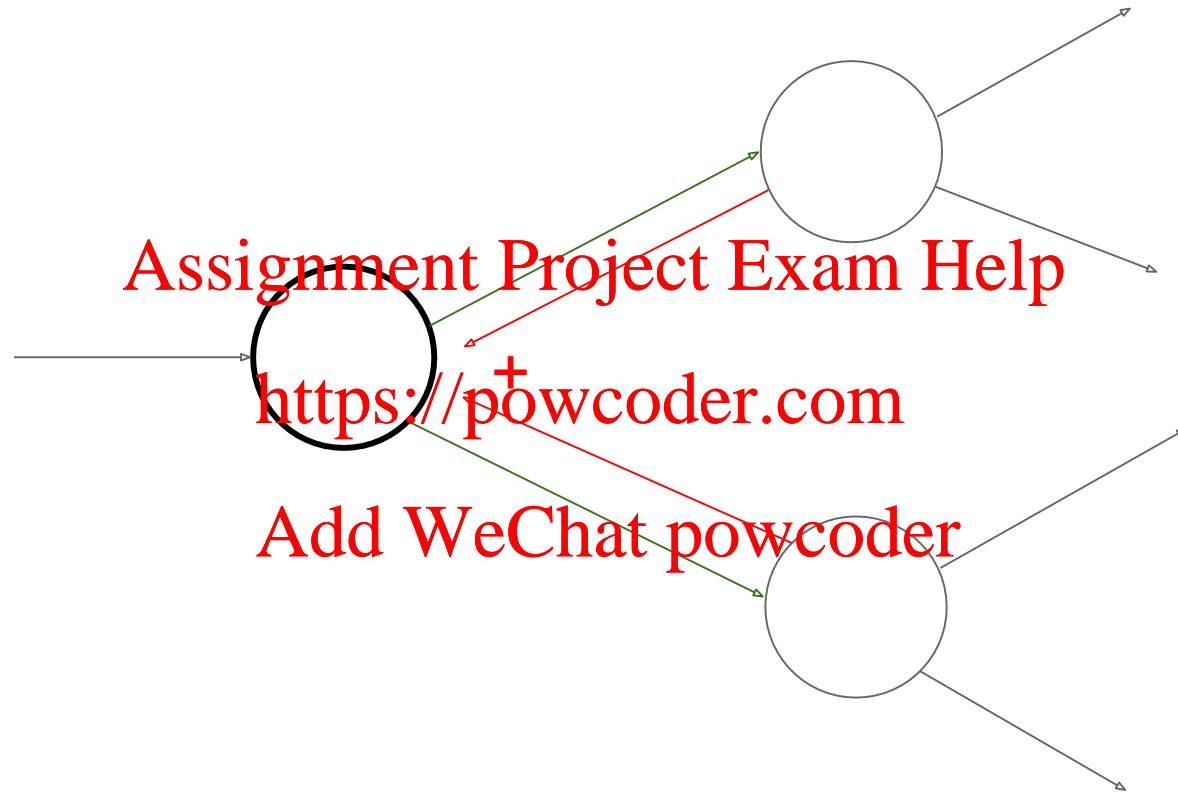
add gate: gradient distributor

max gate: gradient router

mul gate: gradient... "switcher"?



Gradients add at branches





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Neural Networks II

Vectorized Backpropagation

Forward Pass

Require: Network depth, l

Require: $W^{(i)}, i \in \{1, \dots, l\}$, the weight matrices of the model

Require: $b^{(i)}, i \in \{1, \dots, l\}$, the bias parameters of the model

Require: x , the input to process

Require: y , the target output

$h^{(0)} = x$

for $k = 1, \dots, l$ **do**

$a^{(k)} = b^{(k)} + W^{(k)} h^{(k-1)}$

$h^{(k)} = f(a^{(k)})$

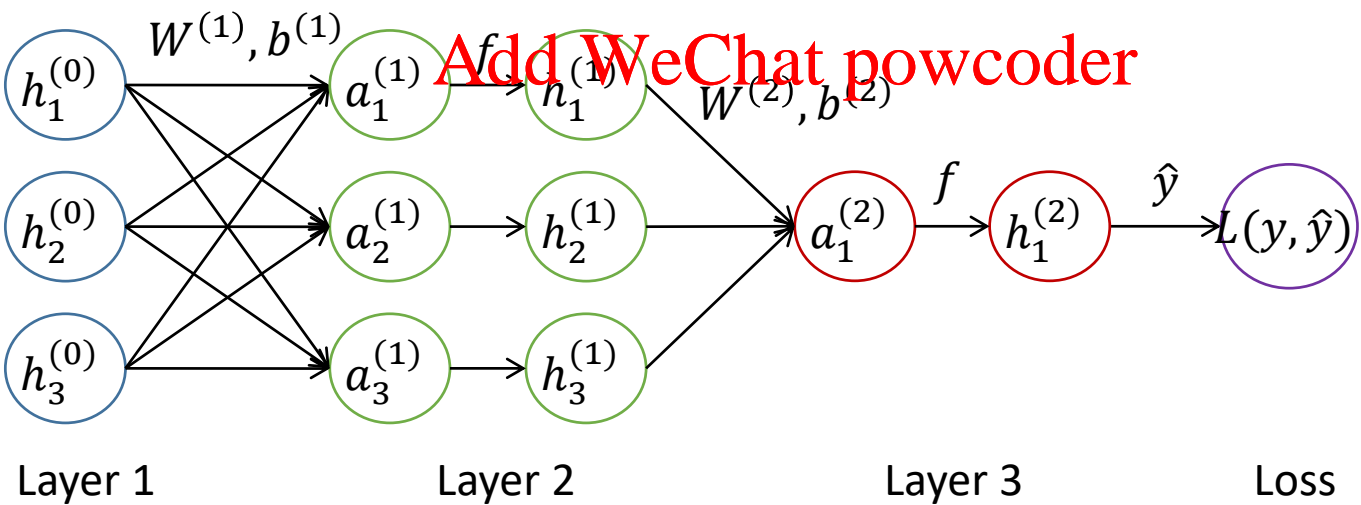
end for

$\hat{y} = h^{(l)}$

$J = L(\hat{y}, y) + \lambda \Omega(\theta)$

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Backward Pass

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

```

$$\mathbf{g} \leftarrow \nabla_{\hat{\mathbf{y}}} J = \nabla_{\hat{\mathbf{y}}} L(\hat{\mathbf{y}}, \mathbf{y})$$
  
for  $k = l, l - 1, \dots, 1$  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):

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

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

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

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

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

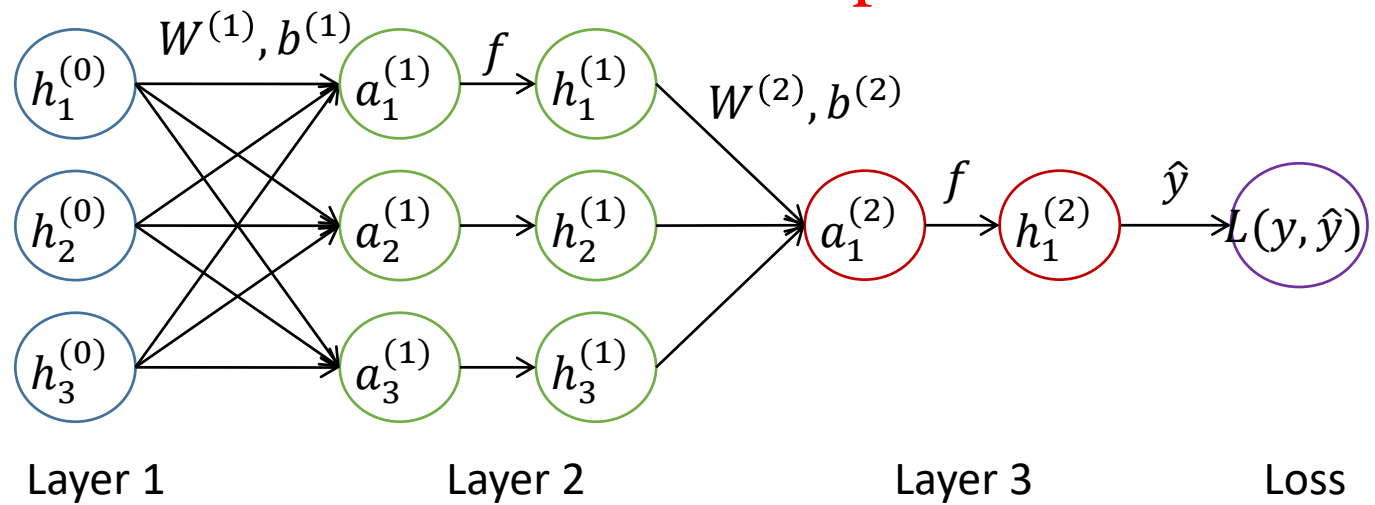
$$\mathbf{g} \leftarrow \nabla_{\mathbf{h}^{(k-1)}} J = \mathbf{W}^{(k)\top} \mathbf{g}$$

```
end for
```

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Backpropagation example with vectorized gradients:

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

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Next Class

Neural Networks III: Convolutional Nets:

Convolutional networks.

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Reading: Bishop Ch 5.5