Computation Graphs

What are Computational graphs ?

- Computational graphs are a type of graph that can be used to represent mathematical expressions.
- In the context of deep learning (and PyTorch) we can think of neural networks as computation graphs.
- These can be used for two different types of calculations:
  - *Forward computation*
  - *Backward computation*

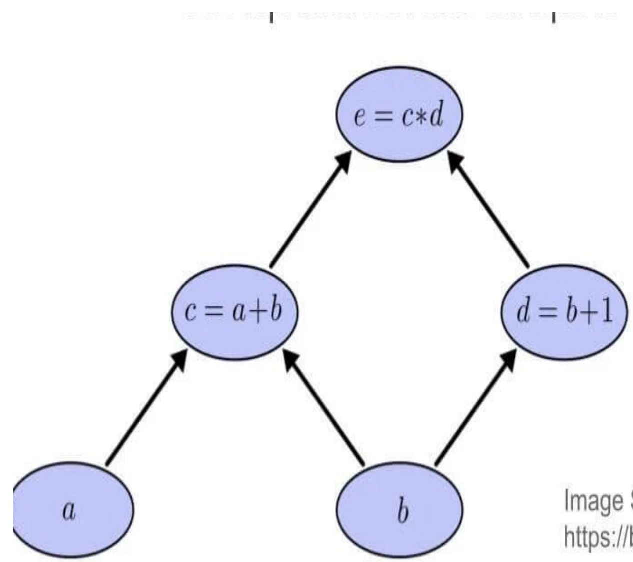
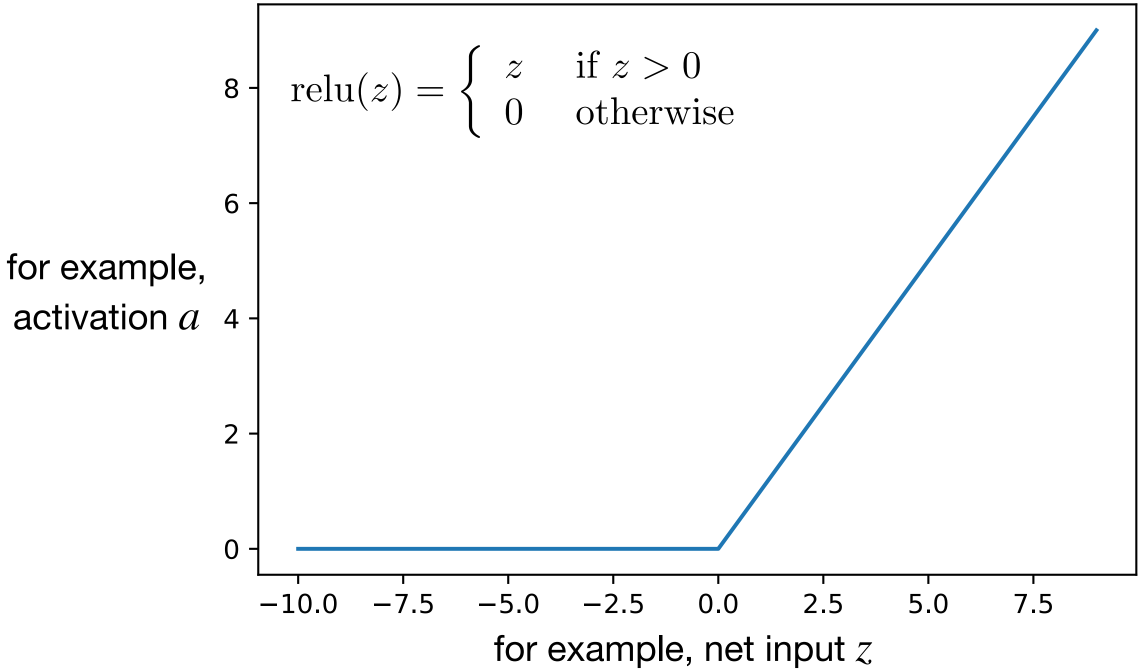


Image Source:
https://bit.ly/2HAxlQP

Computational graphs

Suppose we have the following activation function:

$$a(x,\ w,\ b) = relu(w \cdot x + b)$$



ReLU = Rectified Linear Unit

Computational graphs

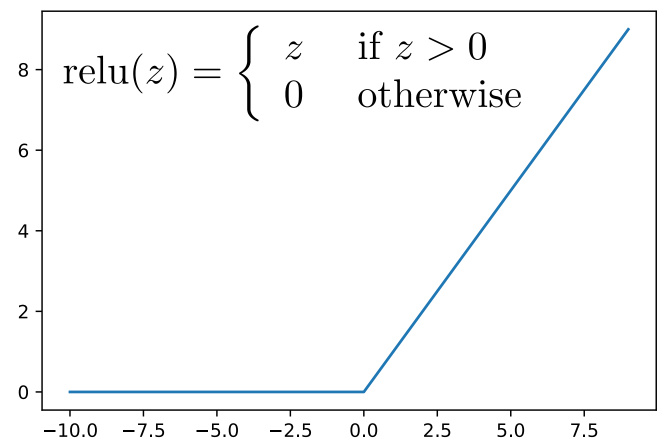
You may note that

$$\sigma'(z) = \begin{cases} 0 & \text{if } z < 0 \\ 1 & \text{if } z > 0 \\ \text{DNE} & \text{if } z = 0 \end{cases}$$

Why not differentiable?
Derivative does not exist (DNE) at 0

But in the machine learning--computer science context, for convenience, we can just say

$$\sigma'(z) = \begin{cases} 0 & \text{if } z \leq 0 \\ 1 & \text{if } z > 0 \end{cases}$$



Computational graphs

Suppose we have the following activation function:

$$a(x,\ w,\ b) = relu(\overbrace{w \cdot x + b}^{\text{net input}})$$

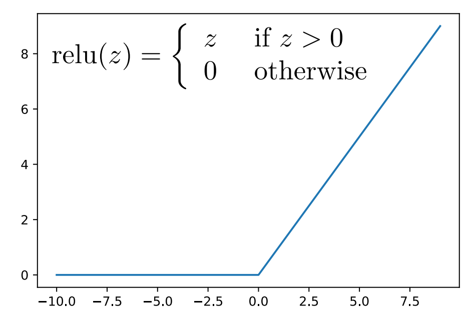
multivariable function

activation function

weight parameter
(assume only 1 input feature)

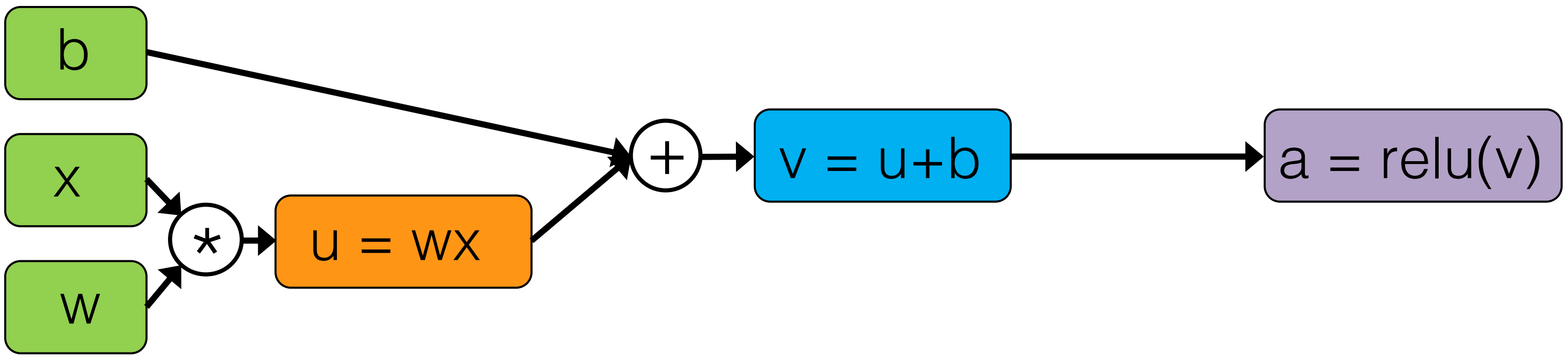
feature
(suppose only 1 training example)

bias

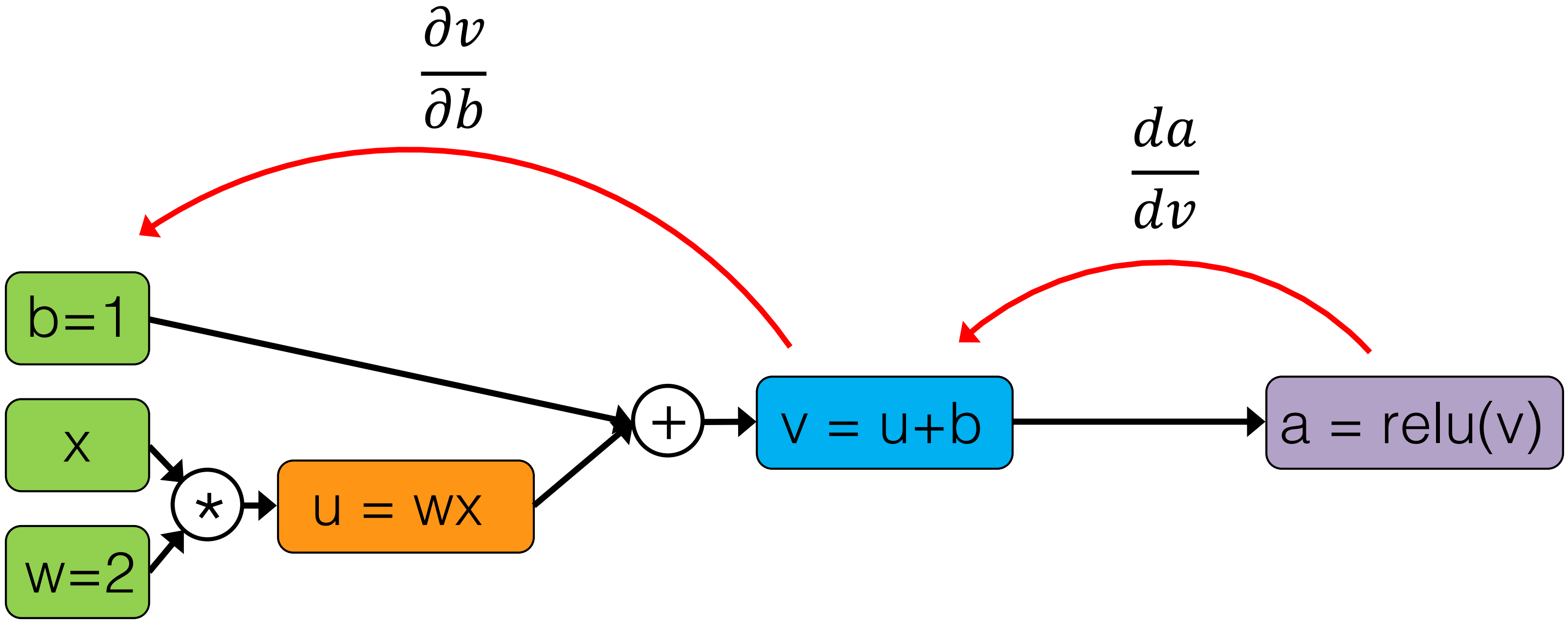


Computational graphs

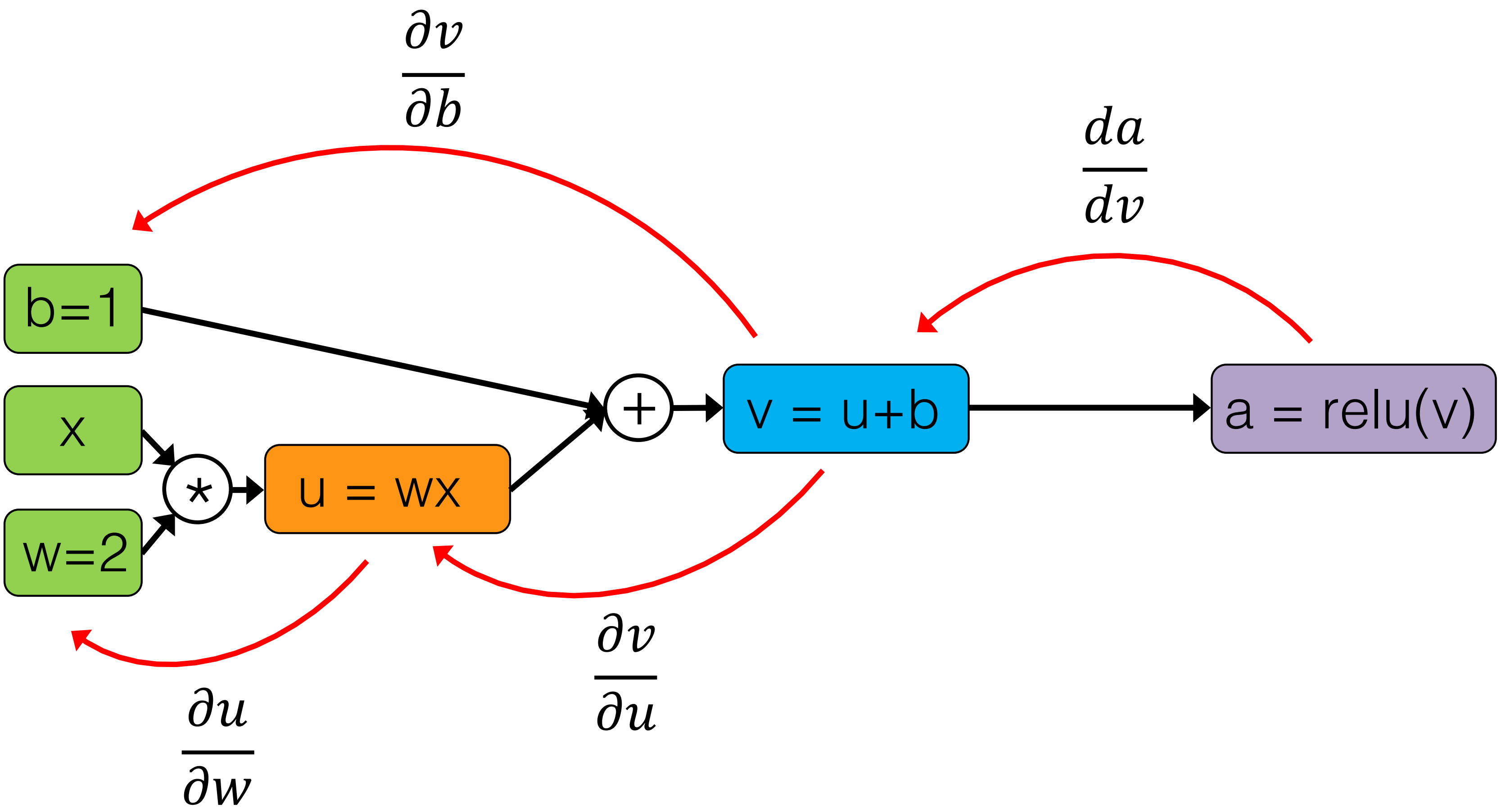
$$a(x,\ w,\ b) = relu(\underbrace{\underbrace{w \cdot x}_{u} + \ b}_{v})$$



Computational graphs

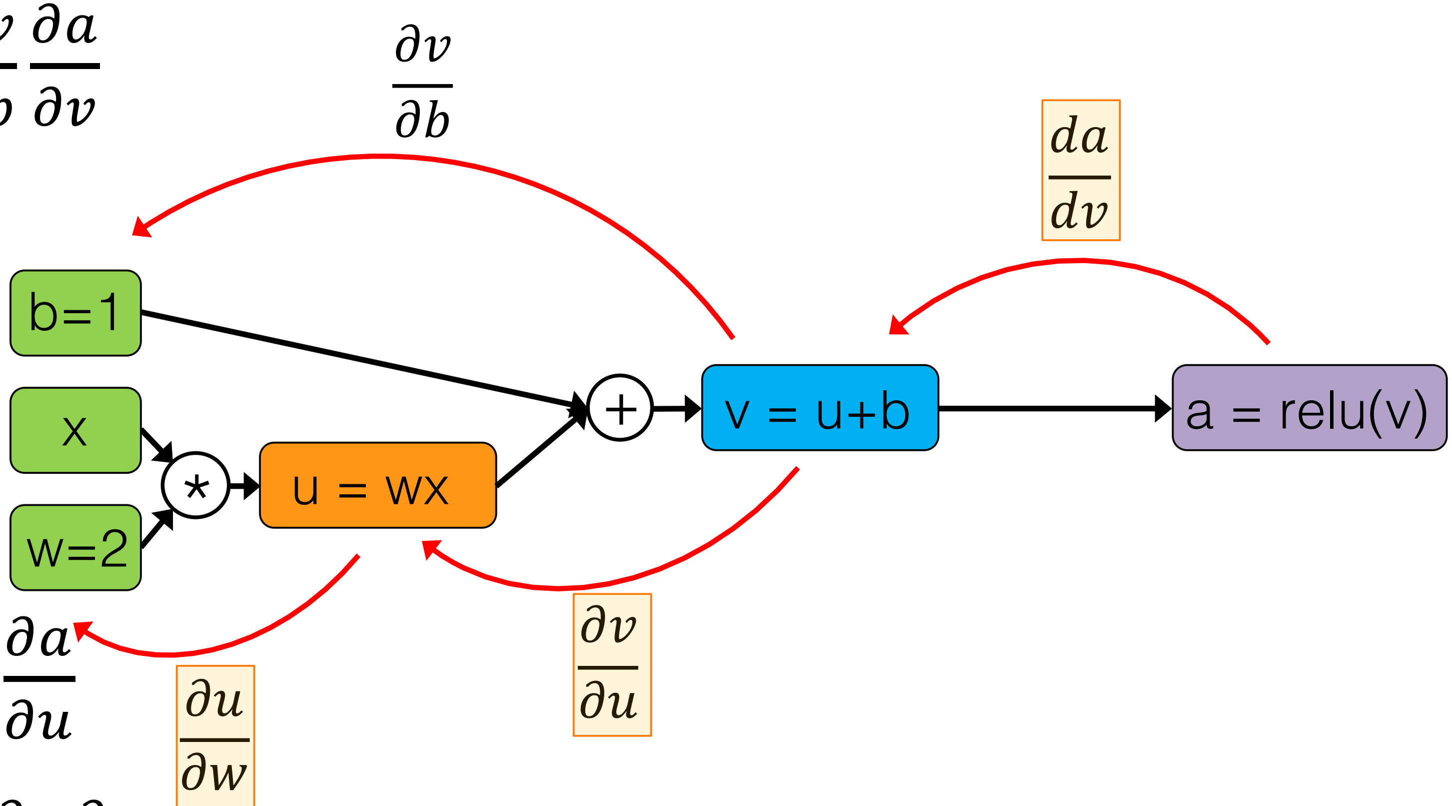


Computational graphs



Computational graphs

$$\frac{\partial a}{\partial b} = \frac{\partial v}{\partial b}\frac{\partial a}{\partial v}$$

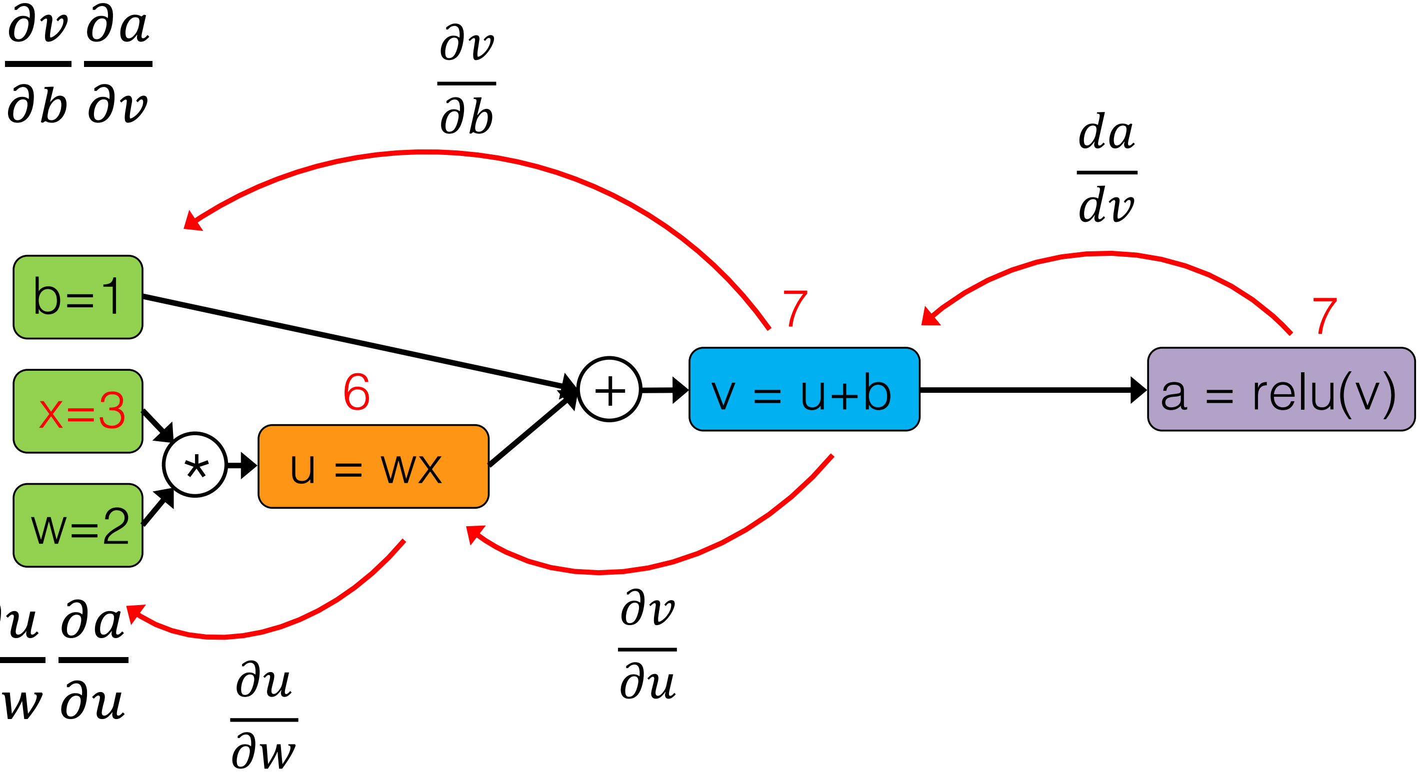


$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

$$= \frac{\partial u}{\partial w}\frac{\partial v}{\partial u}\frac{\partial a}{\partial v}$$

Computational graphs

$$\frac{\partial a}{\partial b} = \frac{\partial v}{\partial b}\frac{\partial a}{\partial v}$$



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Computational graphs

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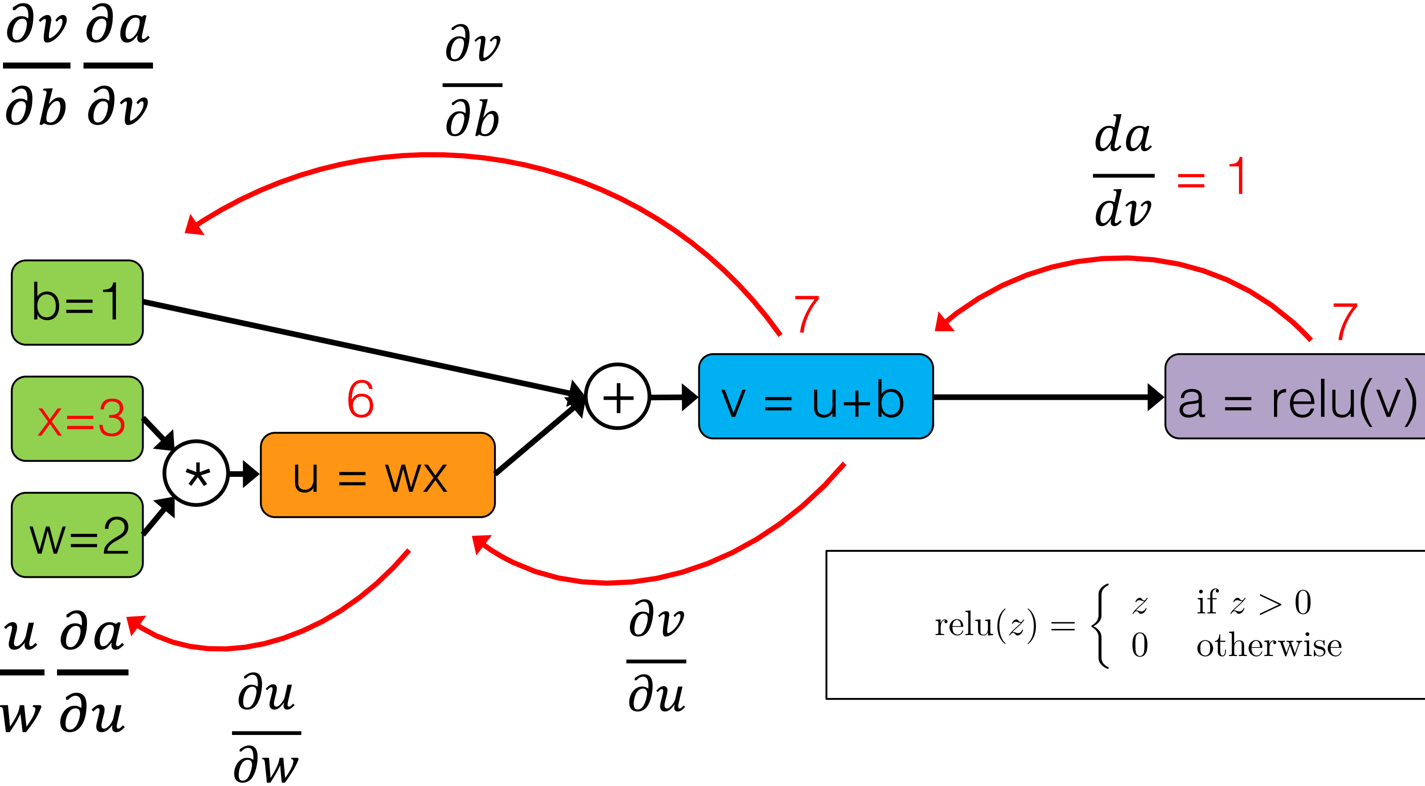


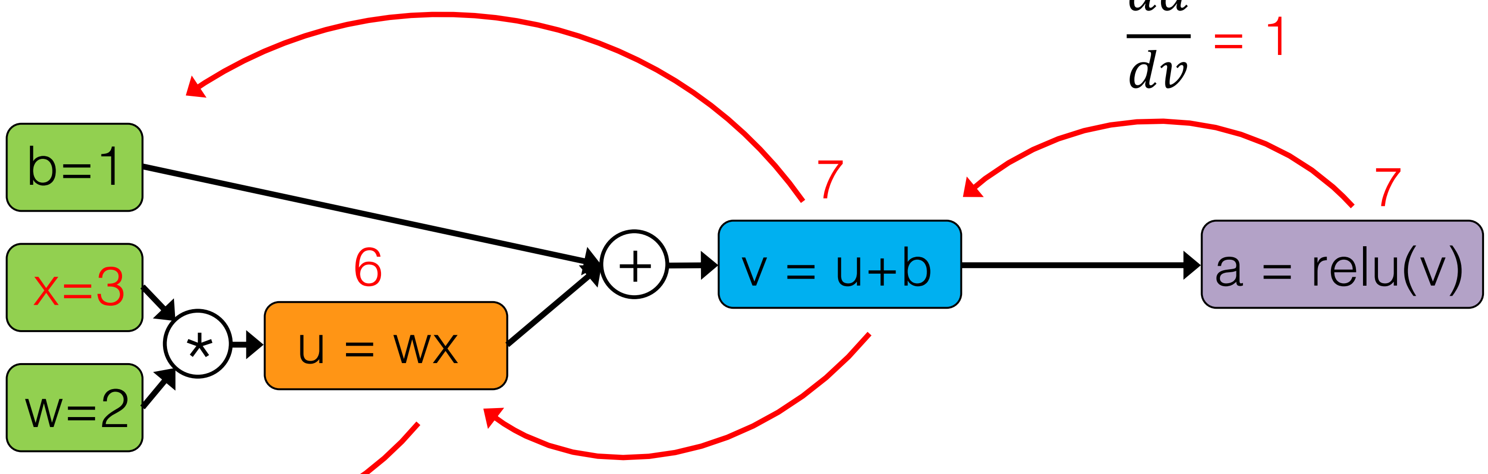
$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

$$= \frac{\partial u}{\partial w}\frac{\partial v}{\partial u}\frac{\partial a}{\partial v}$$

$$\mathrm{relu}(z) = \begin{cases} z & \text{if } z > 0 \\ 0 & \text{otherwise} \end{cases}$$

Computational graphs

$$\frac{\partial a}{\partial b} = \frac{\partial v}{\partial b}\frac{\partial a}{\partial v}$$



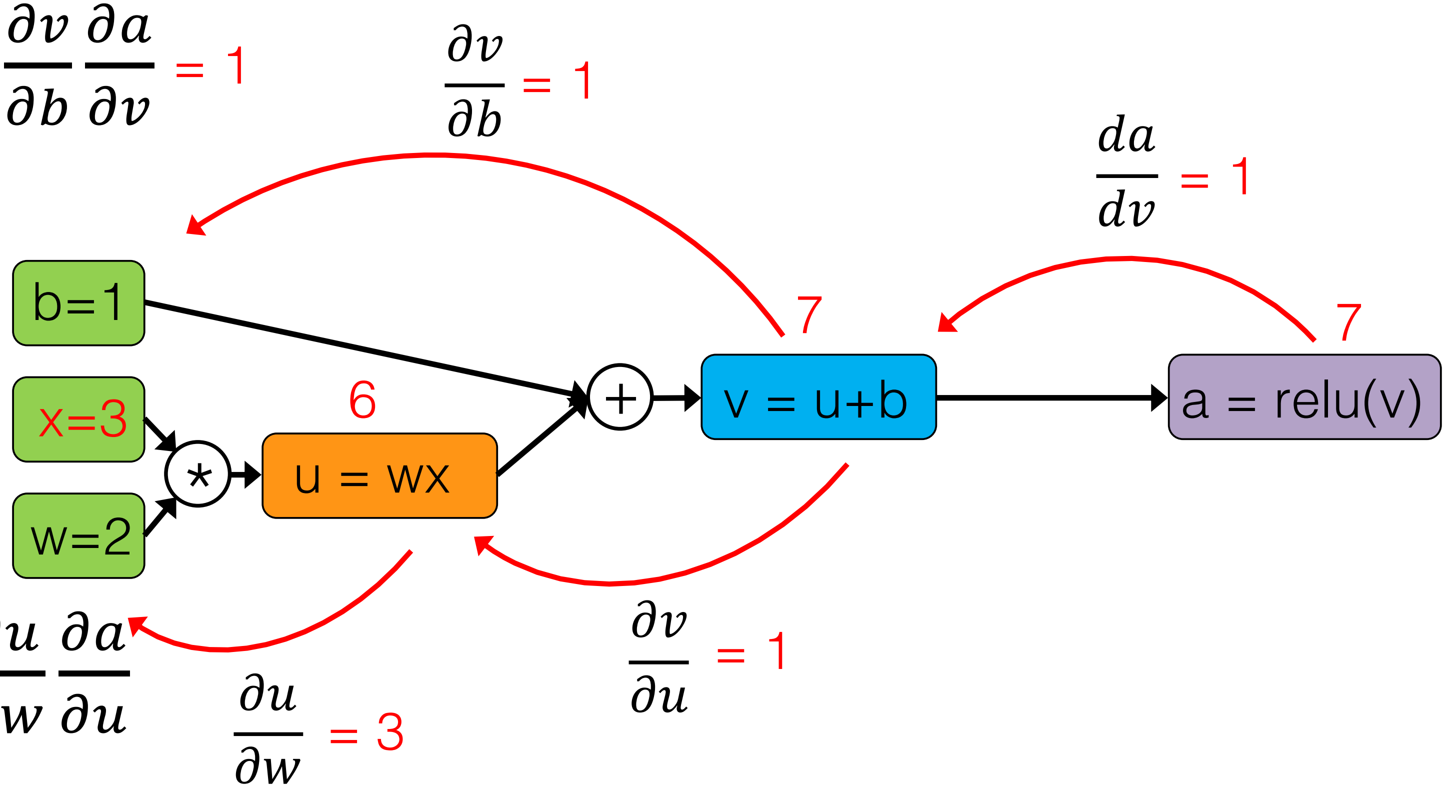
$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

$$= \frac{\partial u}{\partial w}\frac{\partial v}{\partial u}\frac{\partial a}{\partial v}$$

Function	**Derivative**
$f(x) + g(x)$	$f'(x) + g'(x)$

Computational graphs

$$\frac{\partial a}{\partial b} = \frac{\partial v}{\partial b}\frac{\partial a}{\partial v} = 1$$

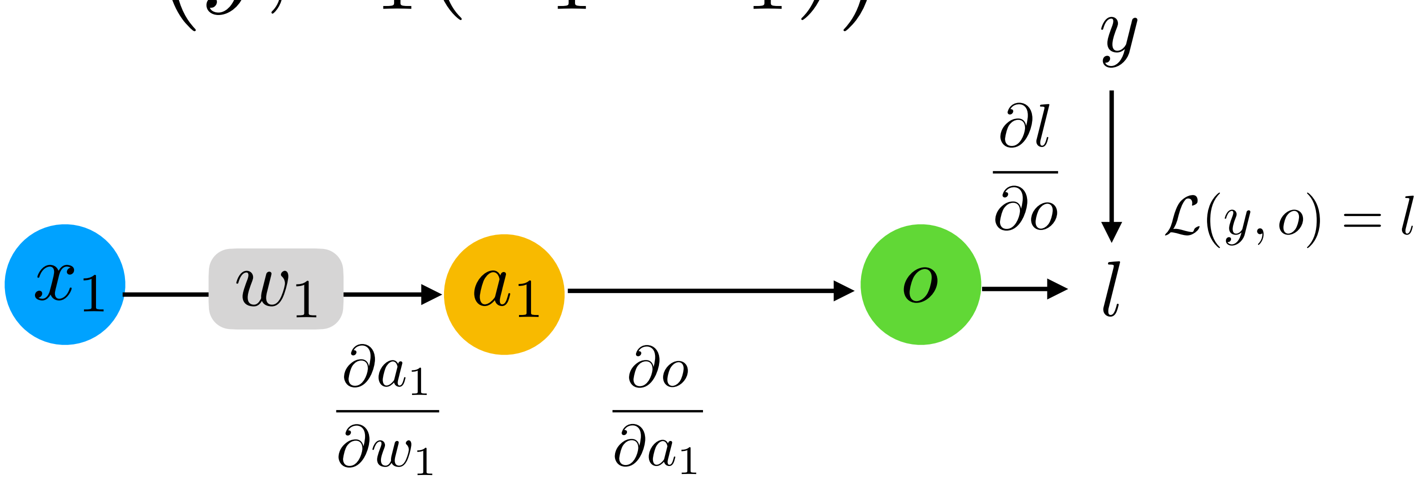


$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

$$= \frac{\partial u}{\partial w}\frac{\partial v}{\partial u}\frac{\partial a}{\partial v} = 3*1*1 = 3$$

Graph with single path

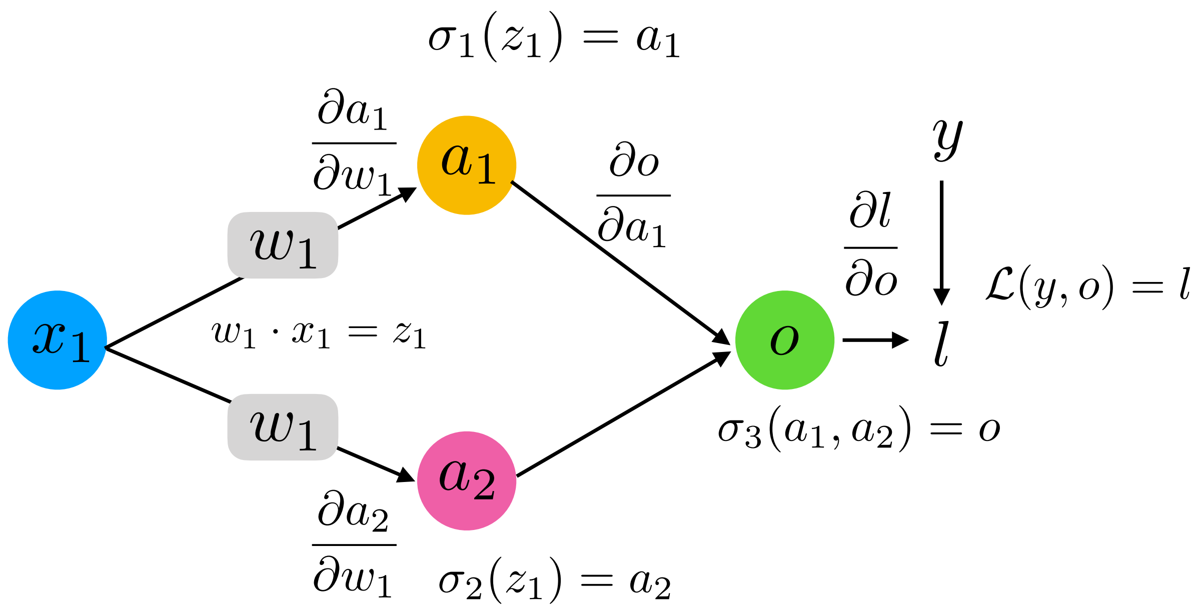
$$\mathcal{L}\big(y, \sigma_1(w_1 \cdot x_1)\big)$$



$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_1} \cdot \frac{\partial a_1}{\partial w_1}$$ (univariate chain rule)

Graph with weight sharing

$$\mathcal{L}\Big(y, \sigma_3\big[\sigma_1(w_1 \cdot x_1), \sigma_2(w_1 \cdot x_1)\big]\Big)$$

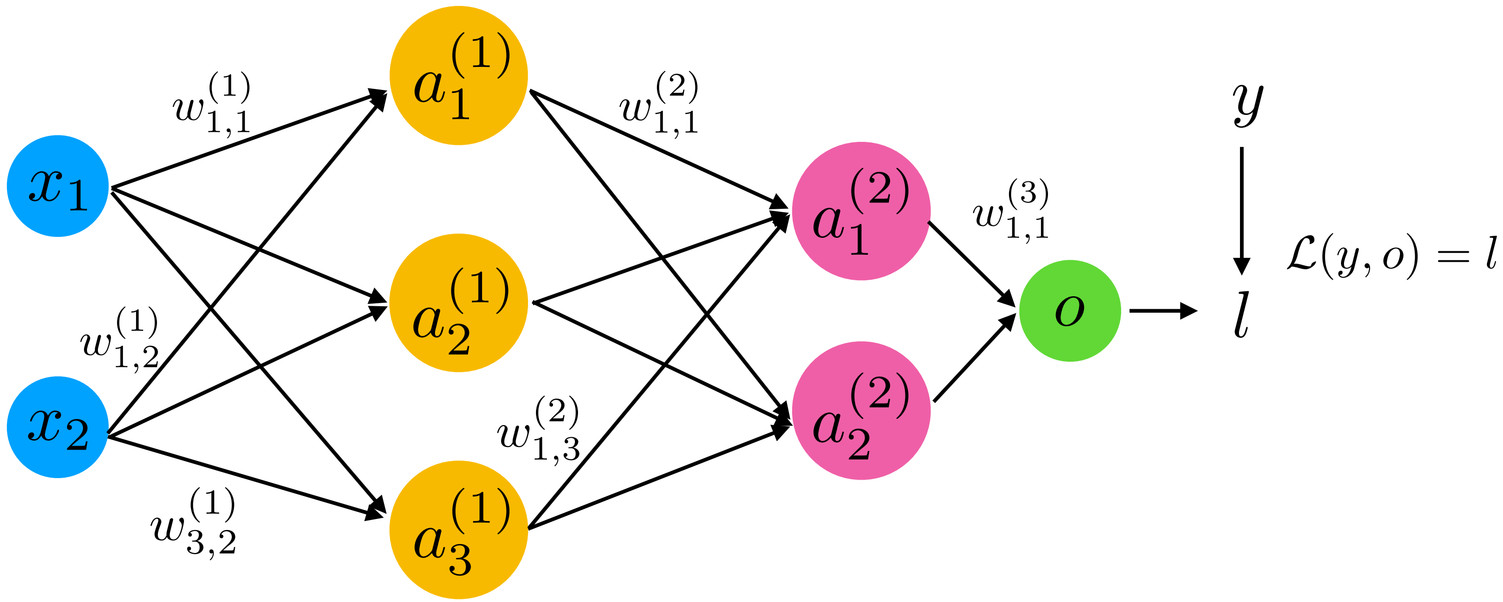


Upper path

$$\frac{\partial l}{\partial w_1} = \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_1} \cdot \frac{\partial a_1}{\partial w_1} + \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_2} \cdot \frac{\partial a_2}{\partial w_1}$$ (multivariable chain rule)

Lower path

Graph with Fully connected layers



$$\frac{\partial l}{\partial w_{1,1}^{(1)}} = \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_1^{(2)}} \cdot \frac{\partial a_1^{(2)}}{\partial a_1^{(1)}} \cdot \frac{\partial a_1^{(1)}}{\partial w_{1,1}^{(1)}}$$
$$+ \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a_2^{(2)}} \cdot \frac{\partial a_2^{(2)}}{\partial a_1^{(1)}} \cdot \frac{\partial a_1^{(1)}}{\partial w_{1,1}^{(1)}}$$

Automatic Differentiation with PyTorch