Lecture 06

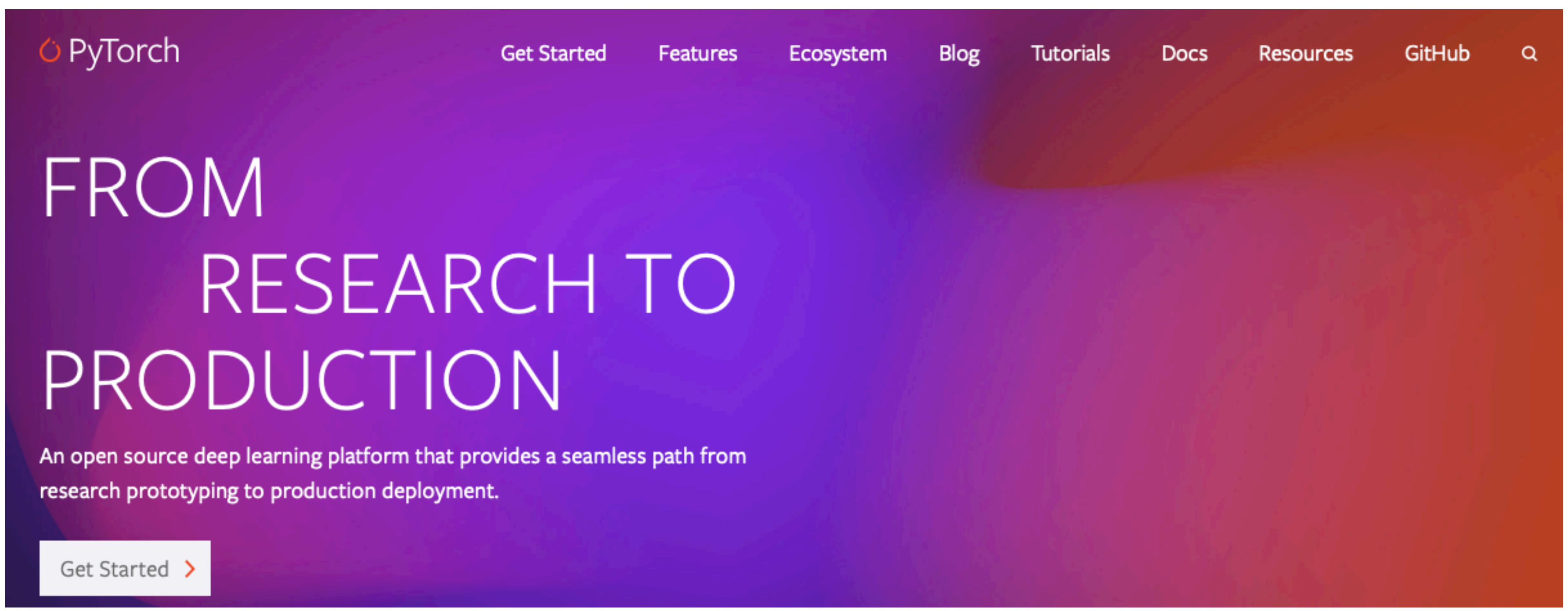
Automatic Differentiation with PyTorch

STAT 479: Deep Learning, Spring 2019

Sebastian Raschka

http://stat.wisc.edu/~sraschka/teaching/stat479-ss2019/

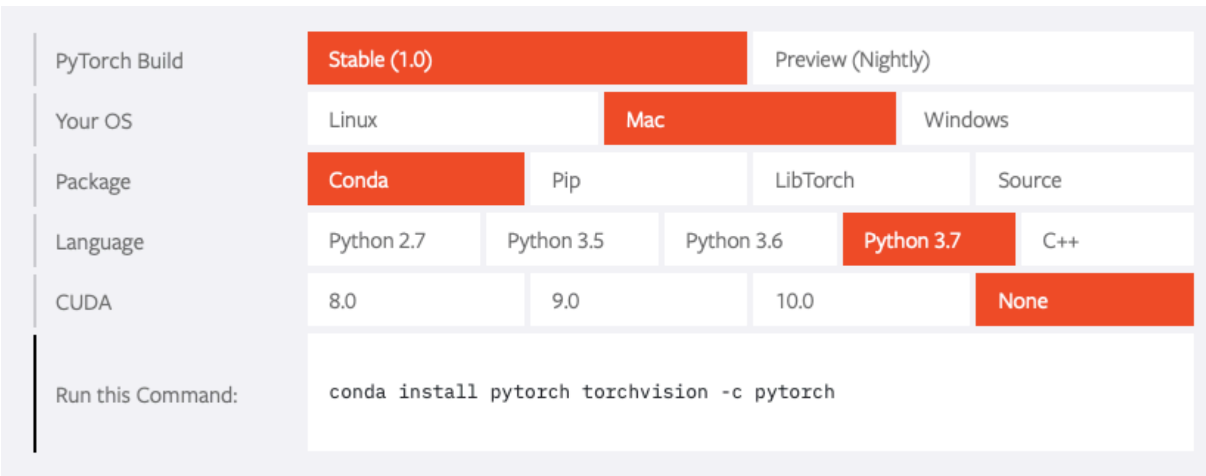
PyTorch



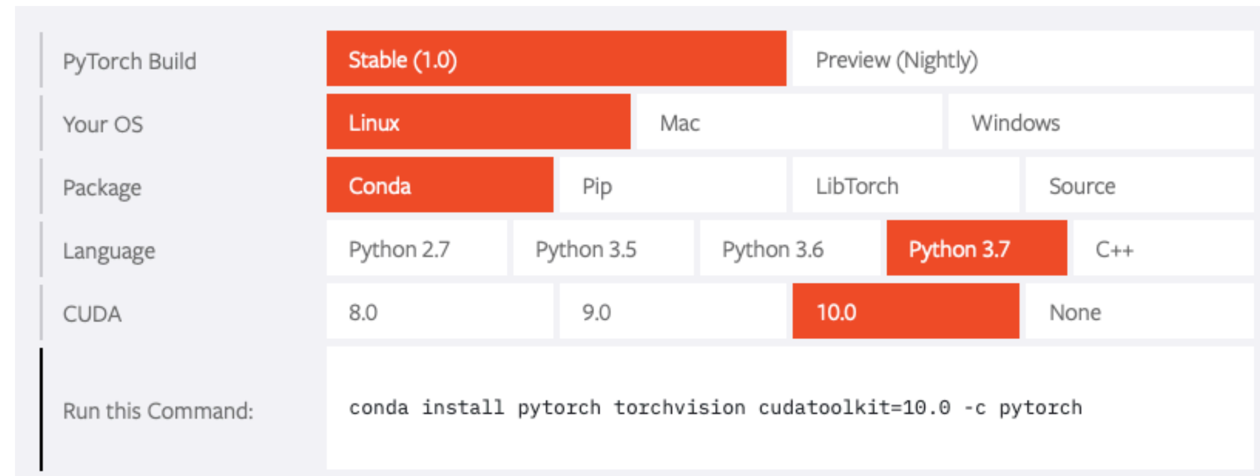
https://pytorch.org/

Installation

Recommendation for Laptop (e.g., MacBook)



Recommendation for Desktop (Linux) with GPU



https://pytorch.org/

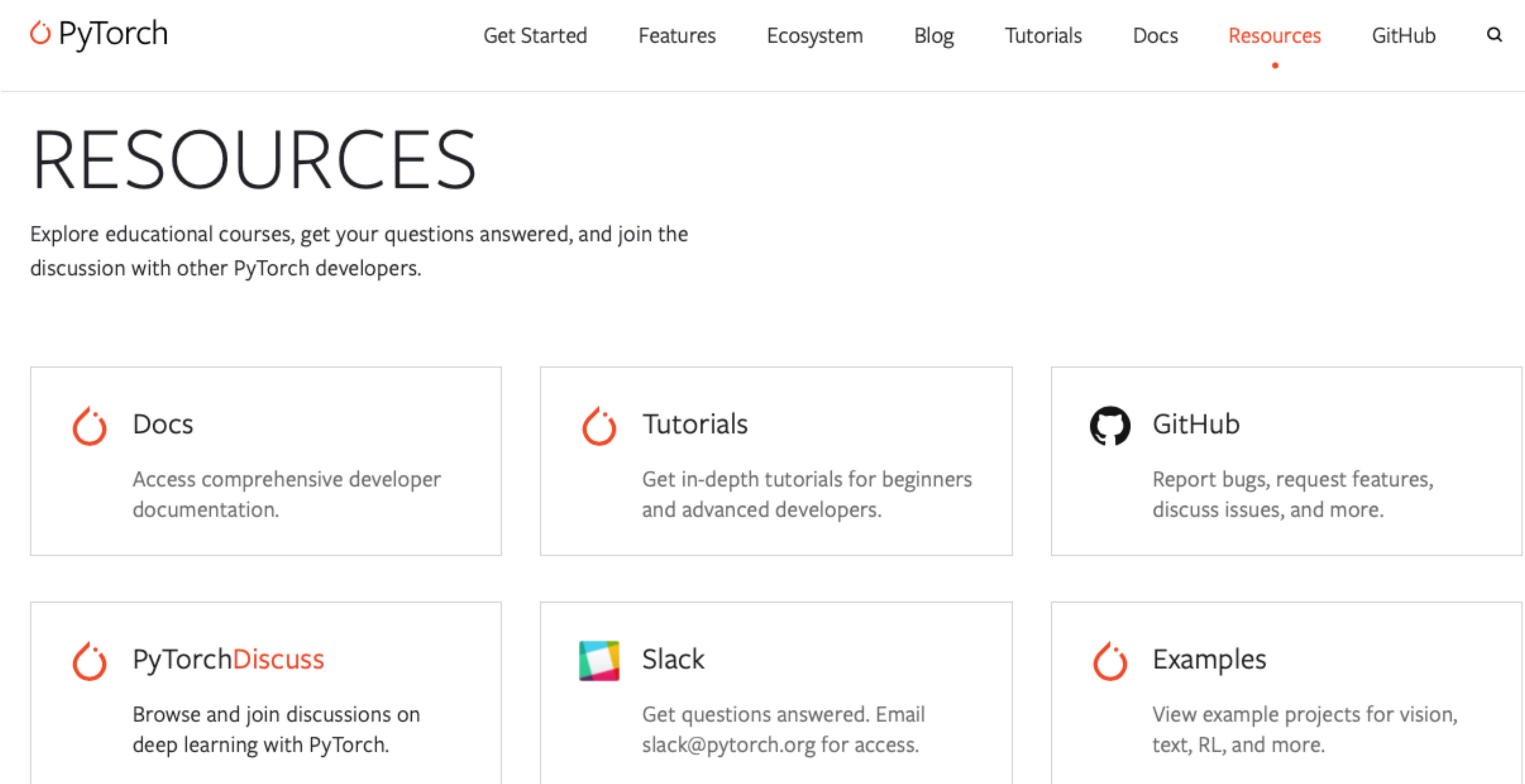
Installation Tips:

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/other/pytorch-installation-tips.md

And don't forget that you import PyTorch as "import torch," not "import pytorch" :)

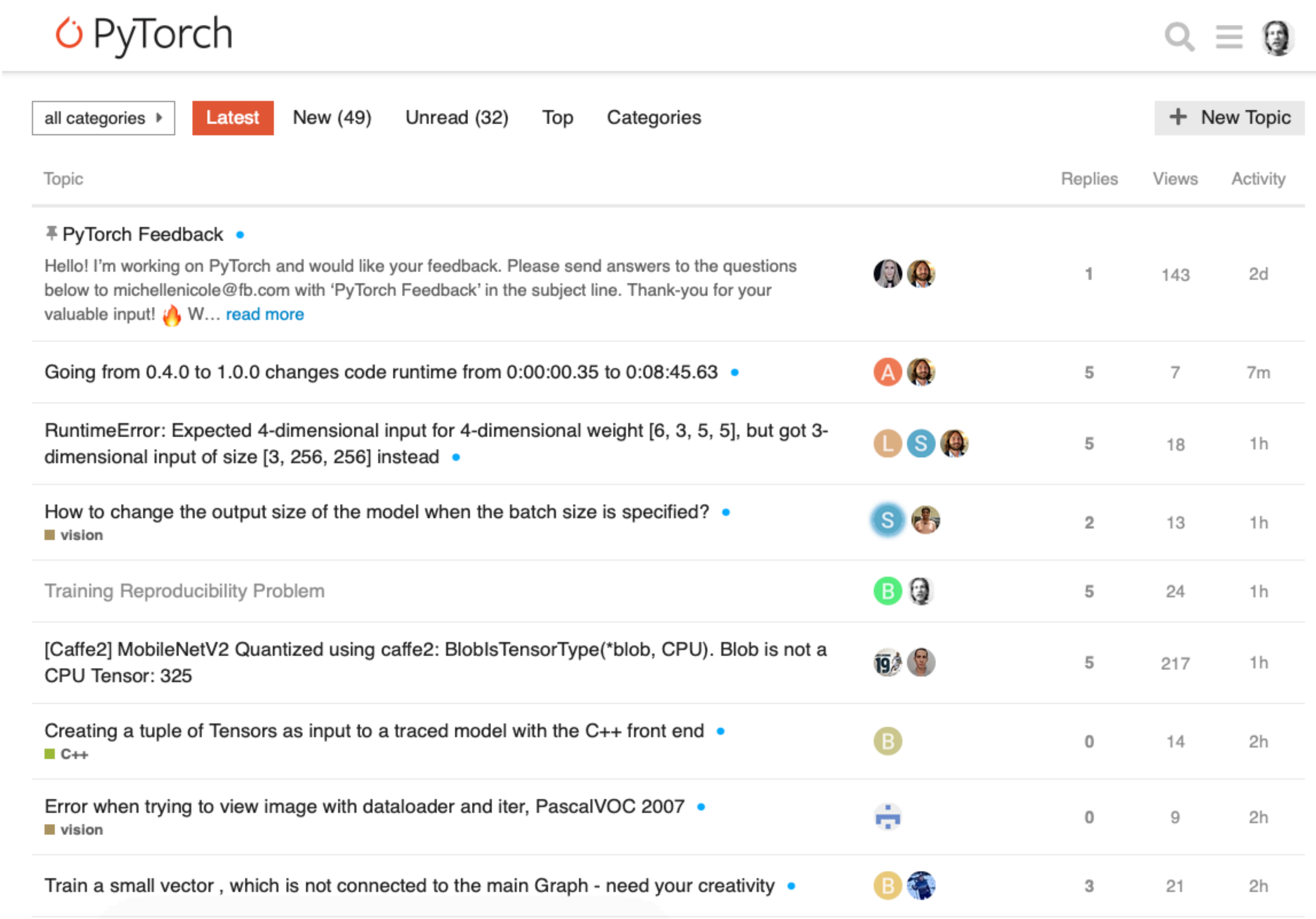
```
In [1]: import torch

In [2]: torch.__version__
Out[2]: '1.0.1'
```

Many Useful Tutorials (recommend that you read some of them)



https://pytorch.org/resources

Very Active & Friendly Community and Help/Discussion Forum



https://pytorch.org/resources

Tutorials > Deep Learning with PyTorch: A 60 Minute Blitz

DEEP LEARNING WITH PYTORCH: A 60 MINUTE BLITZ

Author: Soumith Chintala

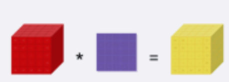
Goal of this tutorial:

- Understand PyTorch's Tensor library and neural networks at a high level.
- Train a small neural network to classify images

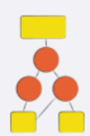
This tutorial assumes that you have a basic familiarity of numpy

NOTE

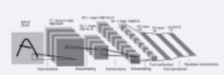
Make sure you have the torch and torchvision packages installed.



What is PyTorch?



Autograd: Automatic Differentiation



Neural Networks

DEEP LEARNING WITH PYTORCH: A 60 MINUTE BLITZ

https://pytorch.org/tutorials/beginner/deep_learning_60min_blitz.html

Generally speaking, `torch.autograd` is an engine for computing vector-Jacobian product. That is, given any vector $v = \begin{pmatrix} v_1 & v_2 & \cdots & v_m \end{pmatrix}^T$, compute the product $v^T \cdot J$. If v happens to be the gradient of a scalar function $l = g(\vec{y})$, that is, $v = \begin{pmatrix} \frac{\partial l}{\partial y_1} & \cdots & \frac{\partial l}{\partial y_m} \end{pmatrix}^T$, then by the chain rule, the vector-Jacobian product would be the gradient of l with respect to $\vec{x}$:

$$J^T \cdot v = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_n} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix} \begin{pmatrix} \frac{\partial l}{\partial y_1} \\ \vdots \\ \frac{\partial l}{\partial y_m} \end{pmatrix} = \begin{pmatrix} \frac{\partial l}{\partial x_1} \\ \vdots \\ \frac{\partial l}{\partial x_n} \end{pmatrix}$$

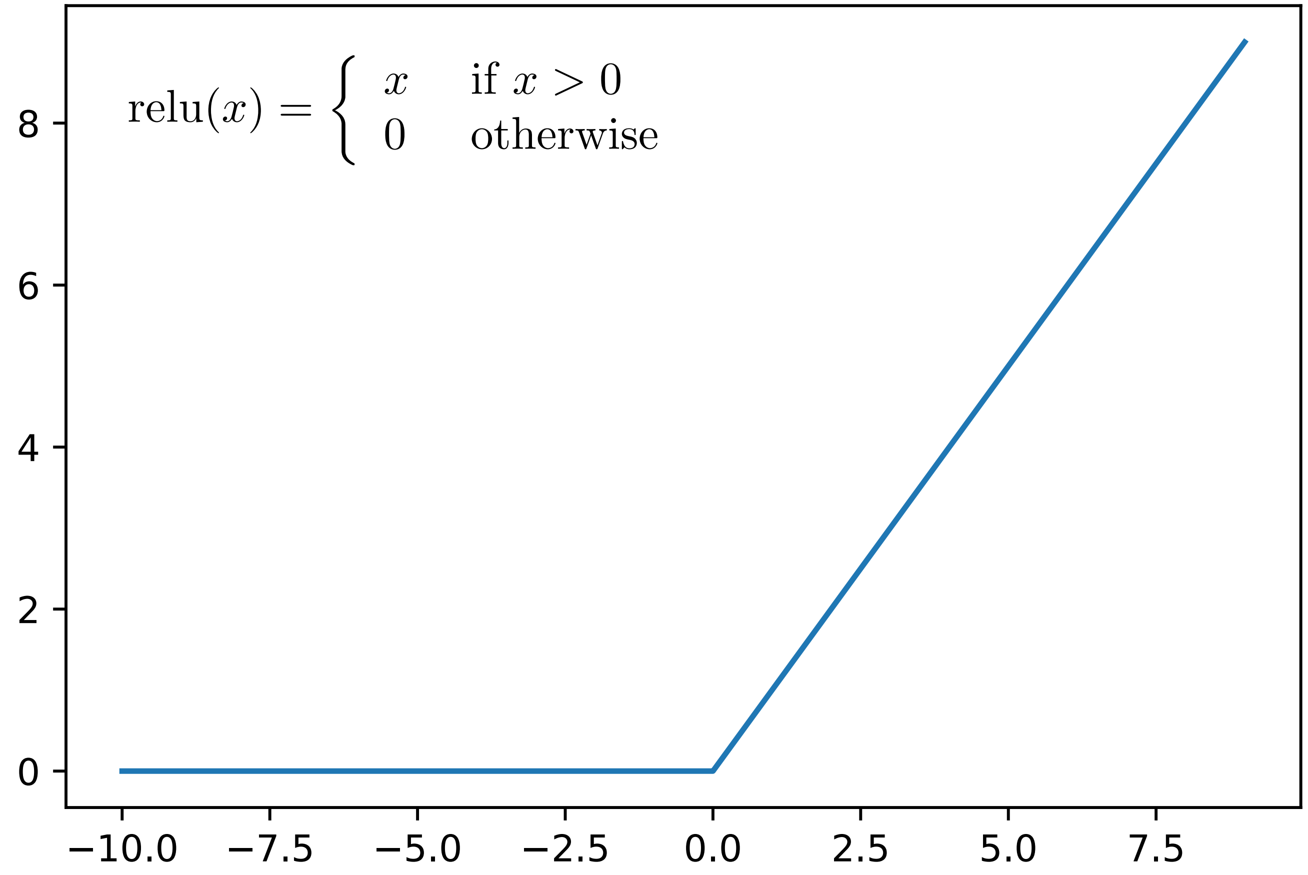
Text source: https://pytorch.org/tutorials/beginner/blitz/autograd_tutorial.html#sphx-glr-beginner-blitz-autograd-tutorial-py

In the context of deep learning (and PyTorch) it is helpful to think about neural networks as computation graphs

Computation Graphs

Suppose we have the following activation function:

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



ReLU = Rectified Linear Unit

(prob. the most commonly used activation function in DL)

Side-note about ReLU Function

You may note that

$$f'(x) = \begin{cases} 0 & \text{if } x < 0 \\ x & \text{if } x > 0 \\ \text{DNE} & \text{if } x = 0 \end{cases}$$

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

$$f'(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}$$

$$f'(x) = \lim_{x \to 0} \frac{\max(0, x + \Delta x) - \max(0, x)}{\Delta x}$$

$$f'(x) = \lim_{x \to 0} \frac{\max(0, x + \Delta x) - \max(0, x)}{\Delta x}$$

$$f'(0) = \lim_{x \to 0^+} \frac{0 + \Delta x - 0}{\Delta x} = 1$$

$$f'(0) = \lim_{x \to 0^-} \frac{0 - 0}{\Delta x} = 0$$

Computation Graphs

Suppose we have the following activation function:

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

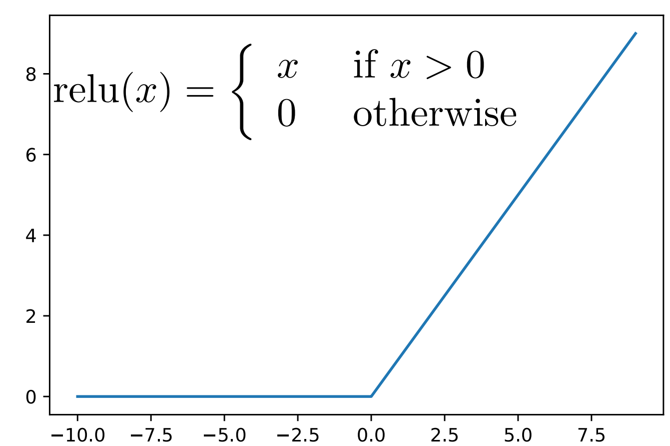
multivariable function

activation function

weight parameter
(assume only 1 input feature)

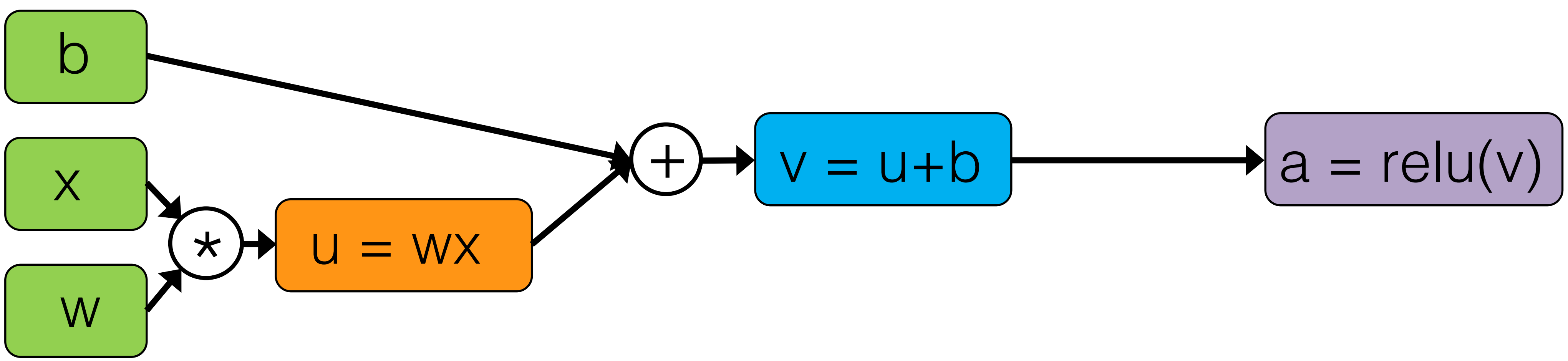
feature
(suppose only 1 training example)

bias



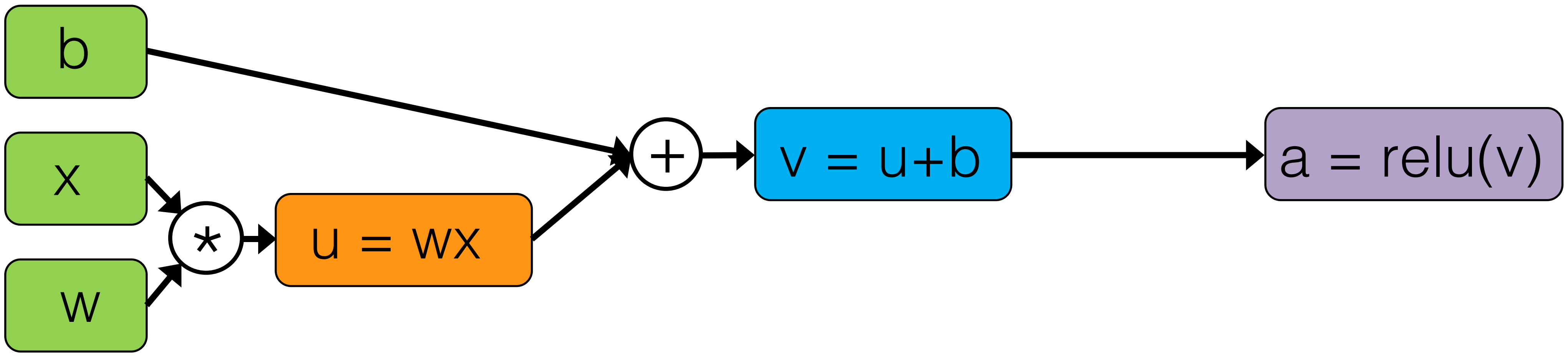
Computation Graphs

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

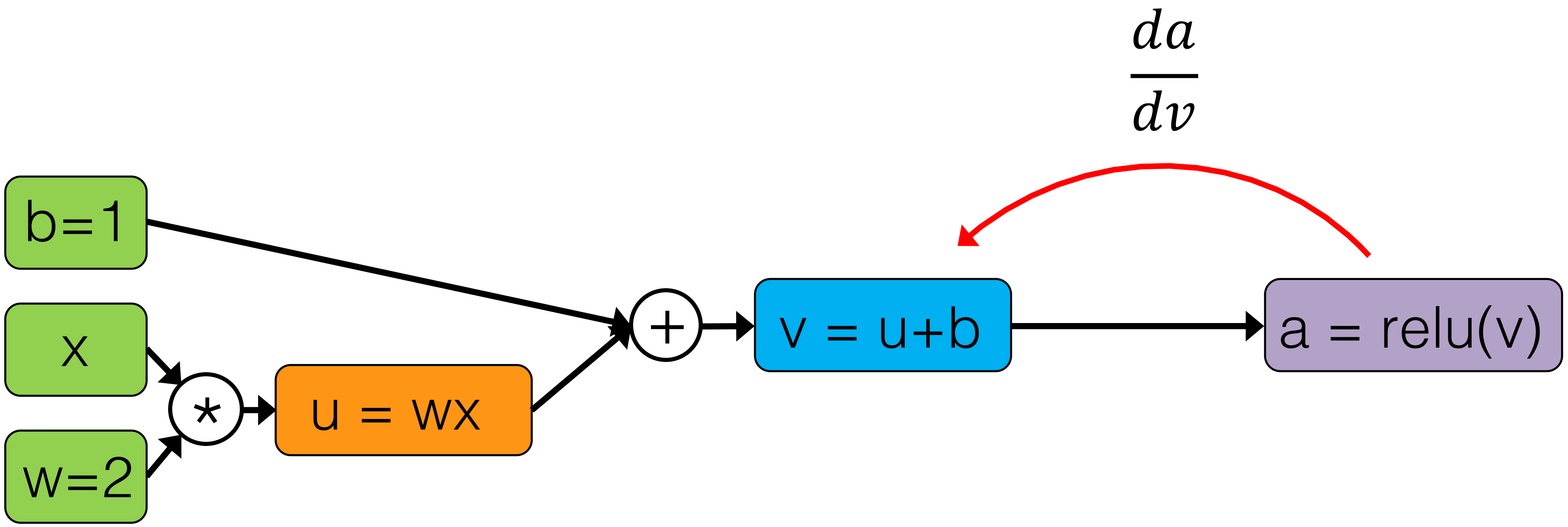


Computation Graphs

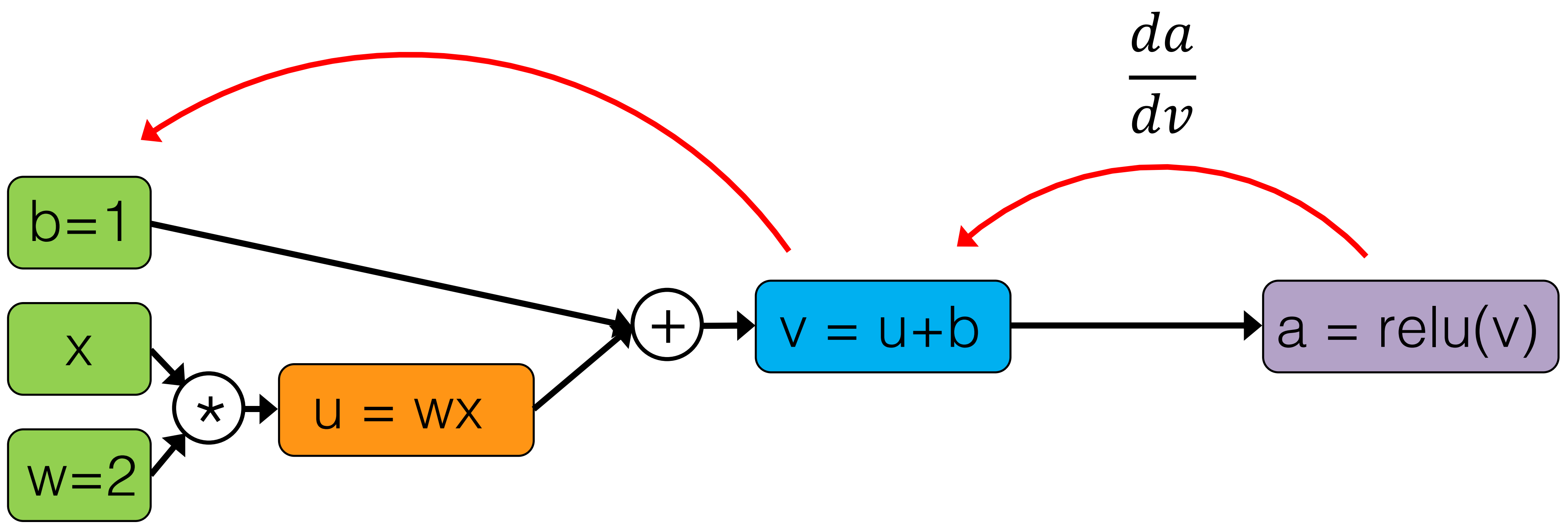
$$a(x,\ w,\ b) = relu(\underbrace{\underbrace{w \cdot x}_{u} + \ b}_{v})$$



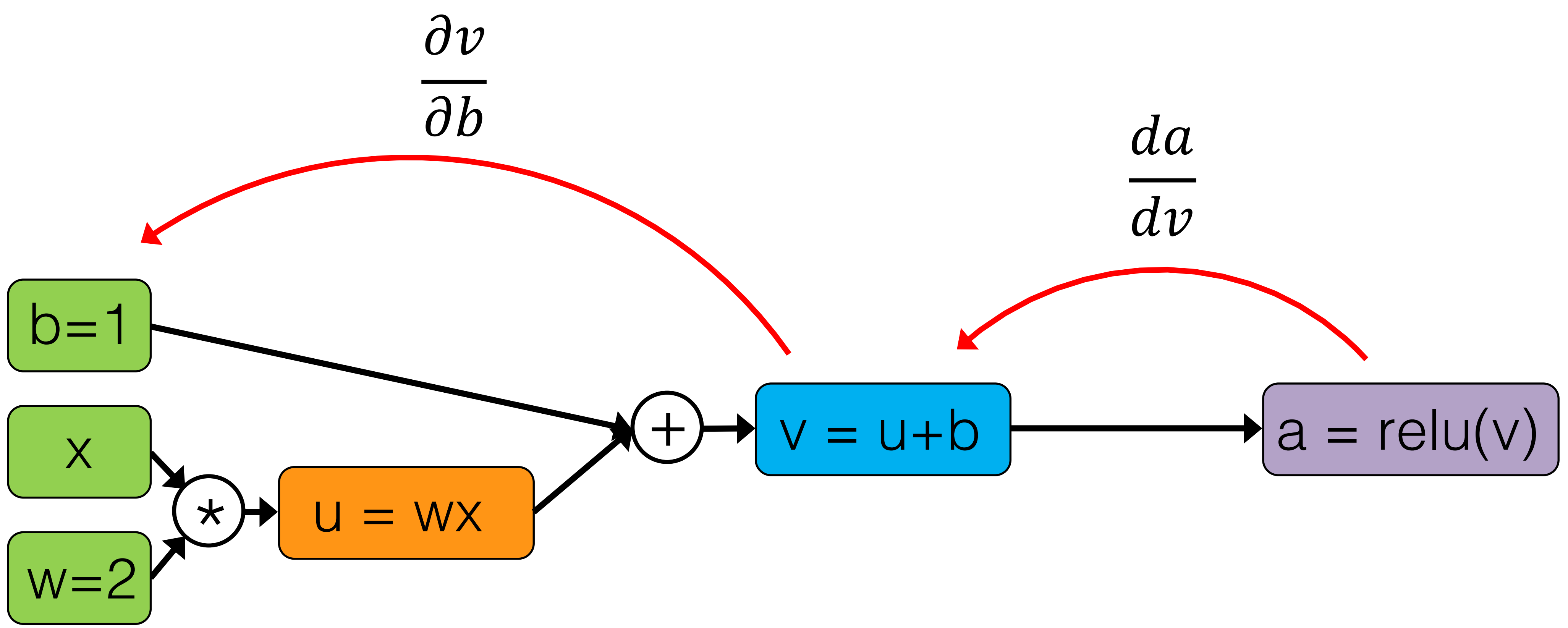
Computation Graphs



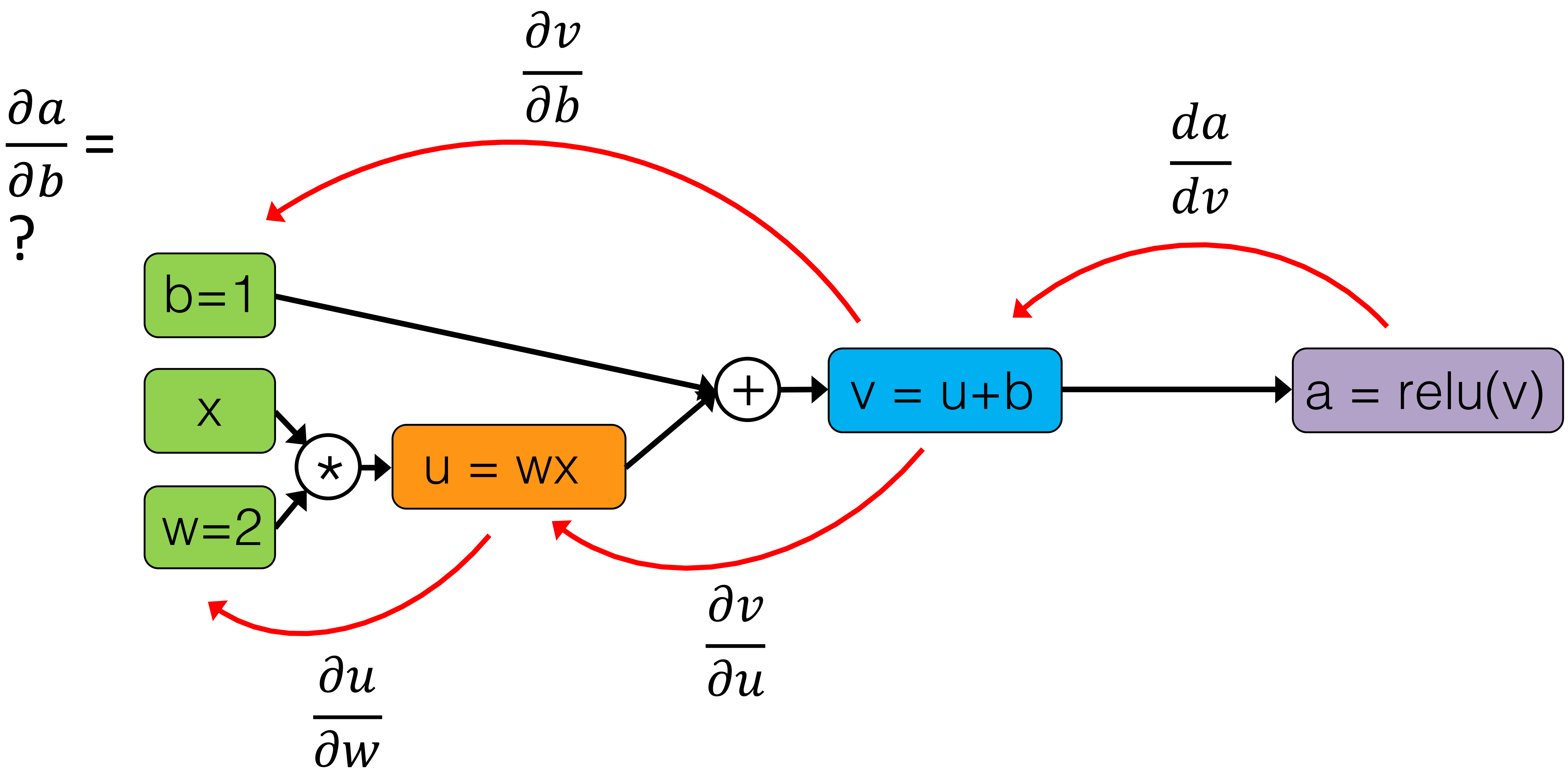
Computation Graphs



Computation Graphs

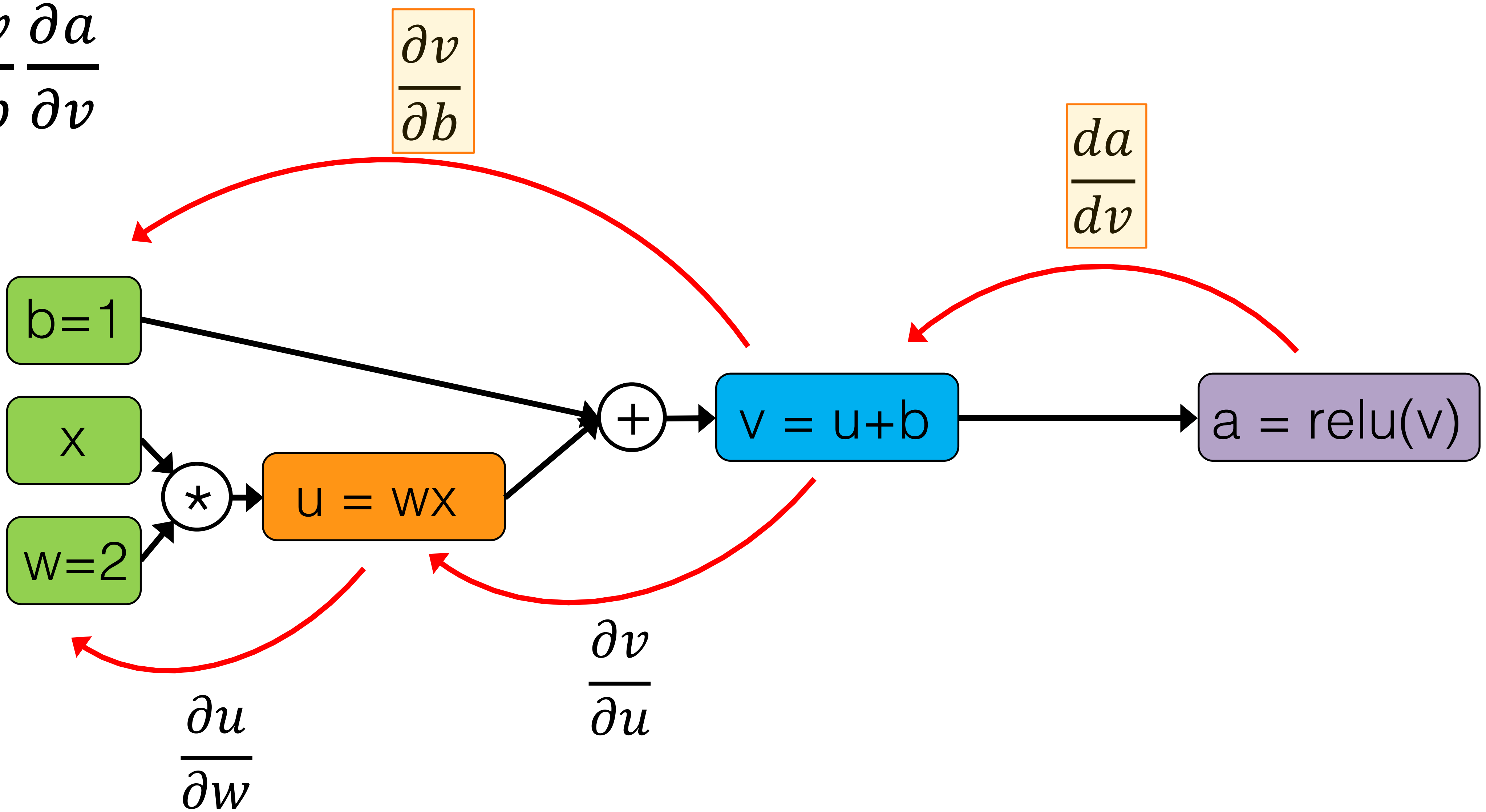


Computation Graphs



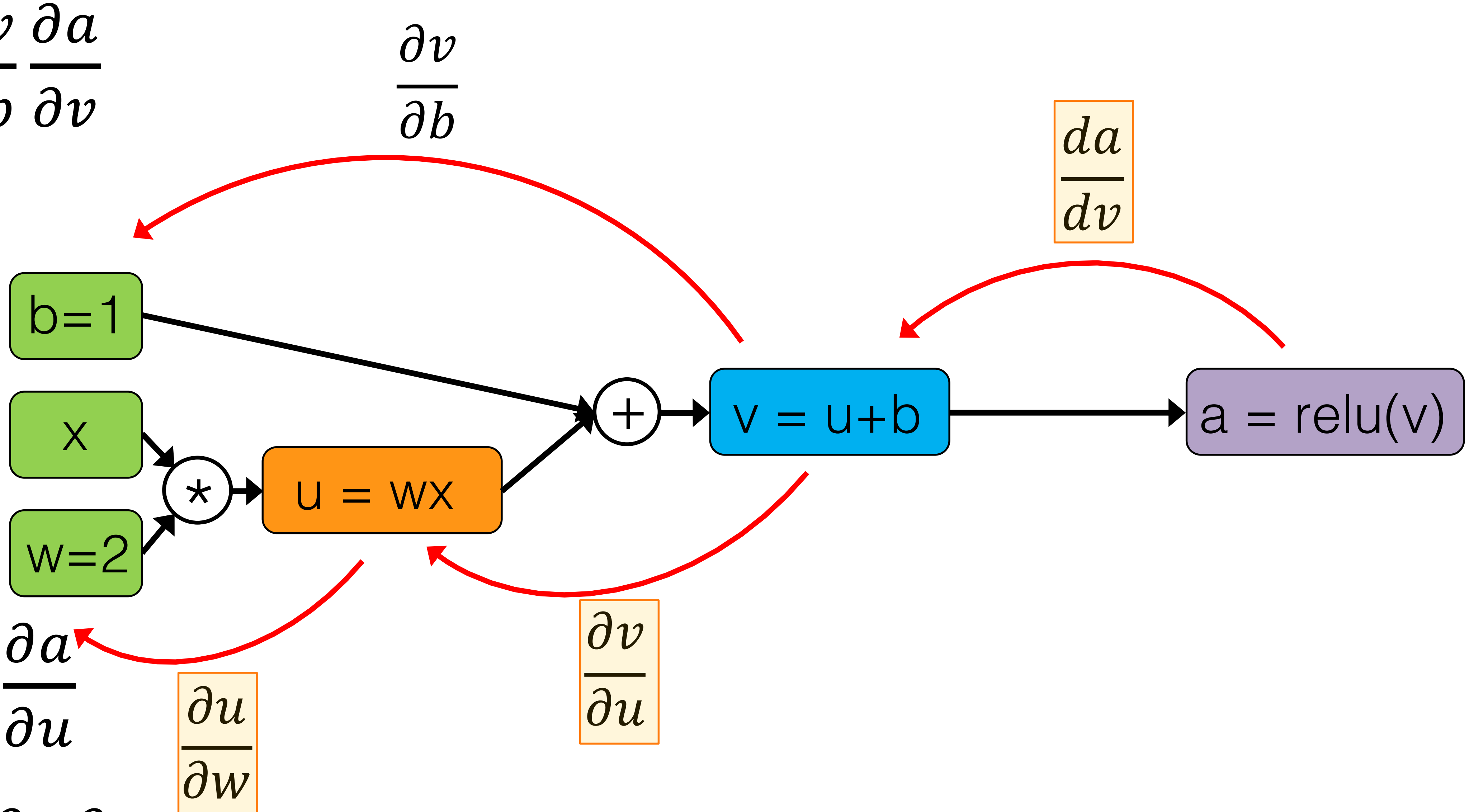
Computation Graphs

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



Computation Graphs

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

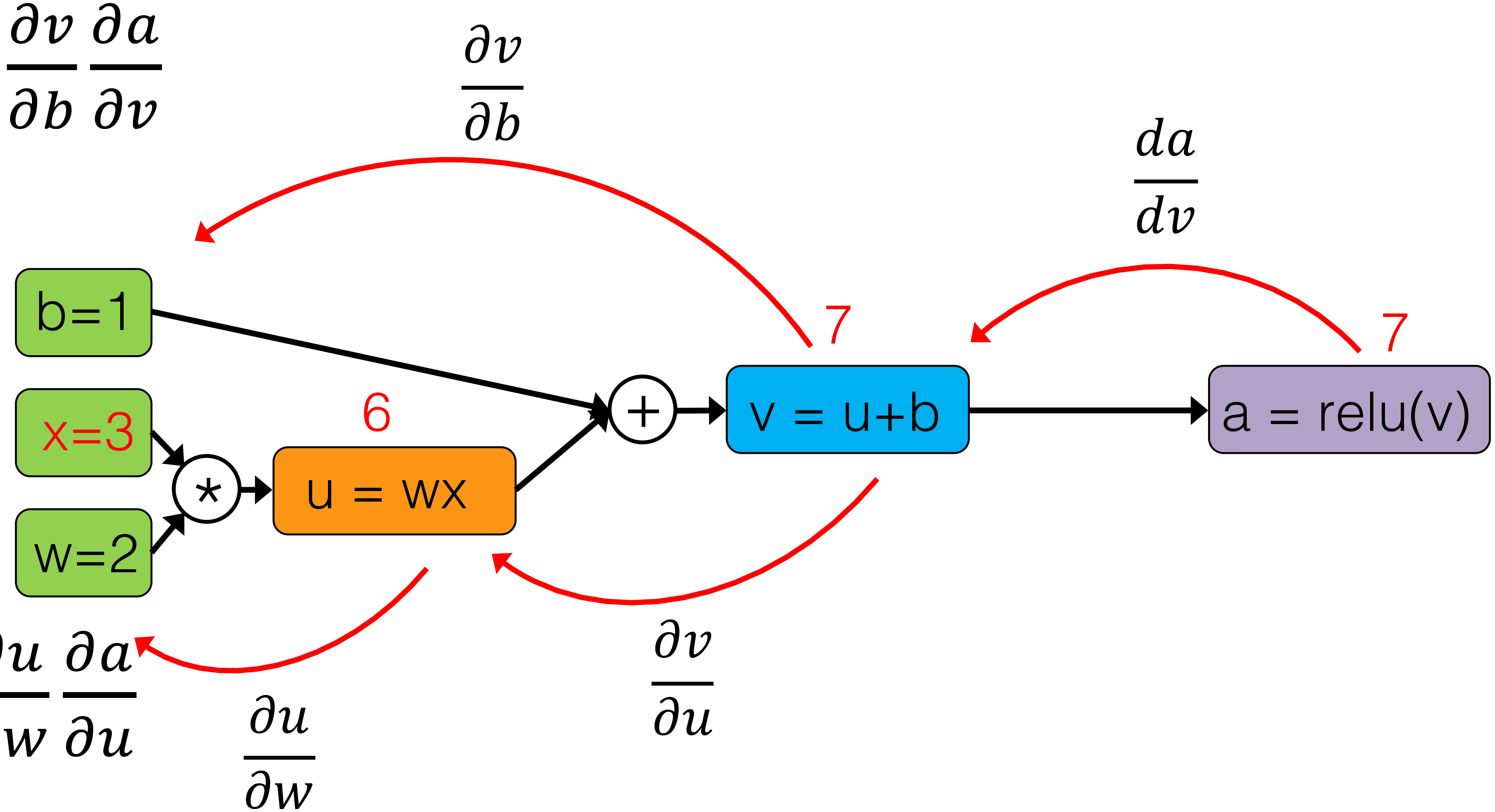


$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

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

Computation Graphs

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

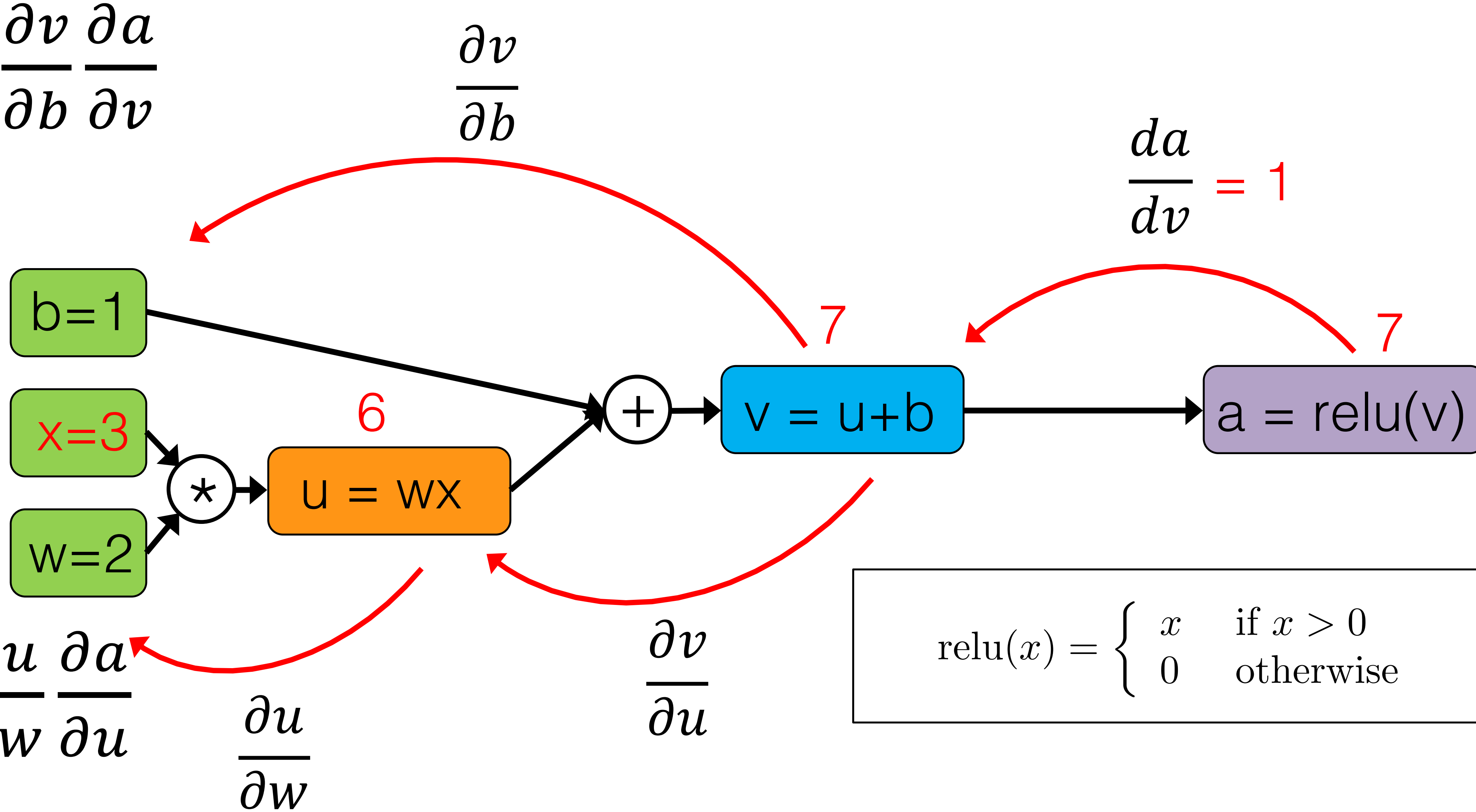


$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

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

Computation Graphs

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



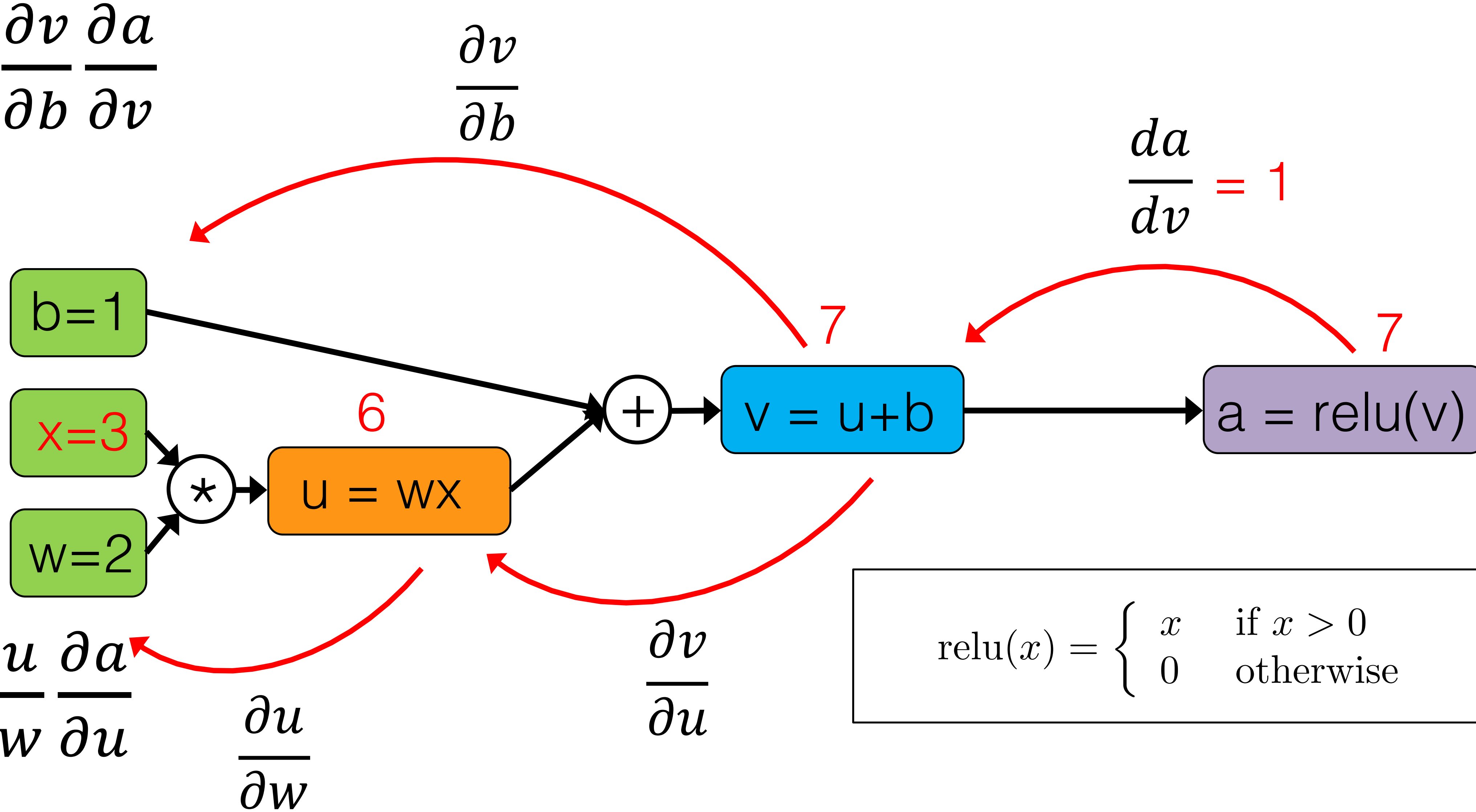
$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

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

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

Computation Graphs

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



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

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

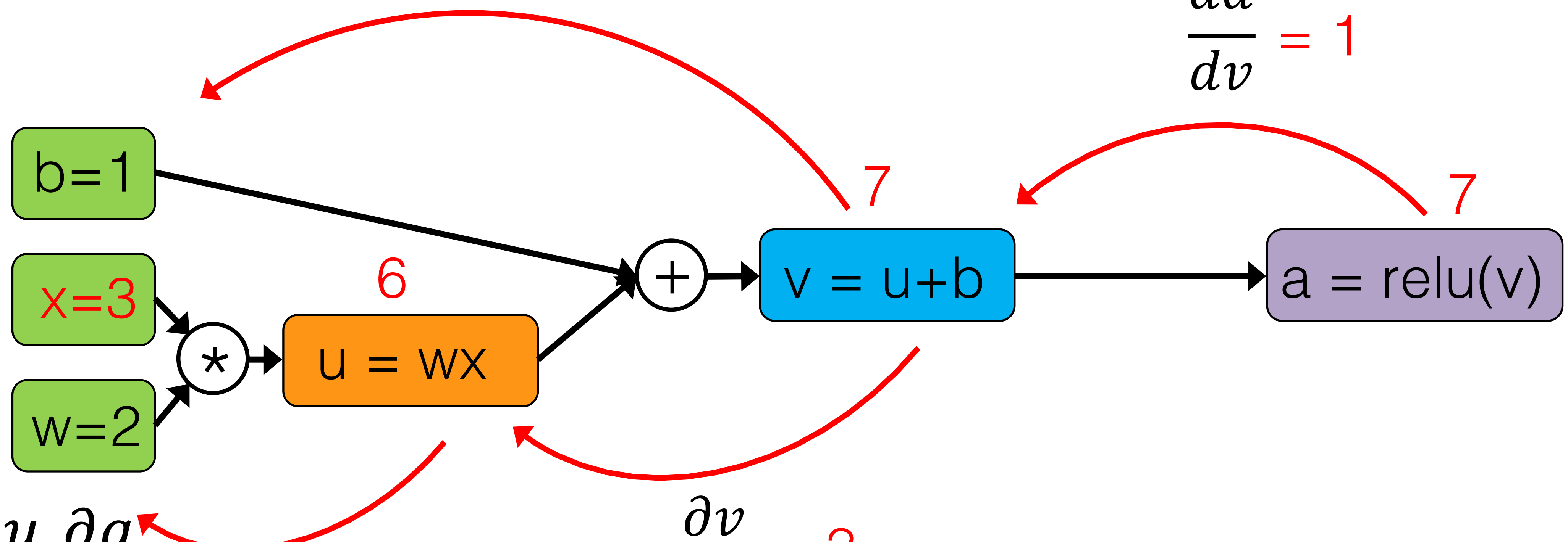
$$= \frac{\partial u}{\partial w}\frac{\partial v}{\partial u}\frac{\partial a}{\partial v}$$

Computation Graphs

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

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

$\frac{da}{dv} = 1$



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

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

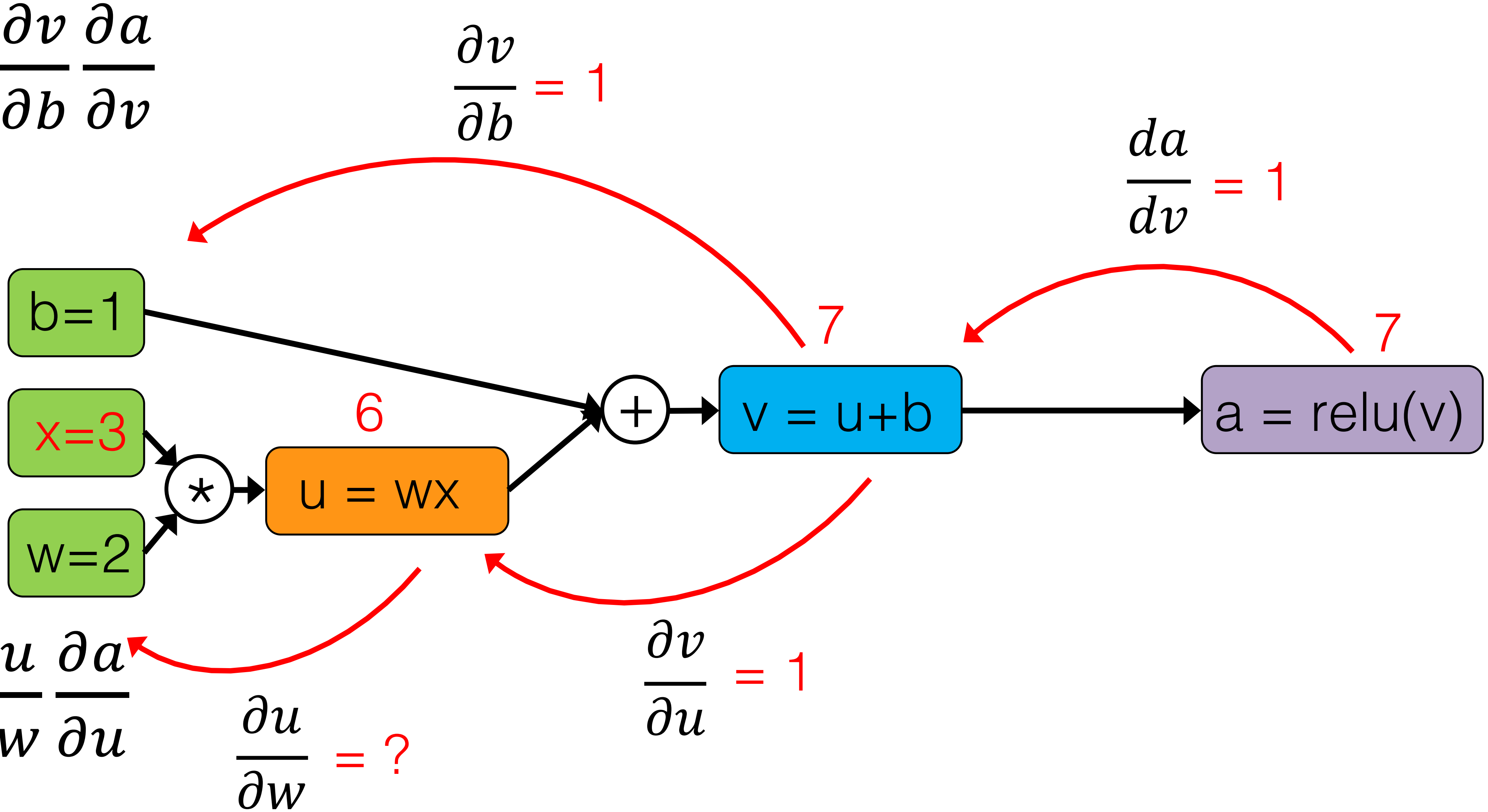
$\frac{\partial u}{\partial w}$

$\frac{\partial v}{\partial u} = ?$

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

Computation Graphs

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



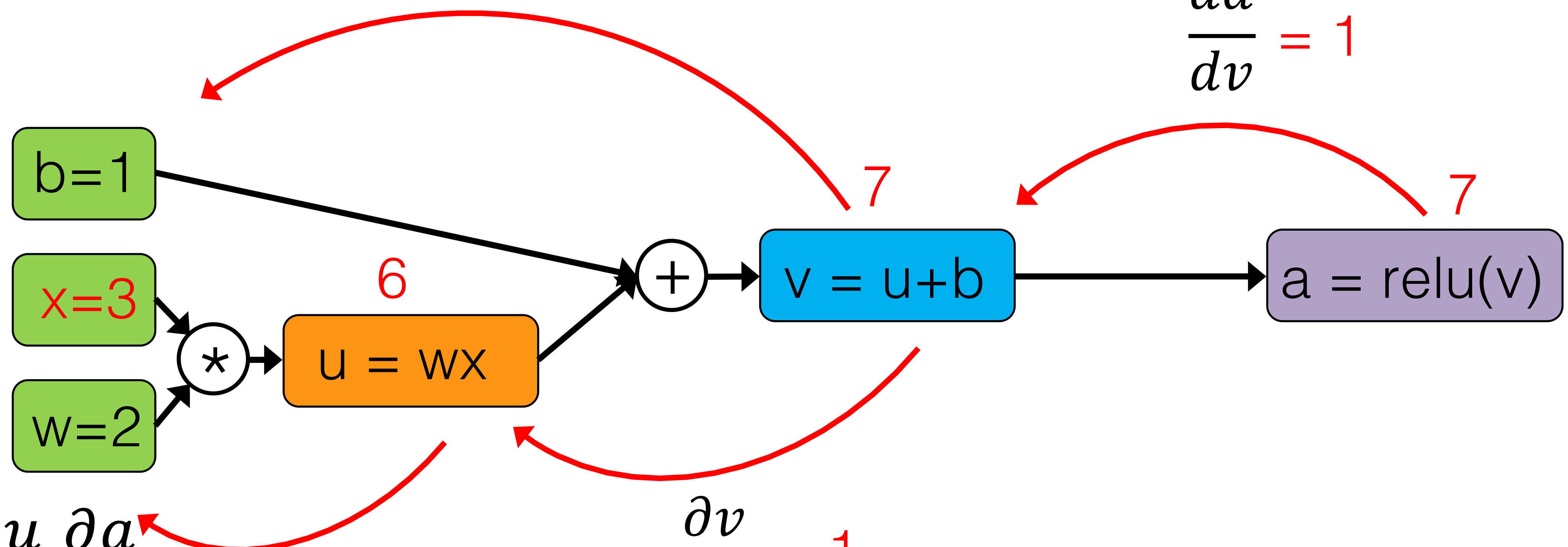
$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

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

Computation Graphs

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

$$\frac{\partial v}{\partial b} = 1 \qquad \frac{da}{dv} = 1$$



$$\frac{\partial v}{\partial u} = 1$$

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

$$\frac{\partial u}{\partial w} = 3$$

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

PyTorch Autograd Example

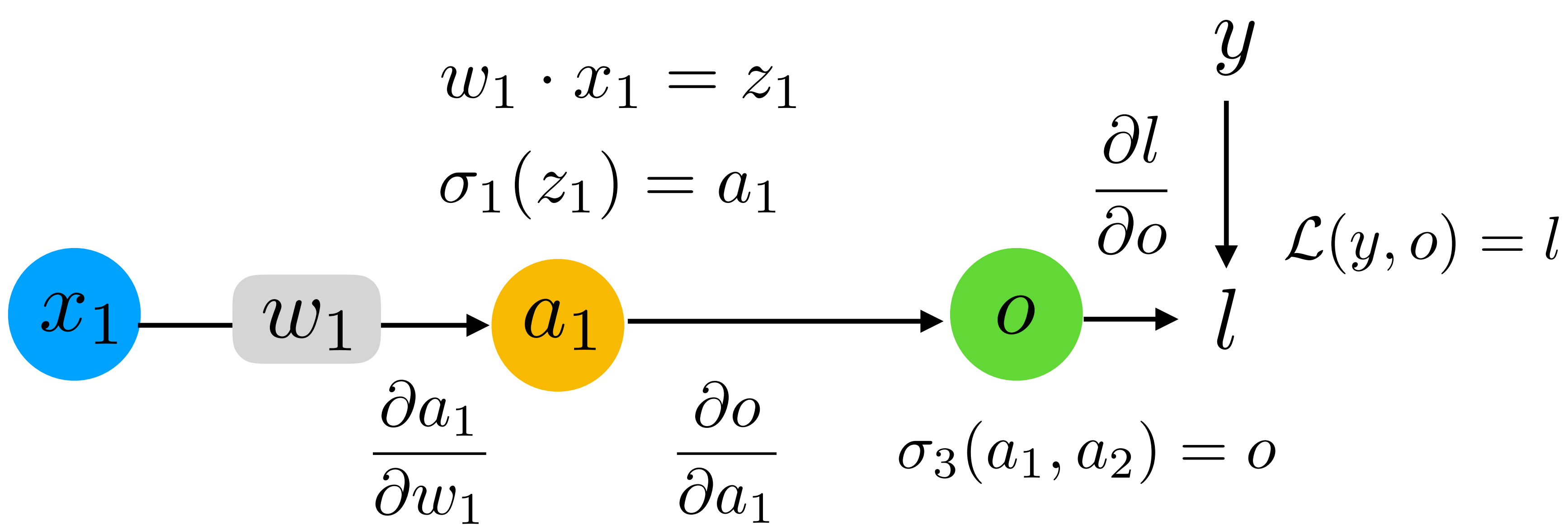
https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L06_pytorch/code/pytorch-autograd.ipynb

Gradients of intermediate variables (usually not required in practice outside research)

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L06_pytorch/code/grad-intermediate-var.ipynb

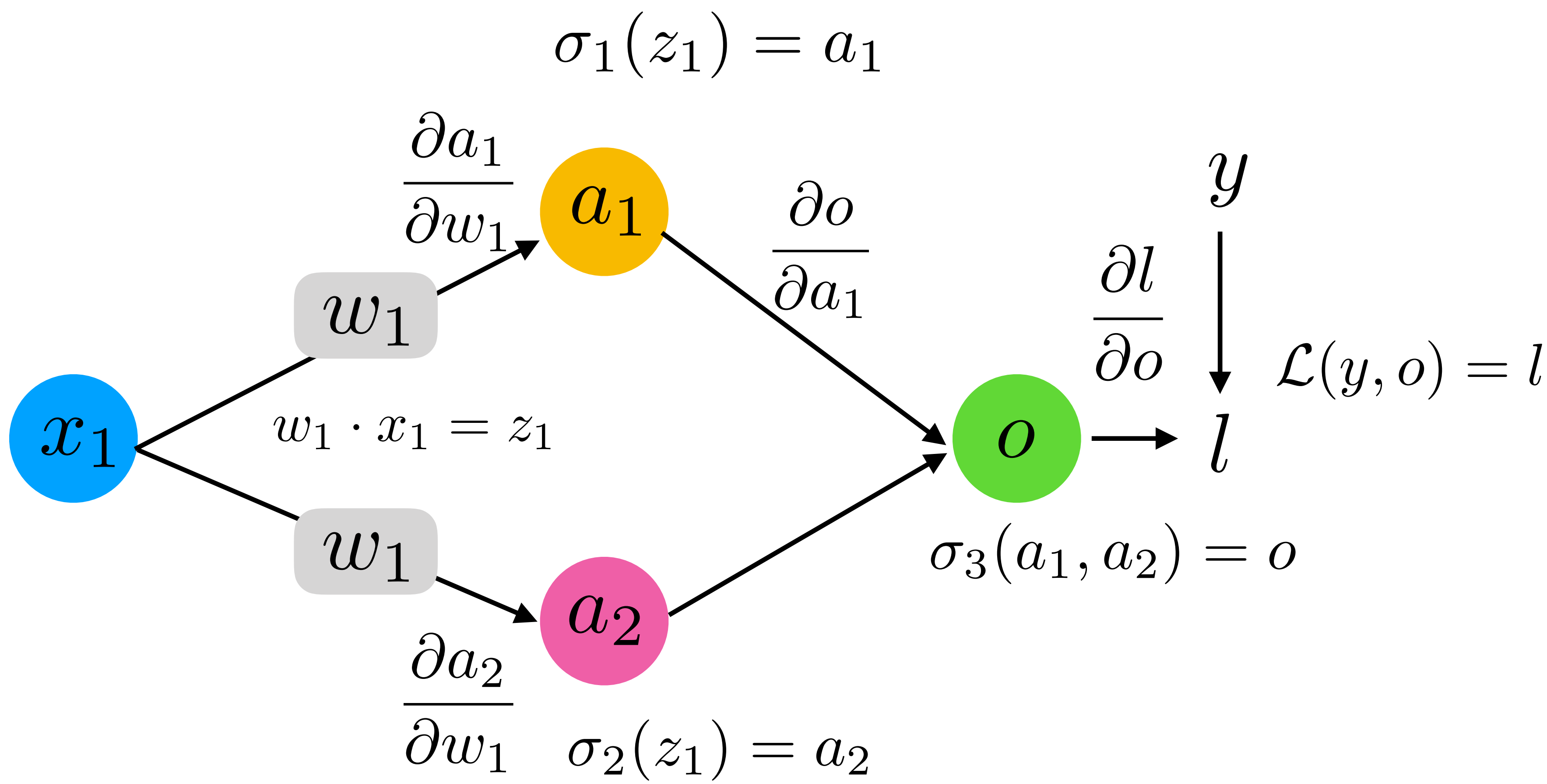
Some More Computation Graphs

Graph with Single Path



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

Graph with Weight Sharing

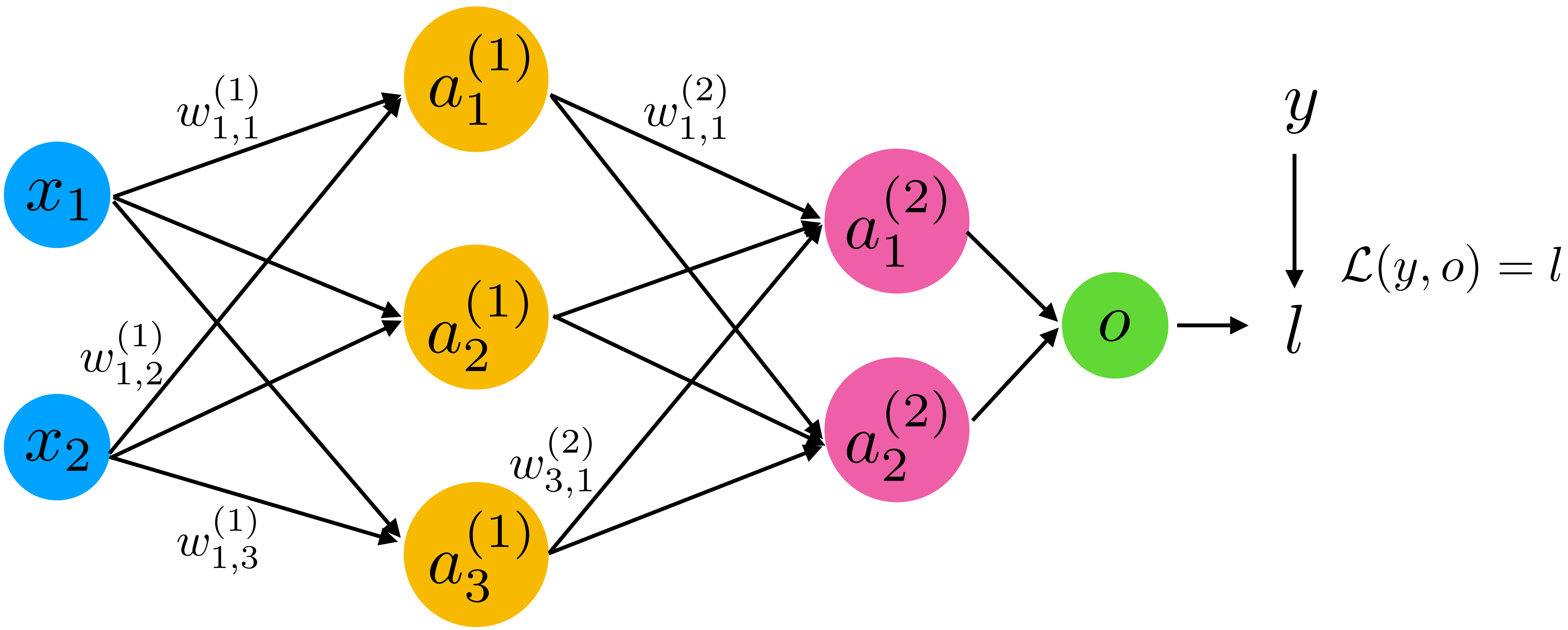


Upper path

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

Lower path

Graph with Fully-Connected Layers (later in this course)



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

PyTorch Usage: Step 1 (Definition)

```
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        ### 1st hidden layer
        self.linear_1 = torch.nn.Linear(num_feat, num_h1)

        ### 2nd hidden layer
        self.linear_2 = torch.nn.Linear(num_h1, num_h2)

        ### Output layer
        self.linear_out = torch.nn.Linear(num_h2, num_classes)

    def forward(self, x):
        out = self.linear_1(x)
        out = F.relu(out)
        out = self.linear_2(out)
        out = F.relu(out)
        logits = self.linear_out(out)
        probas = F.log_softmax(logits, dim=1)
        return logits, probas
```

Backward will be inferred automatically if we use the nn.Module class!

Define model parameters that will be instantiated when created an object of this class

Define how and it what order the model parameters should be used in the forward pass

PyTorch Usage: Step 2 (Creation)

```
torch.manual_seed(random_seed)
model = MultilayerPerceptron(num_features=num_features,
                             num_classes=num_classes)

model = model.to(device)

optimizer = torch.optim.SGD(model.parameters(),
                            lr=learning_rate)
```

Instantiate model
(creates the model parameters)

Define an optimization method

PyTorch Usage: Step 2 (Creation)

```
torch.manual_seed(random_seed)
model = MultilayerPerceptron(num_features=num_features,
                             num_classes=num_classes)

model = model.to(device)

optimizer = torch.optim.SGD(model.parameters(),
                            lr=learning_rate)
```

Optionally move model to GPU, where device e.g. torch.device('cuda:0')

PyTorch Usage: Step 3 (Training)

Run for a specified number of epochs

Iterate over minibatches in epoch

If your model is on the GPU, data should also be on the GPU

```
for epoch in range(num_epochs):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):

        features = features.view(-1, 28*28).to(device)
        targets = targets.to(device)

        ### FORWARD AND BACK PROP
        logits, probas = model(features)
        cost = F.cross_entropy(probas, targets)
        optimizer.zero_grad()

        cost.backward()

        ### UPDATE MODEL PARAMETERS
        optimizer.step()

    model.eval()
    with torch.no_grad():
        # compute accuracy
```

PyTorch Usage: Step 3 (Training)

```
for epoch in range(num_epochs):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):

        features = features.view(-1, 28*28).to(device)
        targets = targets.to(device)

        ### FORWARD AND BACK PROP
        logits, probas = model(features)
        loss = F.cross_entropy(logits, targets)
        optimizer.zero_grad()

        loss.backward()

        ### UPDATE MODEL PARAMETERS
        optimizer.step()

    model.eval()
    with torch.no_grad():
        # compute accuracy
```

This will run the `forward()` method

Define a loss function to optimize

Set the gradient to zero
(could be non-zero from a previous forward pass)

Compute the gradients, the backward is automatically constructed by "autograd" based on the forward() method and the loss function

Use the gradients to update the weights according to the optimization method (defined on the previous slide)
E.g., for SGD, $w := w + \text{learning\_rate} \times \text{gradient}$

PyTorch Usage: Step 3 (Training)

```
for epoch in range(num_epochs):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):

        features = features.view(-1, 28*28).to(device)
        targets = targets.to(device)

        ### FORWARD AND BACK PROP
        logits, probas = model(features)
        loss = F.cross_entropy(logits, targets)
        optimizer.zero_grad()

        loss.backward()

        ### UPDATE MODEL PARAMETERS
        optimizer.step()

    model.eval()
    with torch.no_grad():
        # compute accuracy
```

For evaluation, set the model to eval mode (will be relevant later when we use DropOut or BatchNorm)

This prevents the computation graph for backpropagation from automatically being build in the background to save memory

PyTorch Usage: Step 3 (Training)

```
for epoch in range(num_epochs):
    model.train()
    for batch_idx, (features, targets) in enumerate(train_loader):

        features = features.view(-1, 28*28).to(device)
        targets = targets.to(device)

        ### FORWARD AND BACK PROP
        logits, probas = model(features)
        loss = F.cross_entropy(logits, targets)
        optimizer.zero_grad()

        loss.backward()

        ### UPDATE MODEL PARAMETERS
        optimizer.step()

    model.eval()
    with torch.no_grad():
        # compute accuracy
```

logits because of computational efficiency.
Basically, it internally uses a log_softmax(logits) function that is more stable than log(softmax(logits)).
More on logits ("net inputs" of the last layer) in the next lecture. Please also see
https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/other/pytorch-lossfunc-cheatsheet.md

PyTorch ADALINE (neuron model) Example

https://github.com/rasbt/stat479-deep-learning-ss19/blob/master/L06_pytorch/code/adaline-with-autograd.ipynb

Objected-Oriented vs Functional* API

*Note that with "functional" I mean "functional programming" (one paradigm in CS)

```python
import torch.nn.functional as F

class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        ### 1st hidden layer
        self.linear_1 = torch.nn.Linear(num_features,
                                        num_hidden_1)

        ### 2nd hidden layer
        self.linear_2 = torch.nn.Linear(num_hidden_1,
                                        num_hidden_2)

        ### Output layer
        self.linear_out = torch.nn.Linear(num_hidden_2,
                                          num_classes)

    def forward(self, x):
        out = self.linear_1(x)
        out = F.relu(out)
        out = self.linear_2(out)
        out = F.relu(out)
        logits = self.linear_out(out)
        probas = F.log_softmax(logits, dim=1)
        return logits, probas
```

Unnecessary because these functions don't need to store a state but maybe helpful for keeping track of order of ops (when implementing "forward")

```python
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        ### 1st hidden layer
        self.linear_1 = torch.nn.Linear(num_features,
                                        num_hidden_1)

        self.relu1 = torch.nn.ReLU()

        ### 2nd hidden layer
        self.linear_2 = torch.nn.Linear(num_hidden_1,
                                        num_hidden_2)

        self.relu2 = torch.nn.ReLU()

        ### Output layer
        self.linear_out = torch.nn.Linear(num_hidden_2,
                                          num_classes)

        self.softmax = torch.nn.Softmax()

    def forward(self, x):
        out = self.linear_1(x)
        out = self.relu1(out)
        out = self.linear_2(out)
        out = self.relu2(out)
        logits = self.linear_out(out)
        probas = self.softmax(logits, dim=1)
        return logits, probas
```

Objected-Oriented vs Functional API

Using "Sequential"

```python
import torch.nn.functional as F


class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        ### 1st hidden layer
        self.linear_1 = torch.nn.Linear(num_features,
                                        num_hidden_1)

        ### 2nd hidden layer
        self.linear_2 = torch.nn.Linear(num_hidden_1,
                                        num_hidden_2)

        ### Output layer
        self.linear_out = torch.nn.Linear(num_hidden_2,
                                          num_classes)

    def forward(self, x):
        out = self.linear_1(x)
        out = F.relu(out)
        out = self.linear_2(out)
        out = F.relu(out)
        logits = self.linear_out(out)
        probas = F.log_softmax(logits, dim=1)
        return logits, probas
```

```python
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        self.my_network = torch.nn.Sequential(
            torch.nn.Linear(num_features, num_hidden_1),
            torch.nn.ReLU(),
            torch.nn.Linear(num_hidden_1, num_hidden_2),
            torch.nn.ReLU(),
            torch.nn.Linear(num_hidden_2, num_classes)
        )

    def forward(self, x):
        logits = self.my_network(x)
        probas = F.softmax(logits, dim=1)
        return logits, probas
```

Much more compact and clear, but "forward" may be harder to debug if there are errors (we cannot simply add breakpoints or insert "print" statements

Objected-Oriented vs Functional API

Using "Sequential"

1)

```
class MultilayerPerceptron(torch.nn.Module):

    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()

        self.my_network = torch.nn.Sequential(
            torch.nn.Linear(num_features, num_hidden
            torch.nn.ReLU(),
            torch.nn.Linear(num_hidden_1, num_hidden
            torch.nn.ReLU(),
            torch.nn.Linear(num_hidden_2, num_classe
        )

    def forward(self, x):
        logits = self.my_network(x)
        probas = F.softmax(logits, dim=1)
        return logits, probas
```

Much more compact and clear, but "forward" may be harder to debug if there are errors (we cannot simply add breakpoints or insert "print" statements

2) However, if you use Sequential, you can define "hooks" to get intermediate outputs. For example:

```
[7]: model.net

[7]: Sequential(
       (0): Linear(in_features=784, out_features=128, bias=True)
       (1): ReLU(inplace)
       (2): Linear(in_features=128, out_features=256, bias=True)
       (3): ReLU(inplace)
       (4): Linear(in_features=256, out_features=10, bias=True)
     )
```

If we want to get the output from the 2nd layer during the forward pass, we can register a hook as follows:

```
[8]: outputs = []
     def hook(module, input, output):
         outputs.append(output)

     model.net[2].register_forward_hook(hook)

[8]: <torch.utils.hooks.RemovableHandle at 0x7f659c6685c0>
```

Now, if we call the model on some inputs, it will save the intermediate results in the "outputs" list:

```
[9]: _ = model(features)

     print(outputs)

     [tensor([[0.5341, 1.0513, 2.3542,  ..., 0.0000, 0.0000, 0.0000],
             [0.0000, 0.6676, 0.6620,  ..., 0.0000, 0.0000, 2.4056],
             [1.1520, 0.0000, 0.0000,  ..., 2.5860, 0.8992, 0.9642],
             ...,
             [0.0000, 0.1076, 0.0000,  ..., 1.8367, 0.0000, 2.5203],
             [0.5415, 0.0000, 0.0000,  ..., 2.7968, 0.8244, 1.6335],
             [1.0710, 0.9805, 3.0103,  ..., 0.0000, 0.0000, 0.0000]],
            device='cuda:3', grad_fn=<ThresholdBackward1>)]
```

More PyTorch features will be introduced step-by-step later in this course when we start working with more complex networks, including

- Running code on the GPU
- Using efficient data loaders
- Splitting networks across different GPUs

Reading Assignments

- What is PyTorch
  https://pytorch.org/tutorials/beginner/blitz/tensor_tutorial.html#sphx-glr-beginner-blitz-tensor-tutorial-py

- Autograd: Automatic Differentiation
  https://pytorch.org/tutorials/beginner/blitz/autograd_tutorial.html#sphx-glr-beginner-blitz-autograd-tutorial-py