

Lecture 06

Automatic Differentiation with PyTorch

STAT 453: Deep Learning, Spring 2020

Sebastian Raschka

<http://stat.wisc.edu/~sraschka/teaching/stat453-ss2020/>

Today

Computing partial derivatives more easily
(and automatically) with PyTorch

Overview

1/4 -- PyTorch Resources

2/4 -- Computation Graphs

3/4 -- Automatic Differentiation in PyTorch

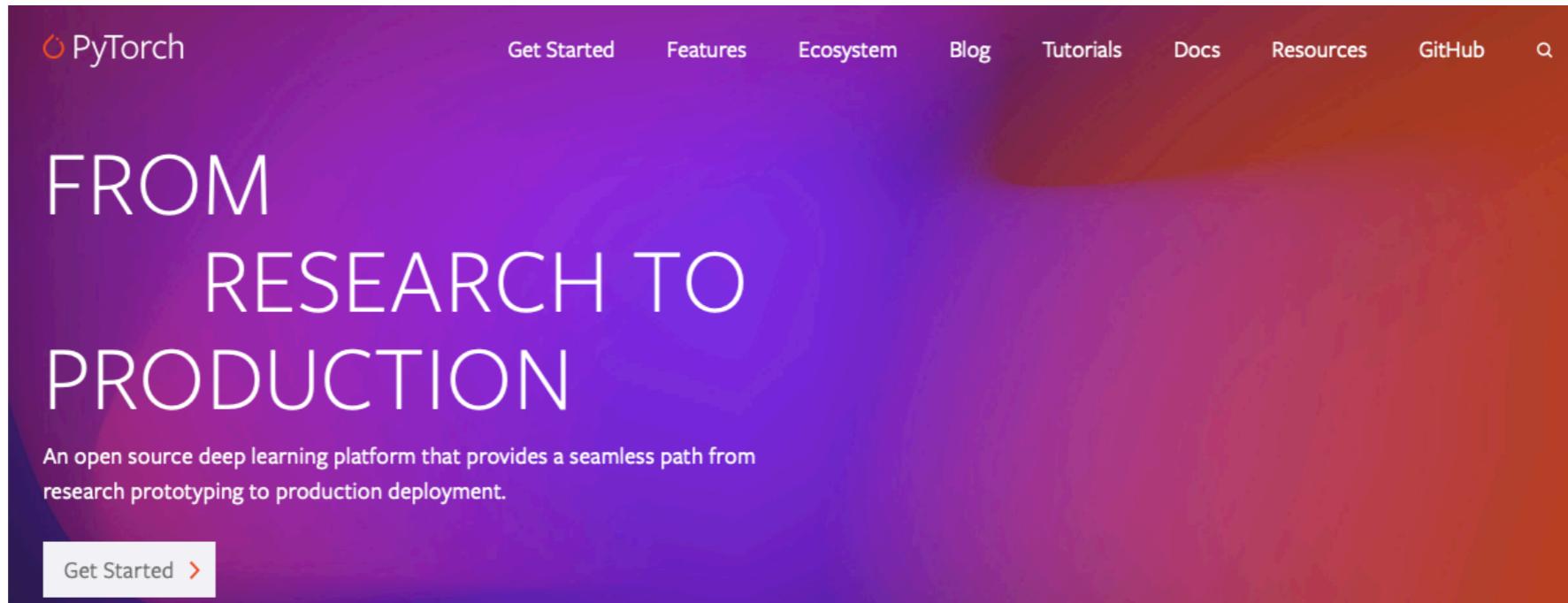
4/4 -- PyTorch API

1/4 -- PyTorch Resources

2/4 -- Computation Graphs

3/4 -- Automatic Differentiation in PyTorch

4/4 -- PyTorch API



The screenshot shows the PyTorch homepage with a purple-to-orange gradient background. At the top, there's a navigation bar with links: Get Started, Features, Ecosystem, Blog, Tutorials, Docs, Resources, GitHub, and a search icon. Below the navigation, the text "FROM RESEARCH TO PRODUCTION" is displayed in large, white, sans-serif capital letters. Underneath this, a subtitle reads: "An open source deep learning platform that provides a seamless path from research prototyping to production deployment." At the bottom left, there's a "Get Started >" button.

<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/stat453-deep-learning-ss20/tree/master/extras/installing-pytorch>

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

```
[In [1]: import torch  
[In [2]: torch.__version__  
Out[2]: '1.4.0'
```

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

PyTorch

Get Started Ecosystem Mobile Blog Tutorials Docs **Resources** GitHub 

RESOURCES

Explore educational courses, get your questions answered, and join the discussion with other PyTorch developers.

 **Docs**
Access comprehensive developer documentation.

 **Tutorials**
Get in-depth tutorials for beginners and advanced developers.

 **GitHub**
Report bugs, request features, discuss issues, and more.

 **PyTorchDiscuss**
Browse and join discussions on deep learning with PyTorch.

 **Slack**
Discuss advanced topics. Request access: <https://bit.ly/ptslack>

 **Examples**
View example projects for vision, text, RL, and more.

 **中文文档**
Docs and tutorials in Chinese, translated by the community.

 **fast.ai**
Get up and running on PyTorch quickly with free learning courses.

 **MobileDemo**
Check out the PyTorch Mobile demo app for iOS and Android.

<https://pytorch.org/resources>

Sebastian Raschka

STAT 453: Intro to Deep Learning and Generative Models

SS 2020

7

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

The screenshot shows the PyTorch website's navigation bar with links for Get Started, Ecosystem, Mobile, Blog, Tutorials (which is highlighted in red), Docs, Resources, and Github. Below the navigation bar, a breadcrumb trail indicates the current page: Tutorials > Deep Learning with PyTorch: A 60 Minute Blitz > What is PyTorch?. On the left sidebar, there are sections for Getting Started (with a link to Deep Learning with PyTorch: A 60 Minute Blitz), Writing Custom Datasets, DataLoaders and Transforms, Visualizing Models, Data, and Training with TensorBoard, and an Image section. The main content area displays the title "WHAT IS PYTORCH?" and a description stating it's a Python-based scientific computing package targeted at two sets of audiences. It lists two bullet points: "A replacement for NumPy to use the power of GPUs" and "a deep learning research platform that provides maximum flexibility and speed".

PyTorch

Get Started Ecosystem Mobile Blog **Tutorials** Docs Resources Github

1.4.0

Tutorials > Deep Learning with PyTorch: A 60 Minute Blitz > What is PyTorch?

Search Tutorials

Run in Google Colab Download Notebook View on GitHub

WHAT IS PYTORCH?

It's a Python-based scientific computing package targeted at two sets of audiences:

- A replacement for NumPy to use the power of GPUs
- a deep learning research platform that provides maximum flexibility and speed

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

DEEP LEARNING WITH PYTORCH: A 60 MINUTE BLITZ ↗

Author: Soumith Chintala

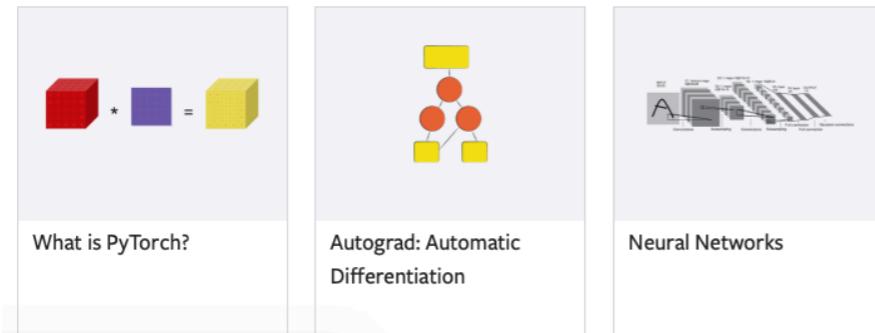
Goal of this tutorial:

- 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.



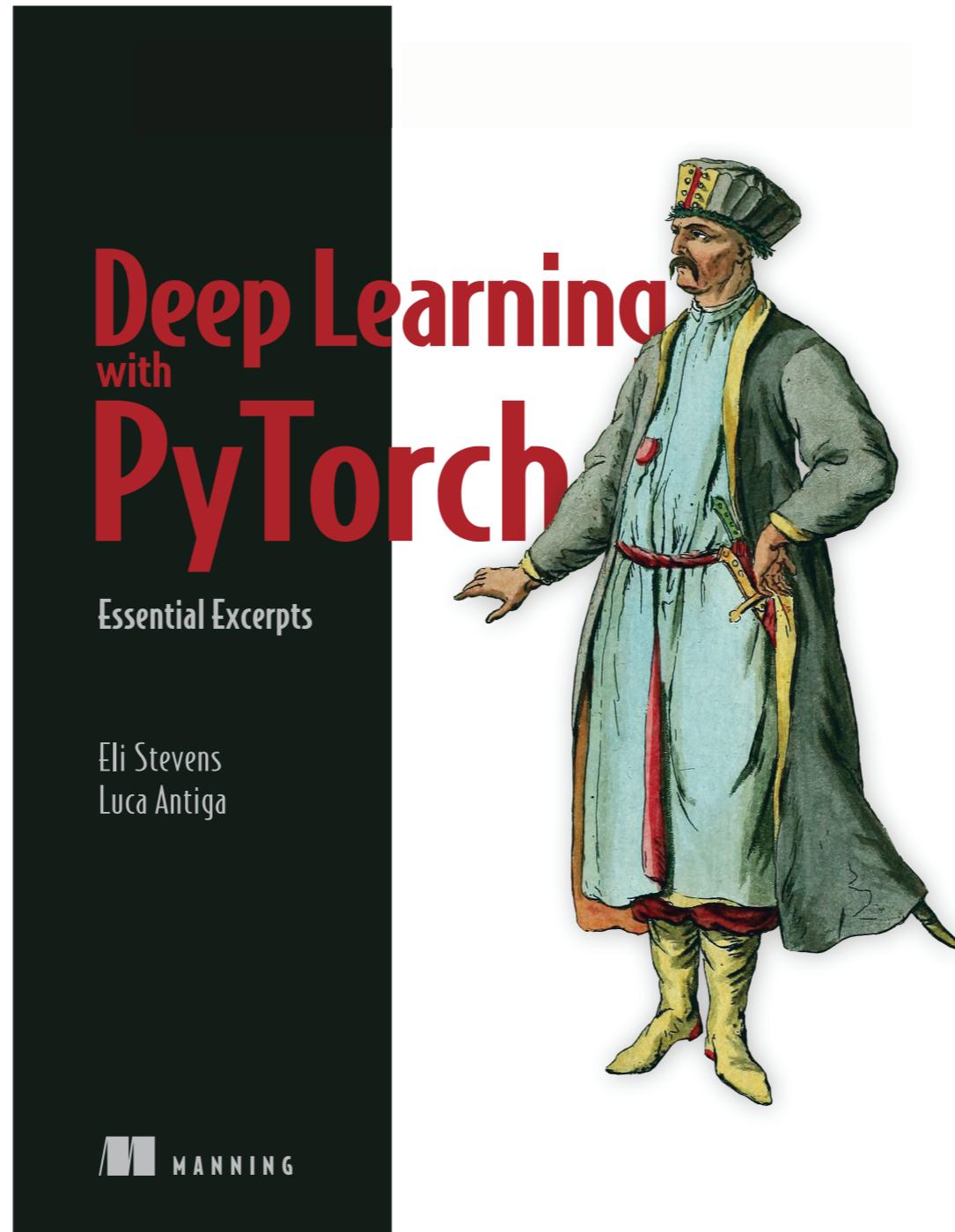
DEEP LEARNING WITH PYTORCH: A 60 MINUTE BLITZ ↗

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 $v = (v_1 \quad v_2 \quad \dots \quad v_m)^T$, compute the product $v^T \cdot J$. If v happens to be the gradient of a scalar function $l = g(y)$, that is, $v = (\frac{\partial l}{\partial y_1} \quad \dots \quad \frac{\partial l}{\partial y_m})^T$, then by the chain rule, the vector-Jacobian product would be the gradient of l with respect to x :

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

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



<https://pytorch.org/assets/deep-learning/Deep-Learning-with-PyTorch.pdf>

Very Active & Friendly Community and Help/Discussion Forum

PyTorch

all categories ▾ Latest New (49) Unread (32) Top Categories + New Topic

Topic	Replies	Views	Activity
PyTorch Feedback • Hello! I'm working on PyTorch and would like your feedback. Please send answers to the questions below to michellenicole@fb.com with 'PyTorch Feedback' in the subject line. Thank-you for your valuable input! 🔥 W... read more	1	143	2d
Going from 0.4.0 to 1.0.0 changes code runtime from 0:00:00.35 to 0:08:45.63 •	5	7	7m
RuntimeError: Expected 4-dimensional input for 4-dimensional weight [6, 3, 5, 5], but got 3-dimensional input of size [3, 256, 256] instead •	5	18	1h
How to change the output size of the model when the batch size is specified? • vision	2	13	1h
Training Reproducibility Problem	5	24	1h
[Caffe2] MobileNetV2 Quantized using caffe2:: BlobIsTensorType(*blob, CPU). Blob is not a CPU Tensor: 325	5	217	1h
Creating a tuple of Tensors as input to a traced model with the C++ front end • C++	0	14	2h
Error when trying to view image with dataloader and iter, PascalVOC 2007 • vision	0	9	2h
Train a small vector , which is not connected to the main Graph - need your creativity •	3	21	2h

<https://pytorch.org/resources>

1/4 -- PyTorch Resources

2/4 -- Computation Graphs

3/4 -- Automatic Differentiation in PyTorch

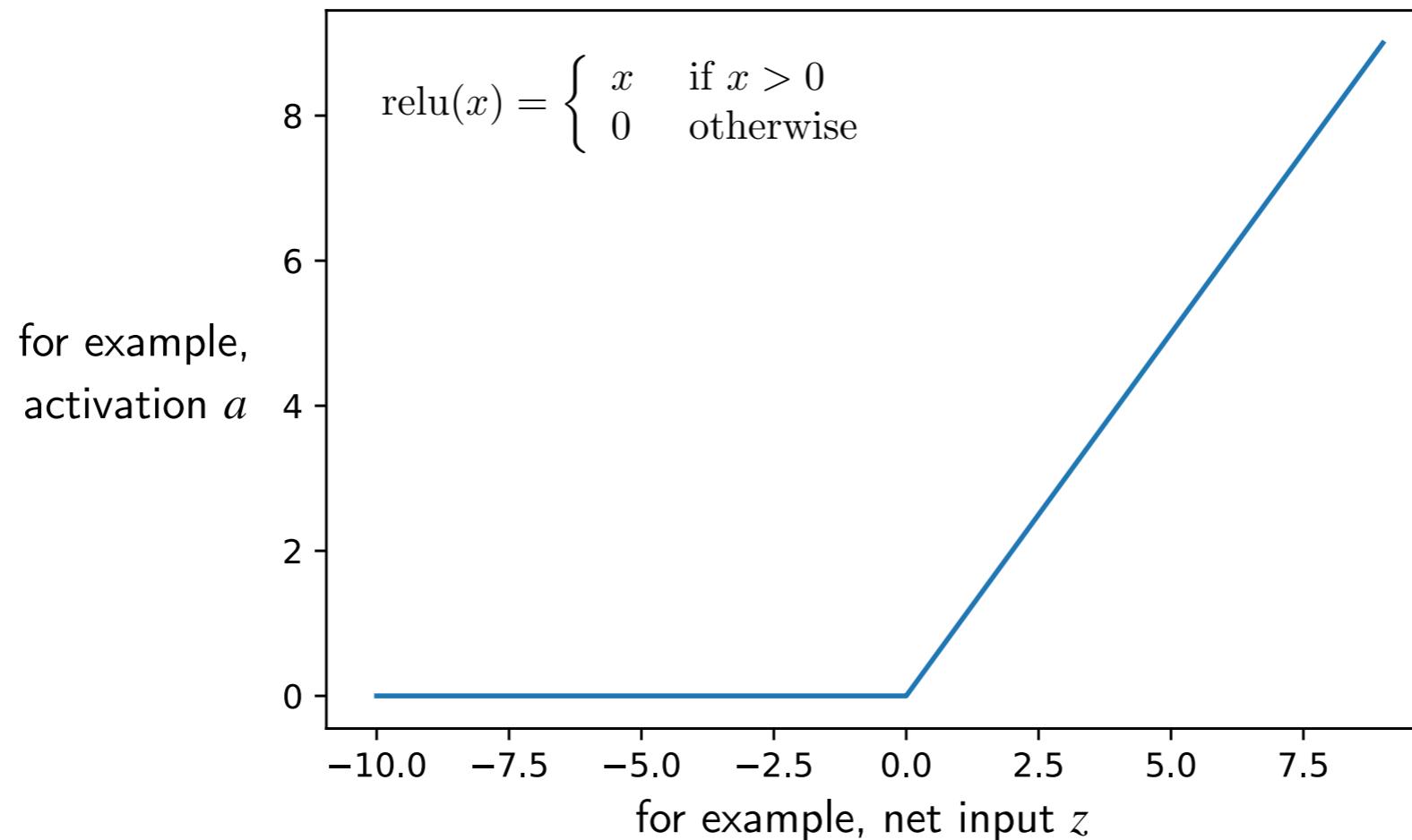
4/4 -- PyTorch API

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:

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



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

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

Why not differentiable?

Derivative does not exist (DNE) at 0, because the derivative is different if we approach the limit from the left or right:

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

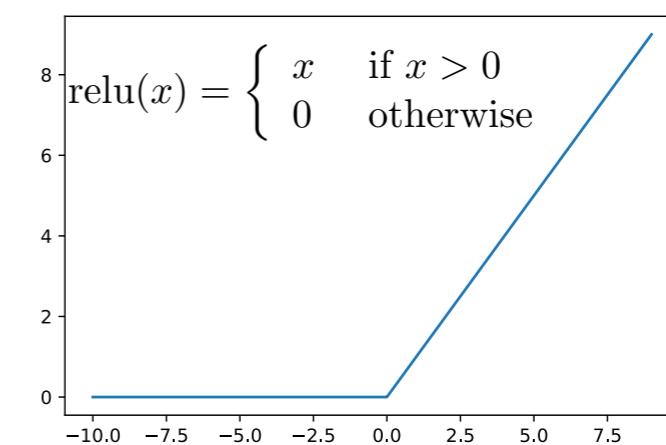
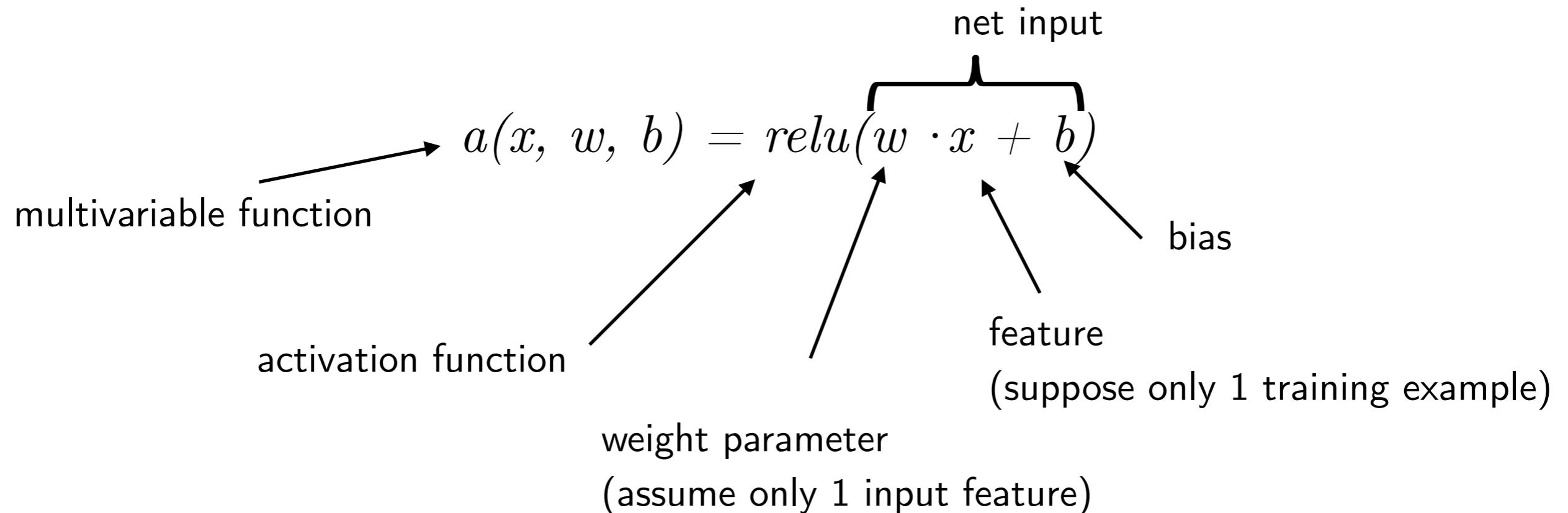
$$f'(x) = \lim_{x \rightarrow 0} \frac{\max(0, x + \Delta x) - \max(0, x)}{\Delta x}$$

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

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

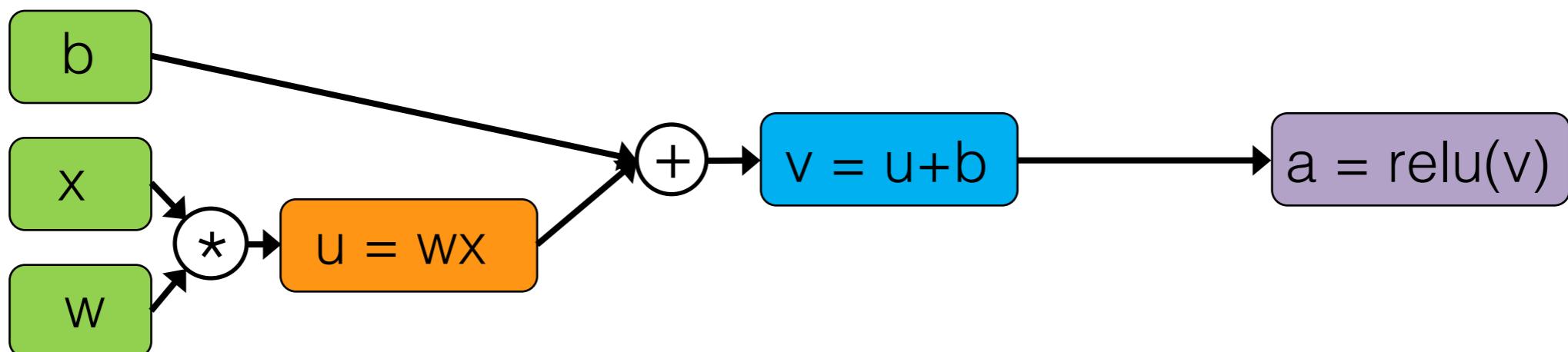
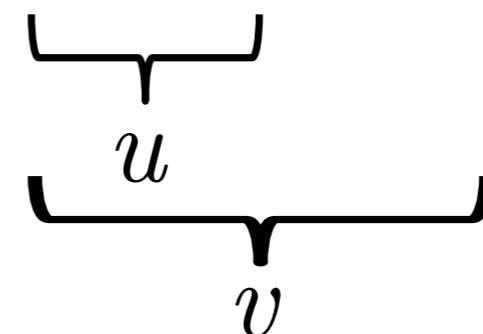
Computation Graphs

Suppose we have the following activation function:



Computation Graphs

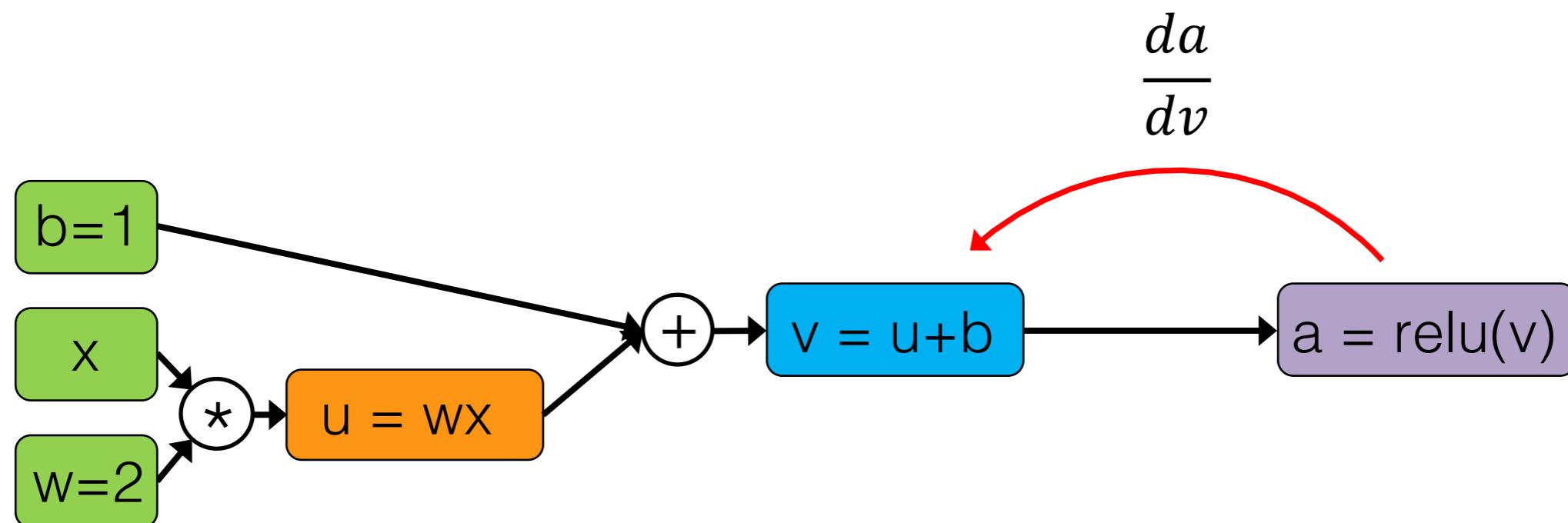
$$a(x, w, b) = \text{relu}(w \cdot x + b)$$



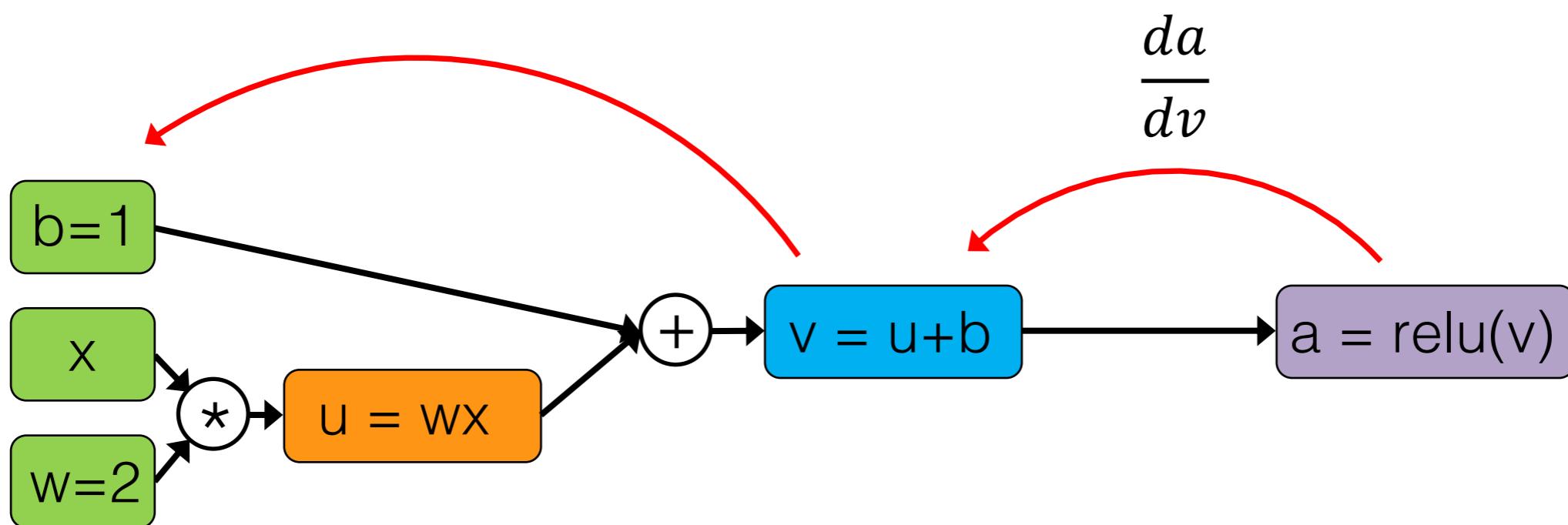
Computation Graphs

Usually, in deep learning (i.e., when we use gradient descent or backprop to optimize a loss function), we are interested in computing the derivative of the loss with respect to the parameters. When we do this, we apply the chain rule, and one component of it is computing the derivative of the activation with respect to the parameters, which we will be doing in the next couple of slides.

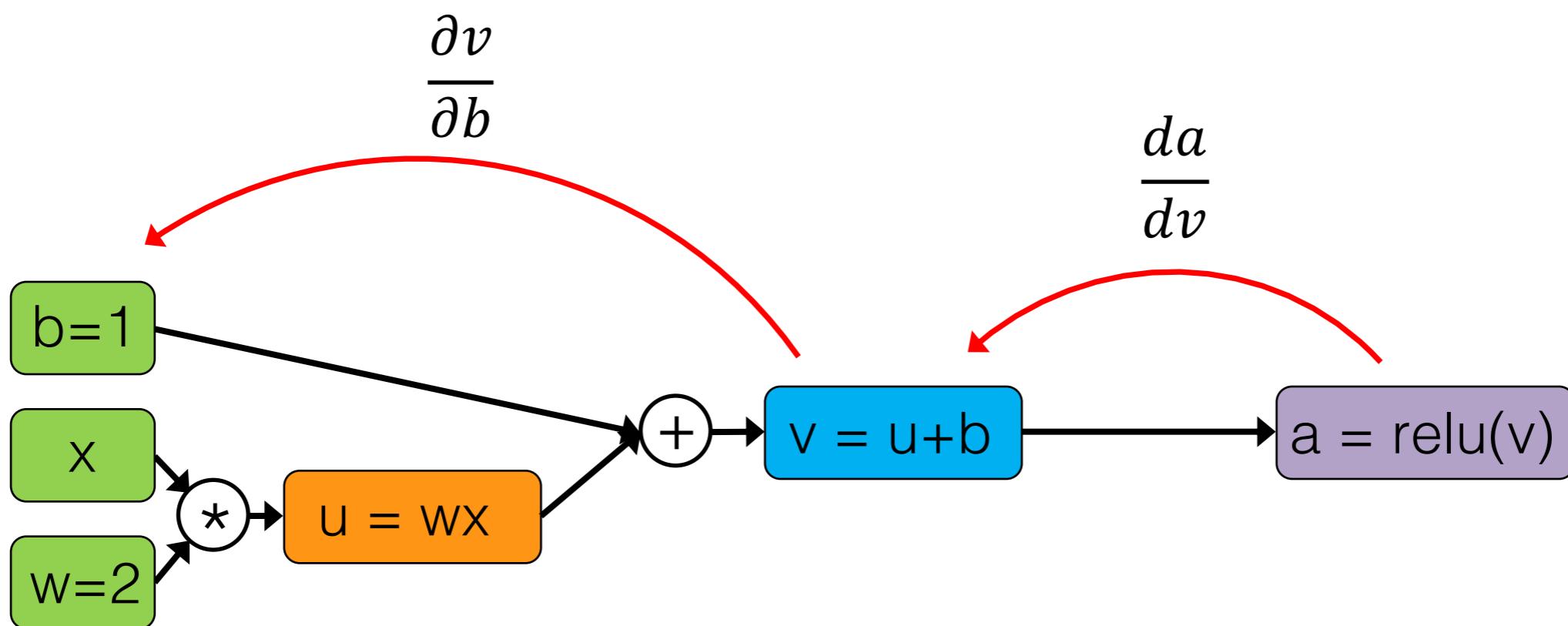
Assuming a "reverse mode" for computing the gradient of the activation with respect to the parameters w and b , we start as follows:



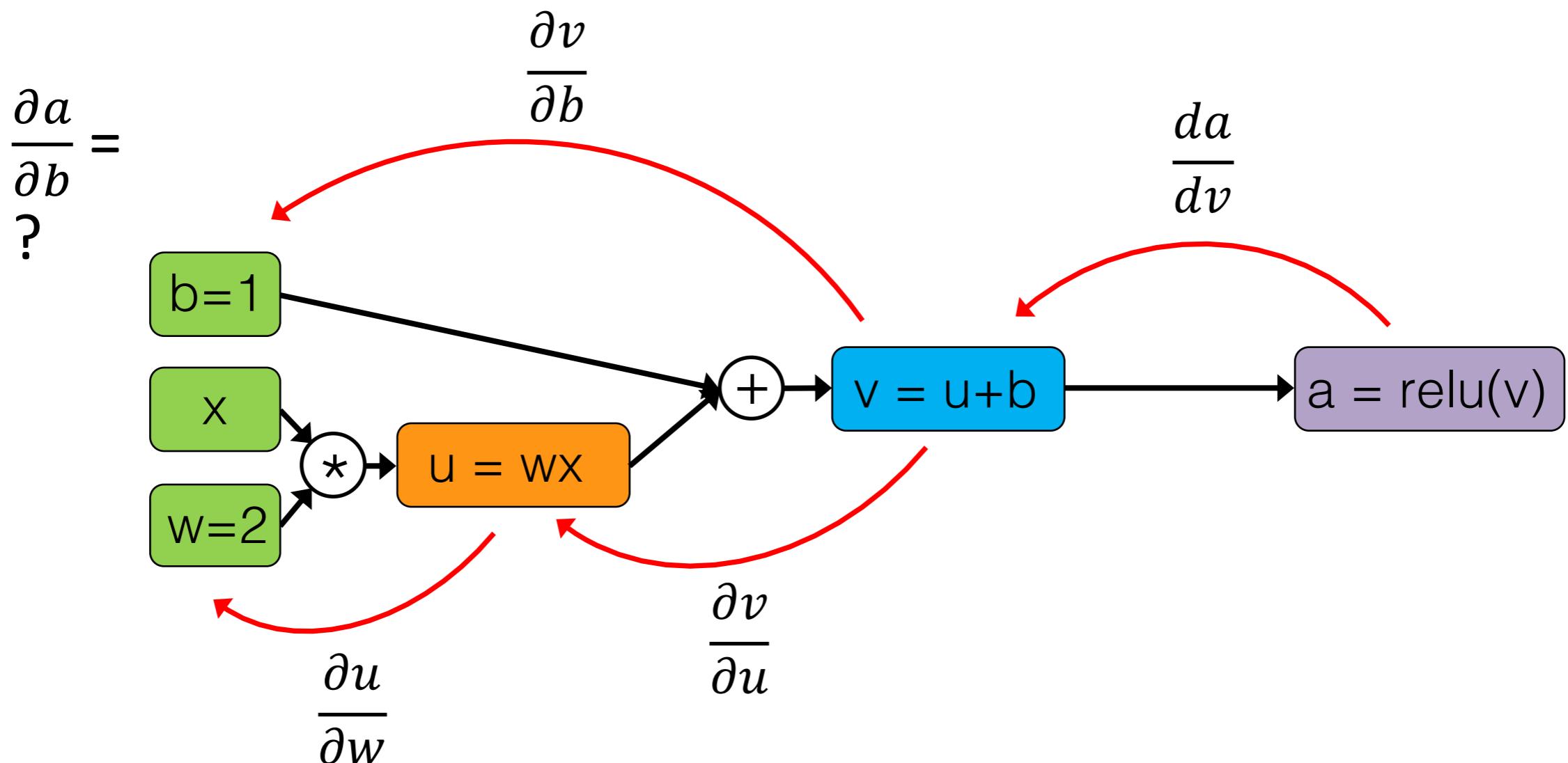
Computation Graphs



Computation Graphs

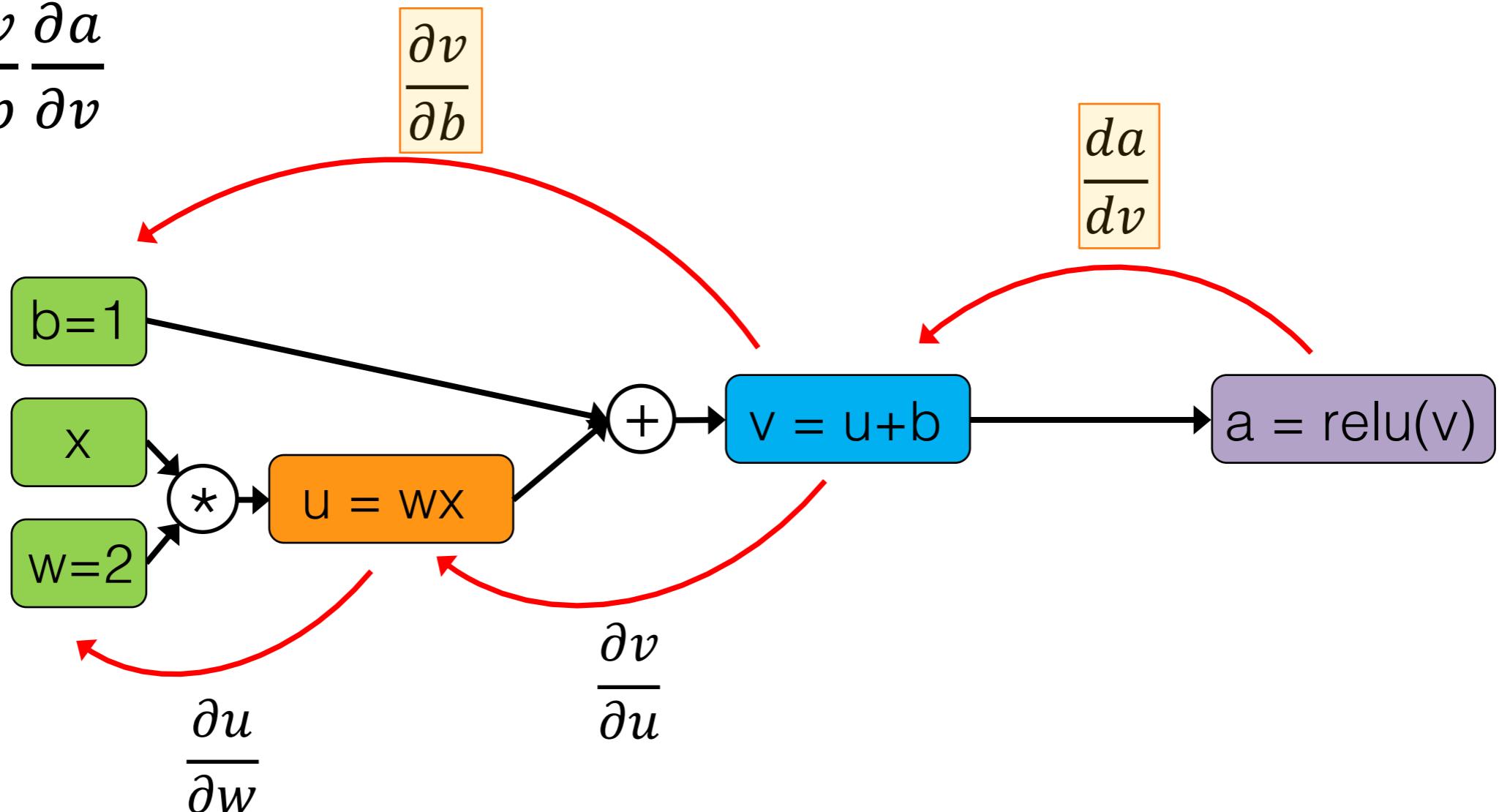


Computation Graphs

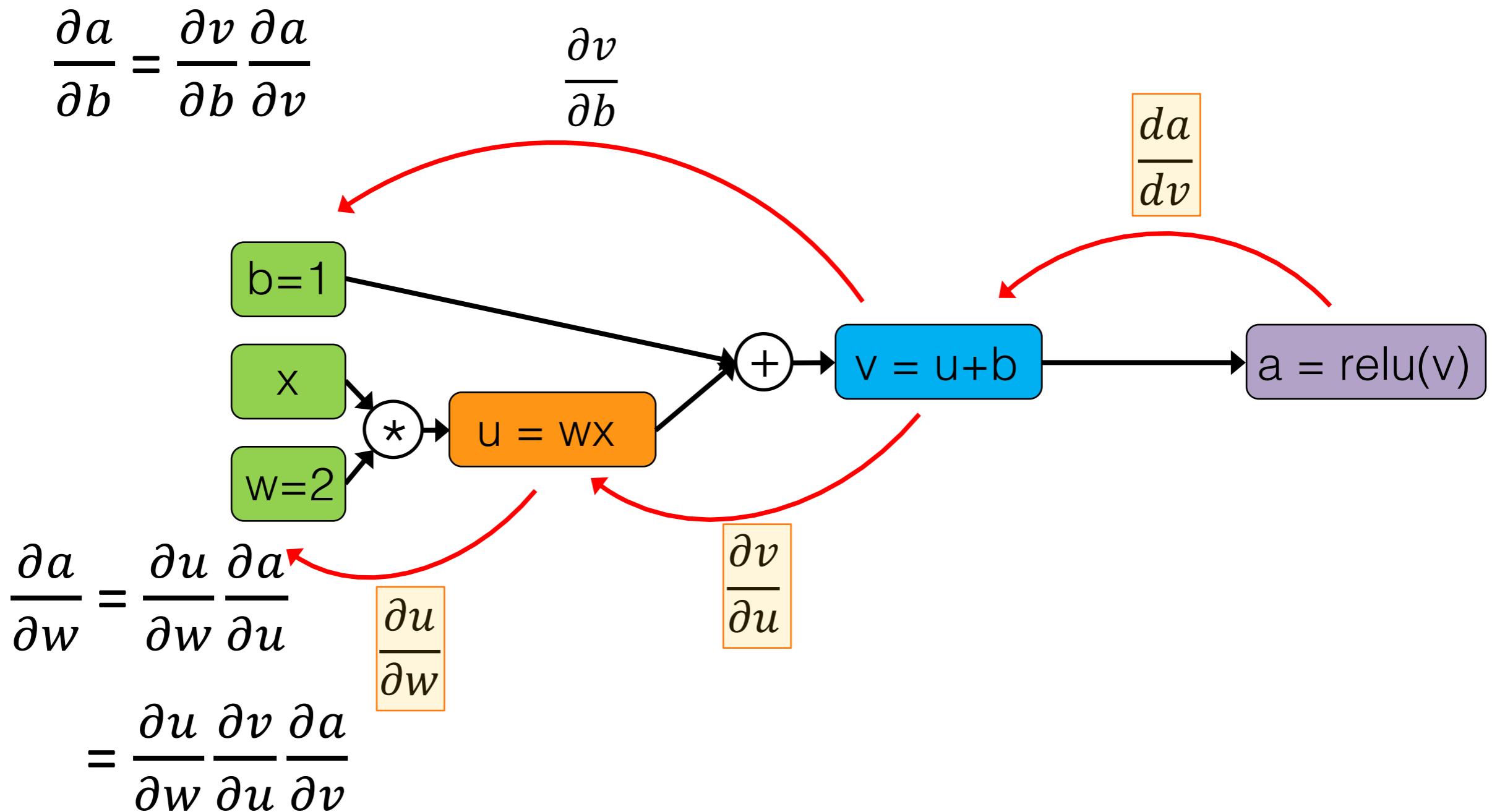


Computation Graphs

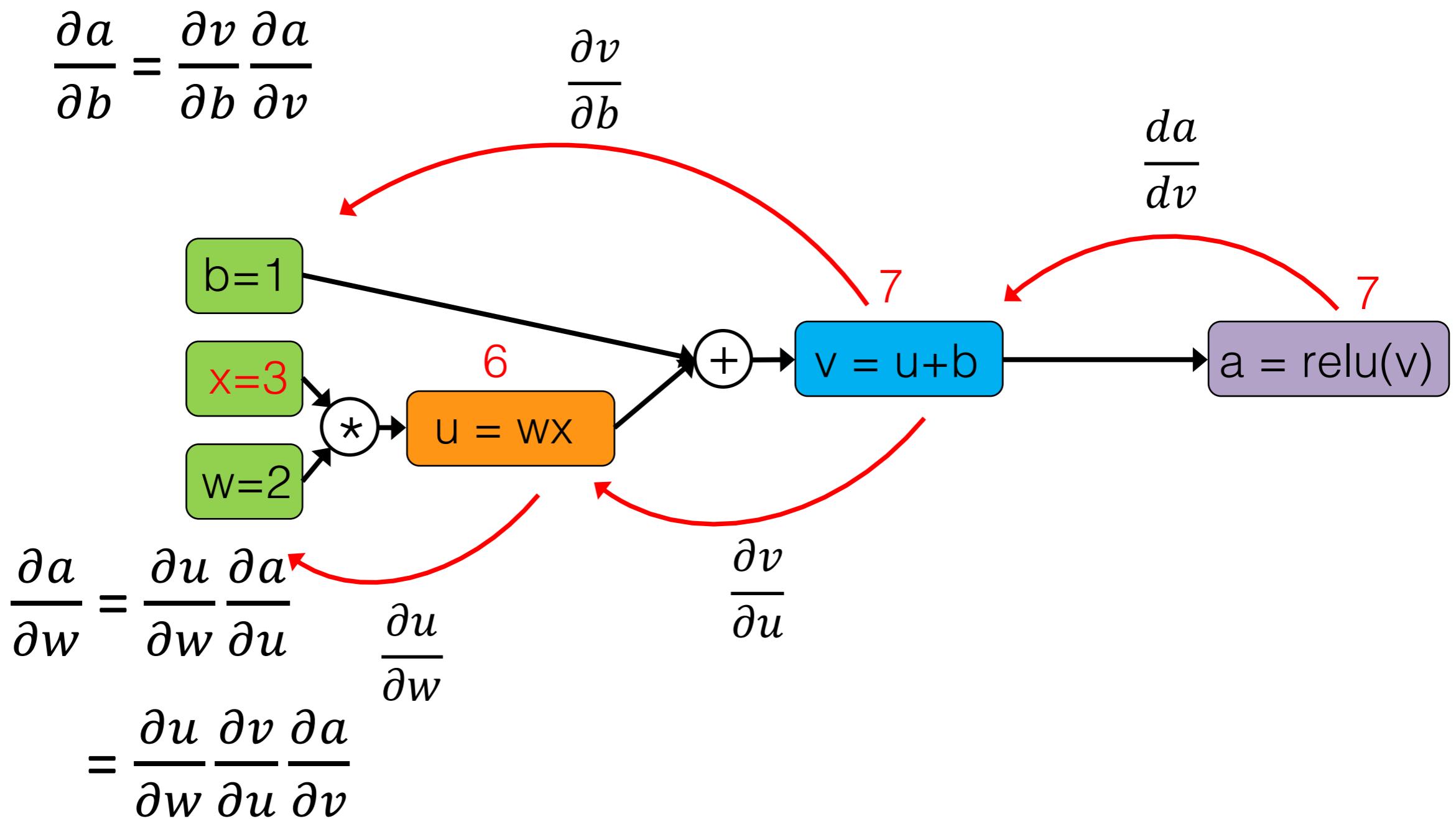
$$\frac{\partial a}{\partial b} = \frac{\partial v}{\partial b} \frac{\partial a}{\partial v}$$



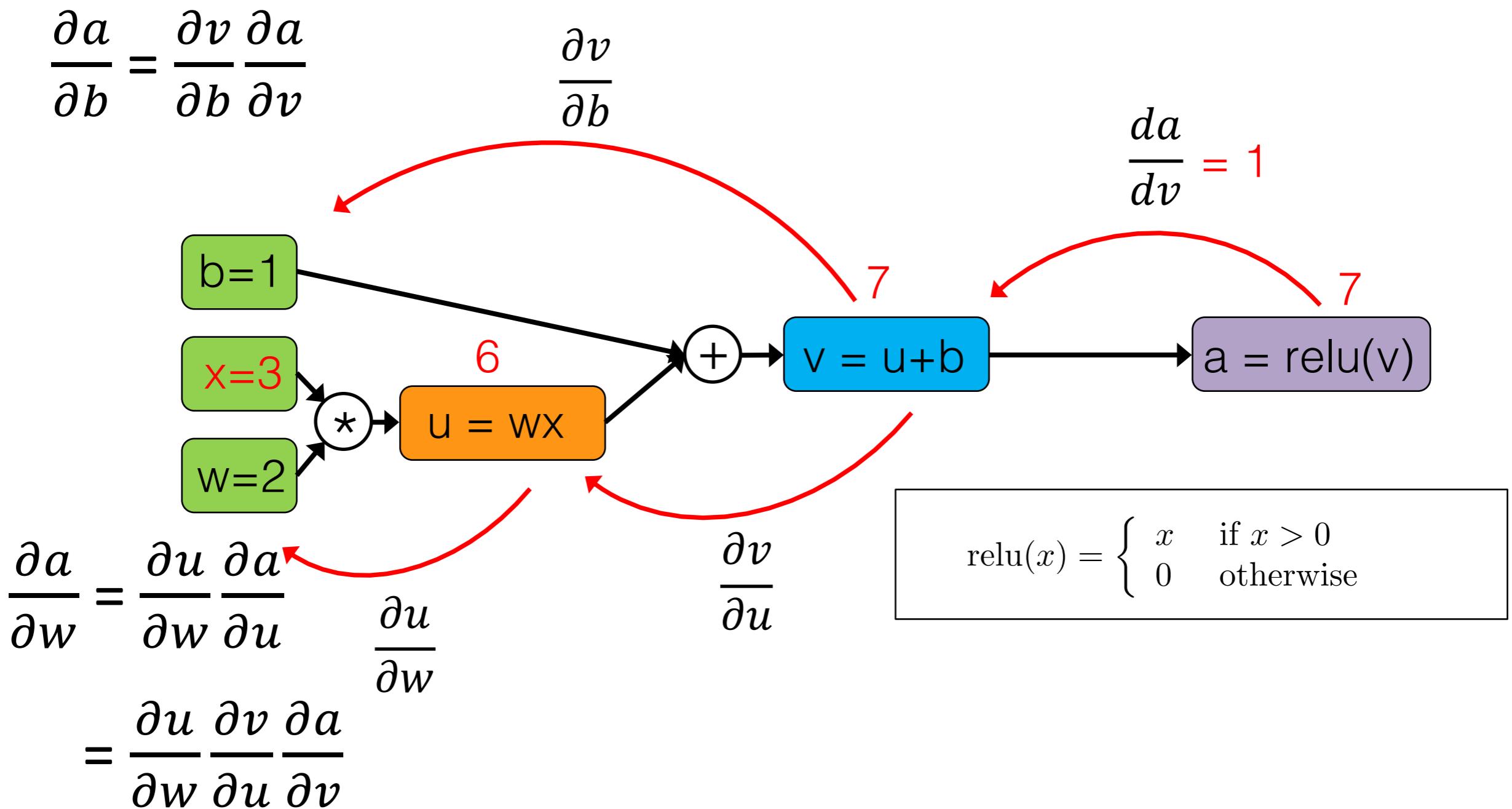
Computation Graphs



Computation Graphs



Computation Graphs

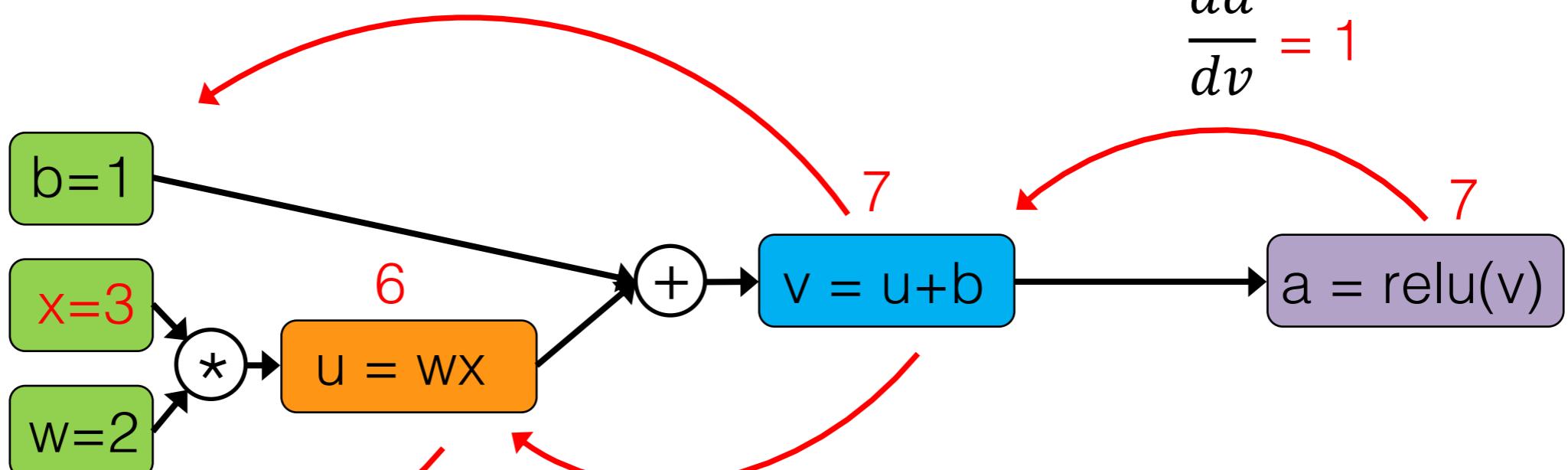


Computation Graphs

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

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

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



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

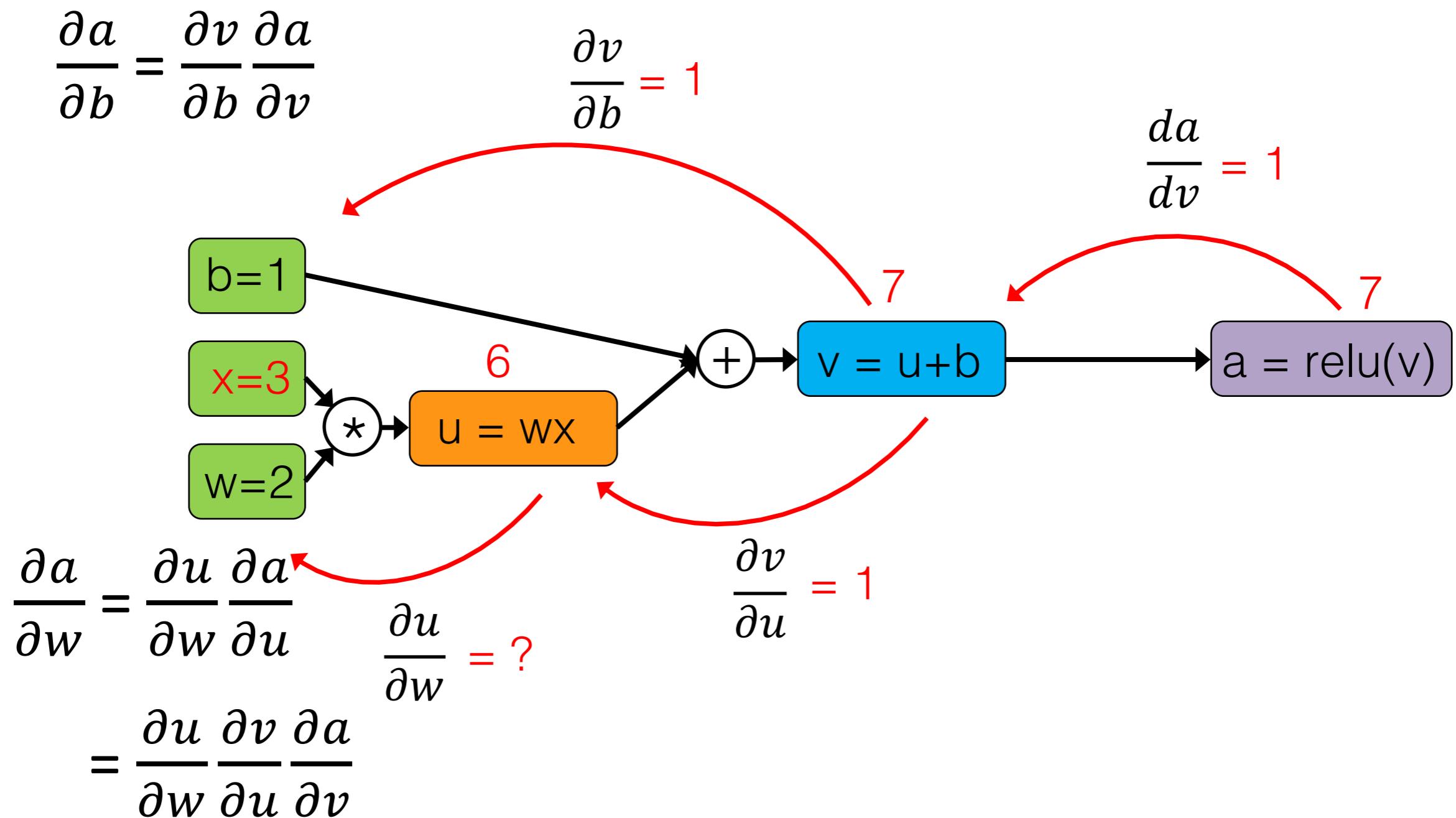
$$\frac{\partial u}{\partial w}$$

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

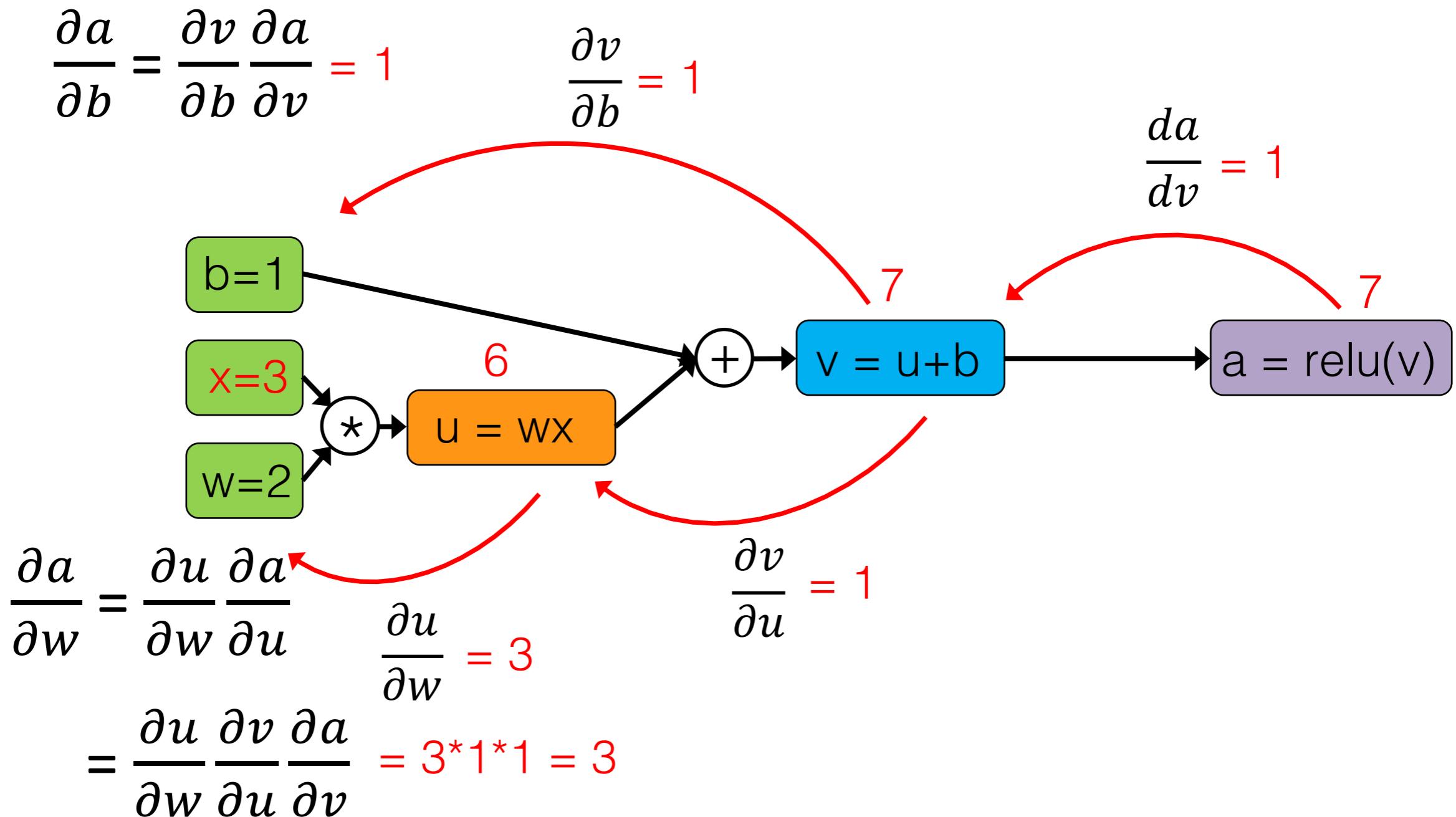
$$\frac{\partial v}{\partial u} = ?$$

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

Computation Graphs

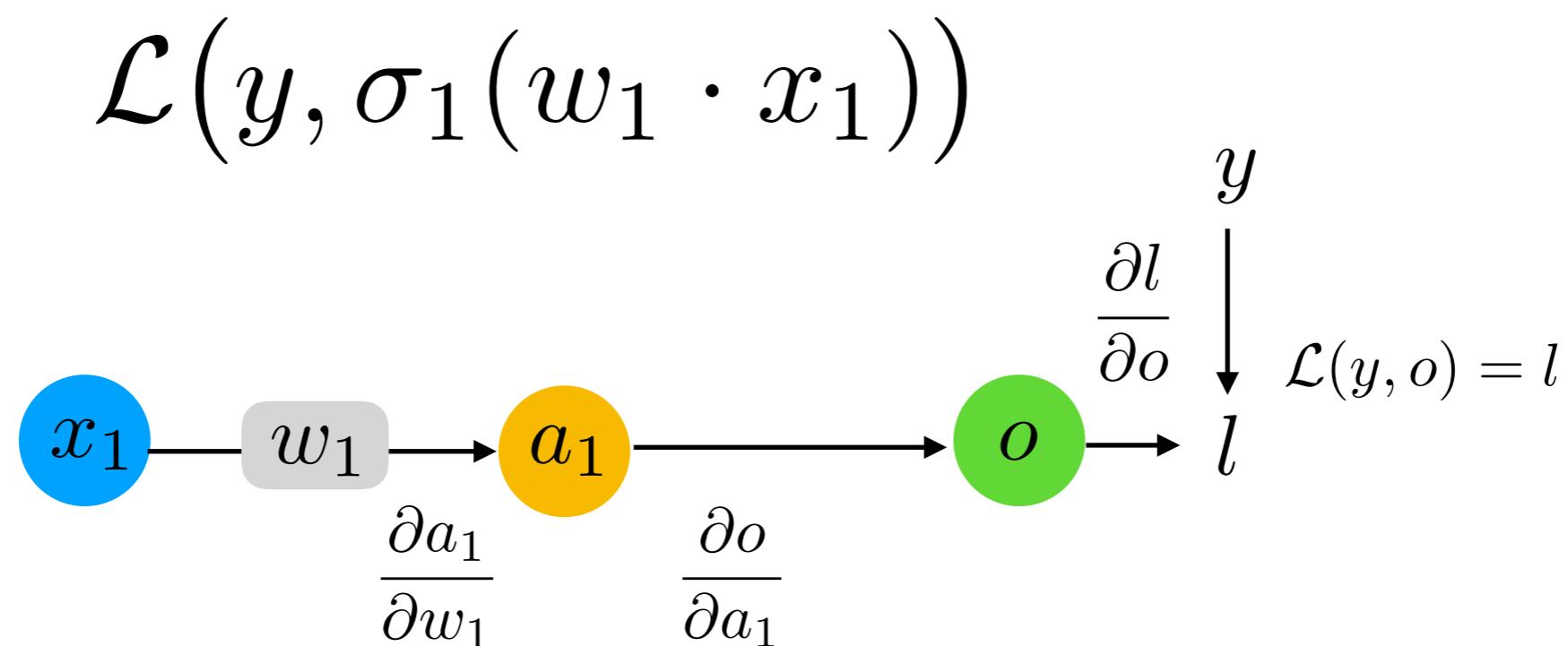


Computation Graphs



Some More Computation Graphs

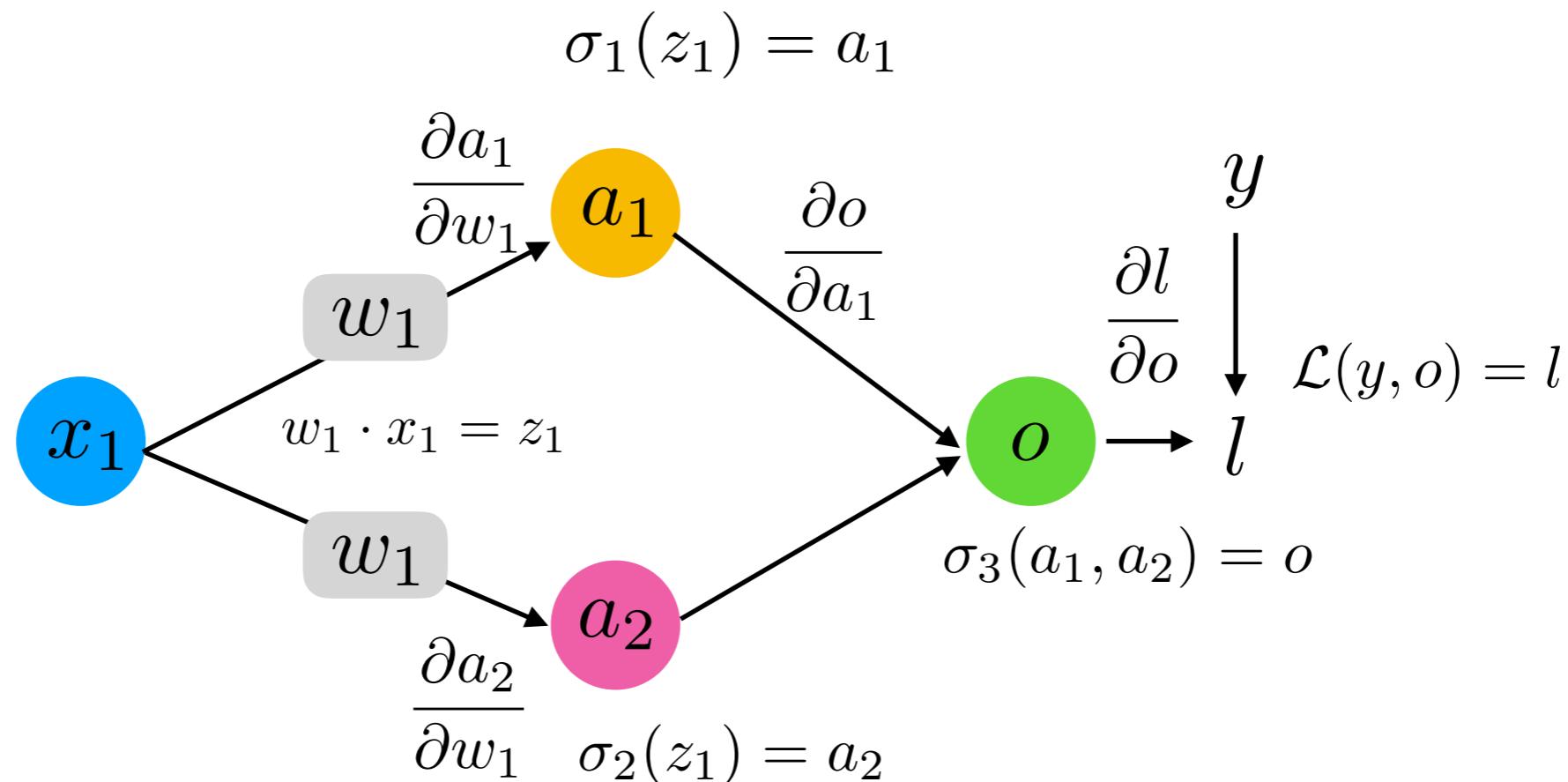
Graph with Single Path



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

Graph with Weight Sharing

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

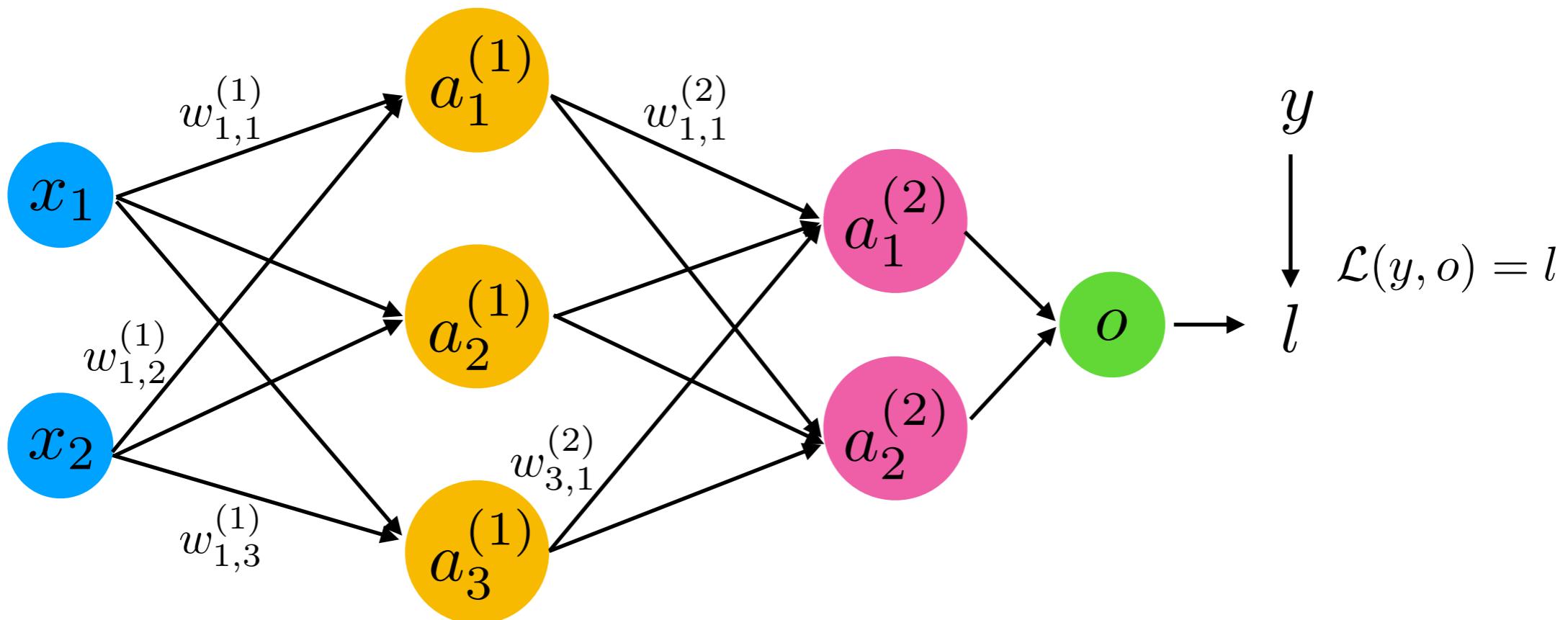


Upper path

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

Lower path

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



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

1/4 -- PyTorch Resources

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4/4 -- PyTorch API

PyTorch Autograd Example

<https://github.com/rasbt/stat453-deep-learning-ss20/tree/master/L06-pytorch/code/pytorch-autograd.ipynb>

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

<https://github.com/rasbt/stat453-deep-learning-ss20/tree/master/L06-pytorch/code/grad-intermediate-var.ipynb>

1/4 -- PyTorch Resources
2/4 -- Computation Graphs
3/4 -- Automatic Differentiation in PyTorch
4/4 -- PyTorch API

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)    | Instantiate model
                                                | (creates the model parameters)

model = model.to(device)

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

```
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
```

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

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) ← This will run the forward() method
        loss = F.cross_entropy(logits, targets) ← Define a loss function to optimize
        optimizer.zero_grad() ← Set the gradient to zero
                                (could be non-zero from a previous forward pass)

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

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

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

PyTorch Usage: Step 3 (Training)

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for epoch in range(num_epochs):
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        logits, probas = model(features)
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        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/stat453-deep-learning-ss20/tree/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)

```
import torch.nn.functional as F

class MultilayerPerceptron(torch.nn.Module):
    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()
        # First hidden layer
        self.linear_1 = torch.nn.Linear(num_features,
                                        num_hidden_1)
        # Second 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")
```

```
class MultilayerPerceptron(torch.nn.Module):
    def __init__(self, num_features, num_classes):
        super(MultilayerPerceptron, self).__init__()
        # First hidden layer
        self.linear_1 = torch.nn.Linear(num_features,
                                        num_hidden_1)
        self.relu1 = torch.nn.ReLU()
        # Second 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"

```
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
```

```
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):

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            torch.nn.ReLU(),
            torch.nn.Linear(num_hidden_1, num_hidden_2),
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            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

2)

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

```
[7]: model.net
[7]: Sequential(
[7]:     (0): Linear(in_features=784, out_features=128, bias=True)
[7]:     (1): ReLU(inplace)
[7]:     (2): Linear(in_features=128, out_features=256, bias=True)
[7]:     (3): ReLU(inplace)
[7]:     (4): Linear(in_features=256, out_features=10, bias=True)
[7]: )
[7]: If we want to get the output from the 2nd layer during the forward pass, we can register a hook as follows:
[8]: outputs = []
[8]: def hook(module, input, output):
[8]:     outputs.append(output)
[8]: model.net[2].register_forward_hook(hook)
[8]: <torch.utils.hooks.RemovableHandle at 0x7f659c6685c0>
[8]: Now, if we call the model on some inputs, it will save the intermediate results in the "outputs" list:
[9]: _ = model(features)
[9]: print(outputs)
[9]: [tensor([[0.5341, 1.0513, 2.3542, ..., 0.0000, 0.0000, 0.0000],
[9]:         [0.0000, 0.6676, 0.6620, ..., 0.0000, 0.0000, 2.4056],
[9]:         [1.1520, 0.0000, 0.0000, ..., 2.5860, 0.8992, 0.9642],
[9]:         ...,
[9]:         [0.0000, 0.1076, 0.0000, ..., 1.8367, 0.0000, 2.5203],
[9]:         [0.5415, 0.0000, 0.0000, ..., 2.7968, 0.8244, 1.6335],
[9]:         [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

- PyTorch Book: <https://pytorch.org/assets/deep-learning/Deep-Learning-with-PyTorch.pdf>

Chapter 1: Introducing deep learning and the PyTorch library

Chapter 2: It starts with a tensor