STAT 453: Introduction to Deep Learning and Generative Models

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Lecture 06: Automatic Differentiation with PyTorch

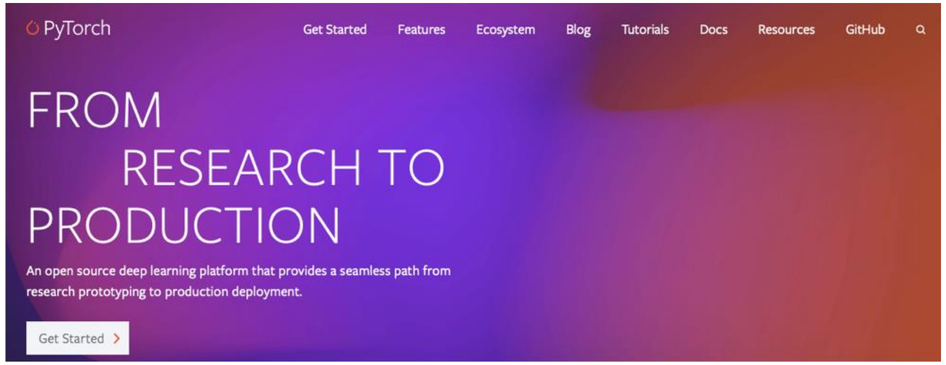
September 22, 2025

Today: Computing partial derivatives with PyTorch

1. **PyTorch Resources**
2. Computation Graphs
3. Automatic Differentiation in PyTorch
4. A Closer Look at the PyTorch API

PyTorch

PyTorch



https://pytorch.org/

At a Glance:

- Based on Torch 7, which was based on Lua and inspired by Lush
- PyTorch started in 2016
- Focuses on flexibility and minimizing cognitive overhead
- Dynamic nature of autograd API inspired by Chainer
- Core features
  - **Automatic differentiation**
  - **Dynamic computation graphs**
  - NumPy integration
- written in C++ and CUDA (CUDA is like C++ for the GPU)
- Python is the usability glue

Installing PyTorch

Recommendation for Laptop (e.g., MacBook)

PyTorch Build	Stable (1.7.1)		Preview (Nightly)		
Your OS	Linux	Mac		Windows	
Package	Conda	Pip	LibTorch	Source	
Language	Python		C++ / Java		
CUDA	9.2	10.1	10.2	11.0	None
Run this Command:	**NOTE:** Python 3.9 users will need to add '-c=conda-forge' for installation conda install pytorch torchvision torchaudio -c pytorch				

Recommendation for Desktop (Linux) with GPU

PyTorch Build	Stable (1.7.1)		Preview (Nightly)		
Your OS	Linux	Mac		Windows	
Package	Conda	Pip	LibTorch	Source	
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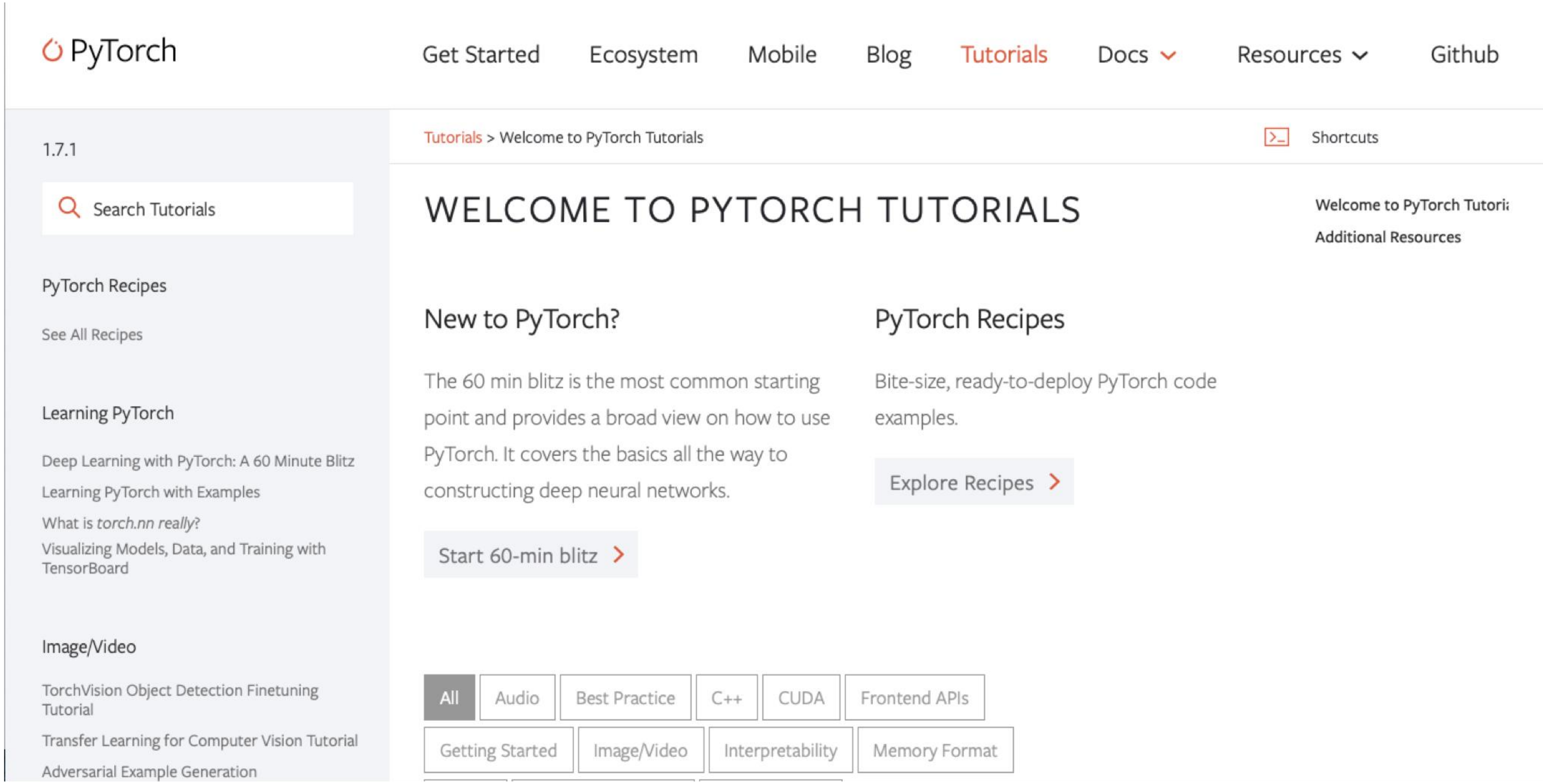
https://pytorch.org/

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

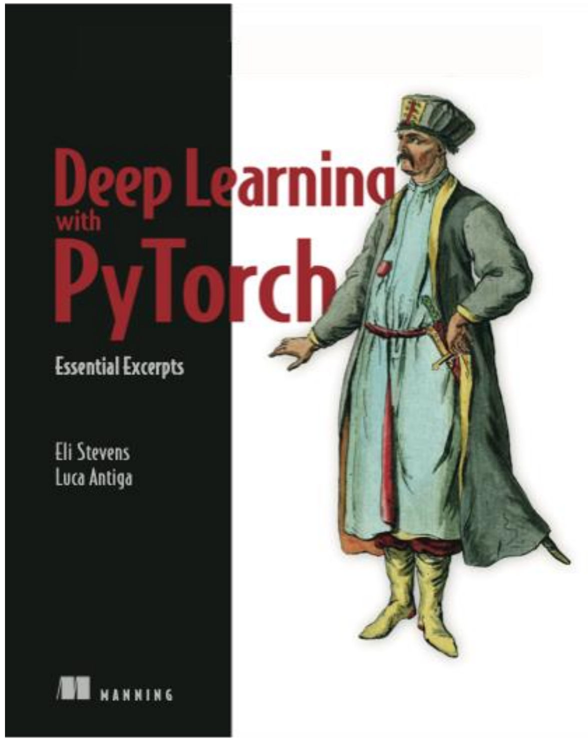
```
In [1]: import torch

In [2]: torch.__version__
Out[2]: '1.7.0'

In [3]:
```

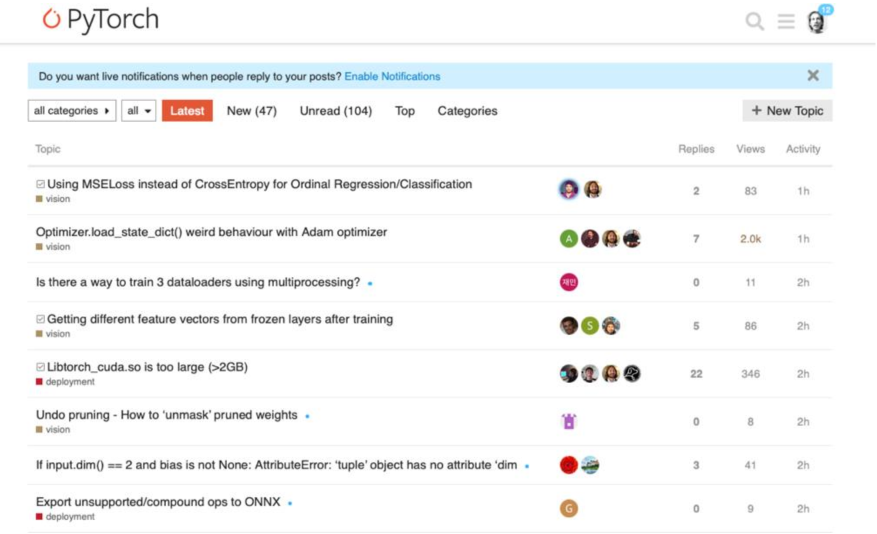
Many useful tutorials (recommend you read some)



https://pytorch.org/tutorials/

Other resources





https://discuss.pytorch.org

And…

Ask ChatGPT/Claude if your PyTorch code is not working ☺

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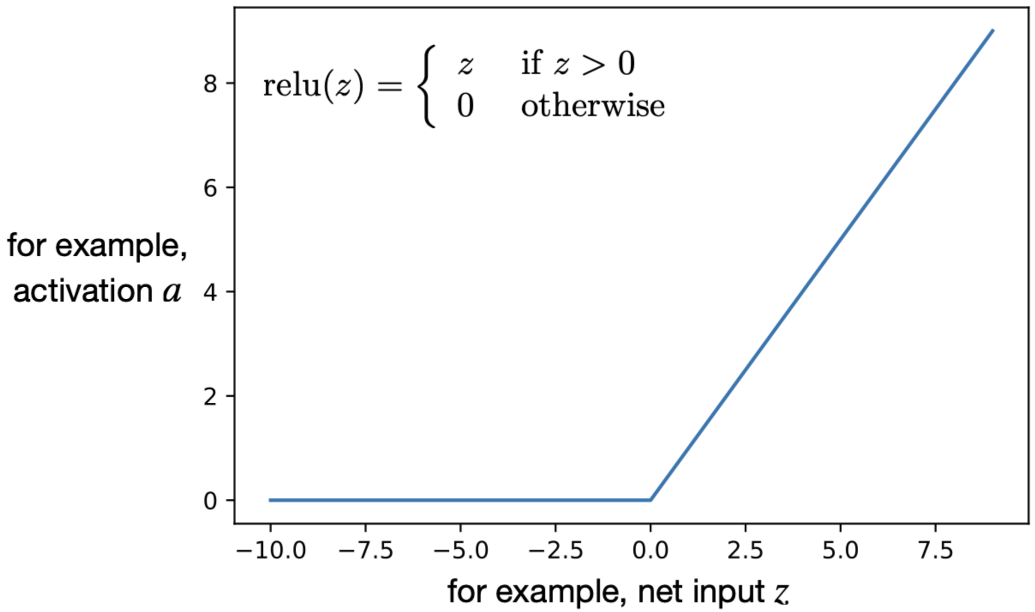
Computation graphs: ReLU

Suppose we have the following activation function:

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

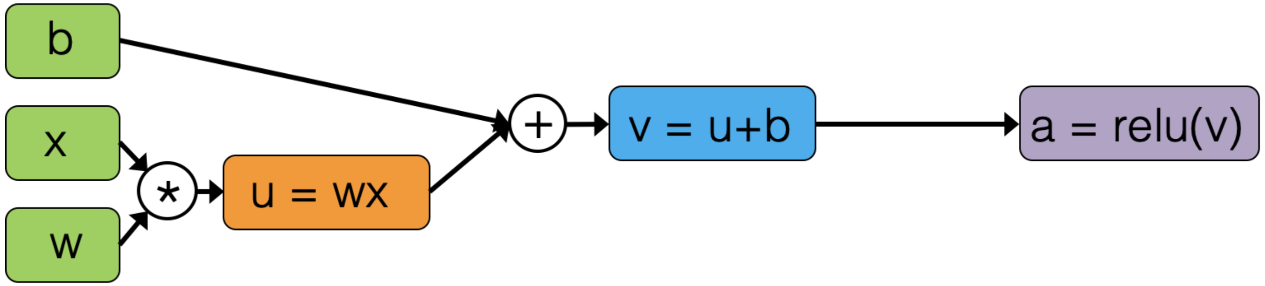


ReLU = Rectified Linear Unit

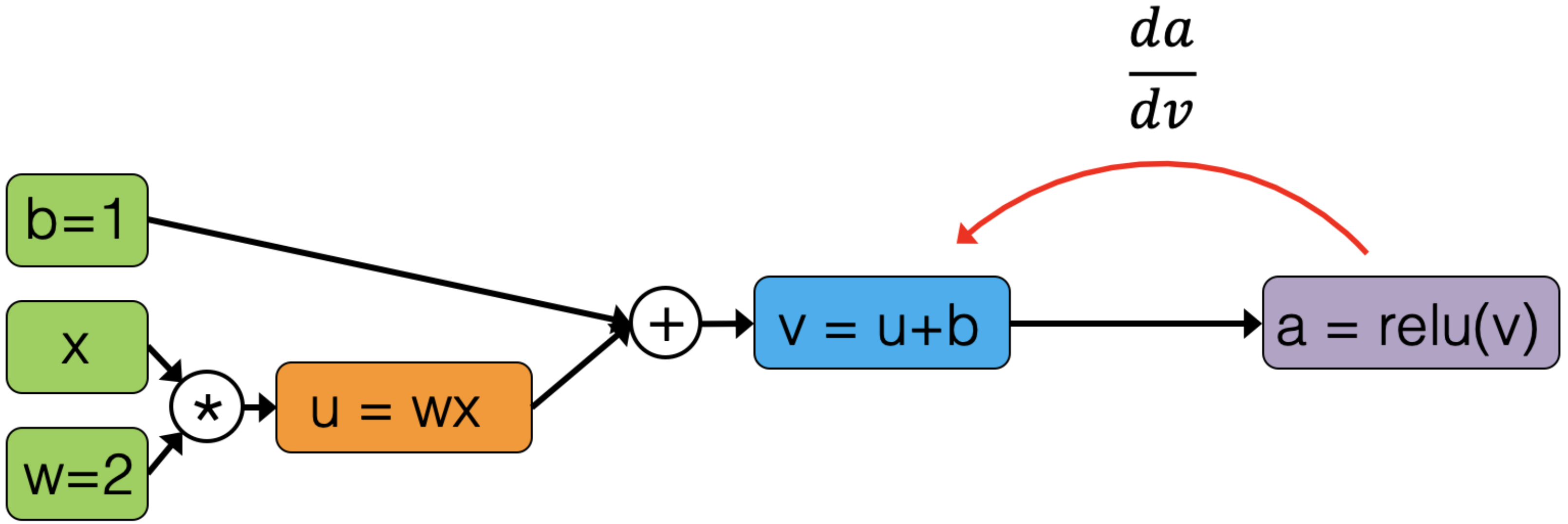
(prob. the most commonly used activation function in DL)

Computation graphs: ReLU

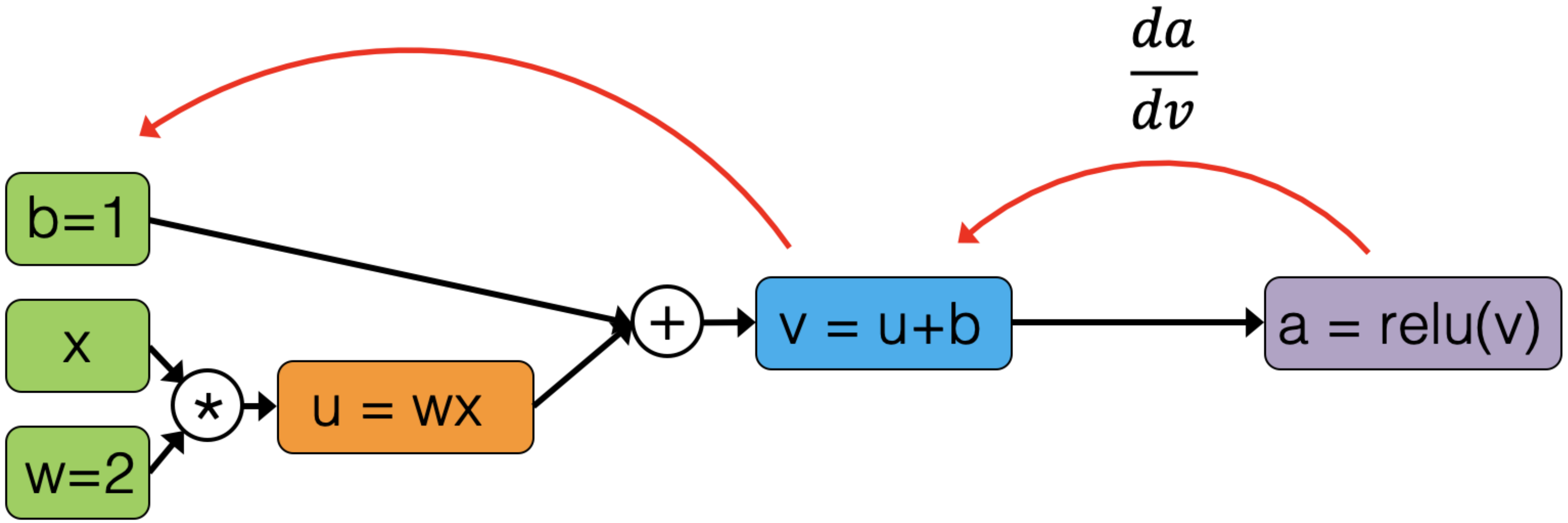
$$a(x, w, b) = relu(\underbrace{\underbrace{w \cdot x}_{u} + b}_{v})$$



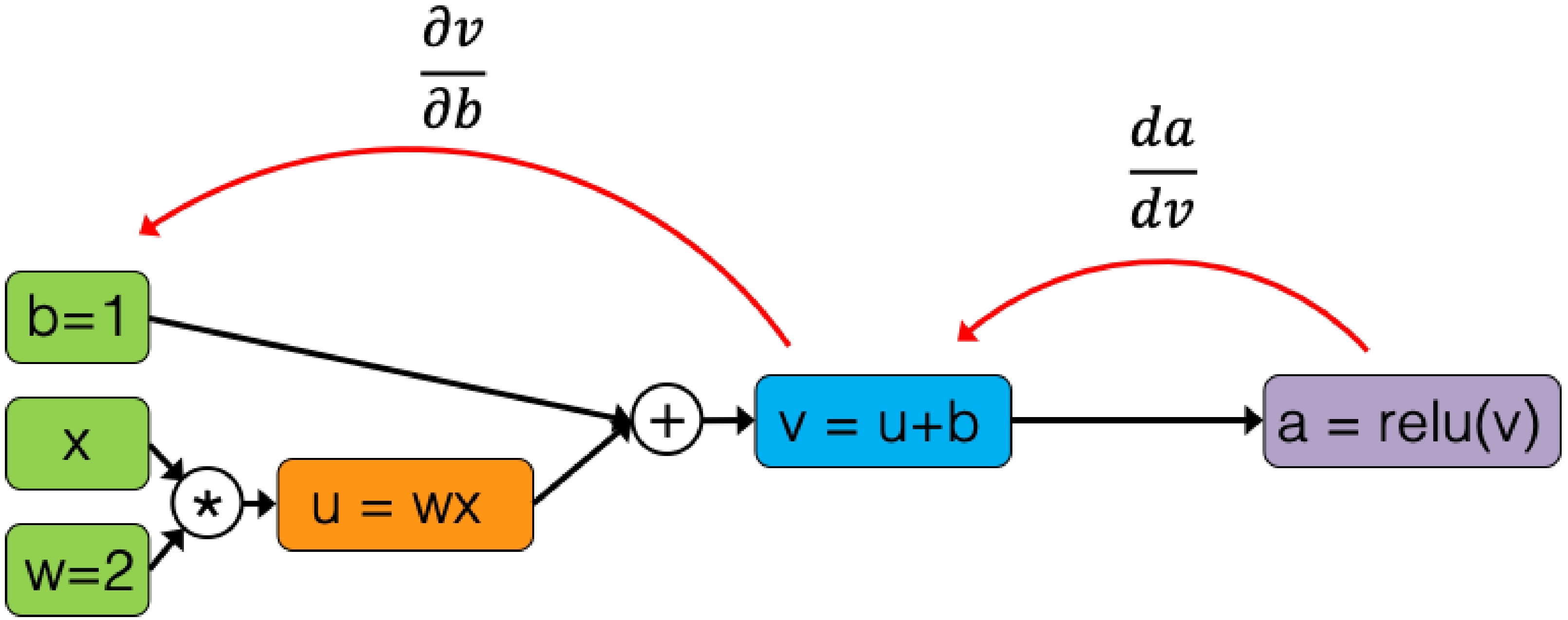
Computation graphs: ReLU



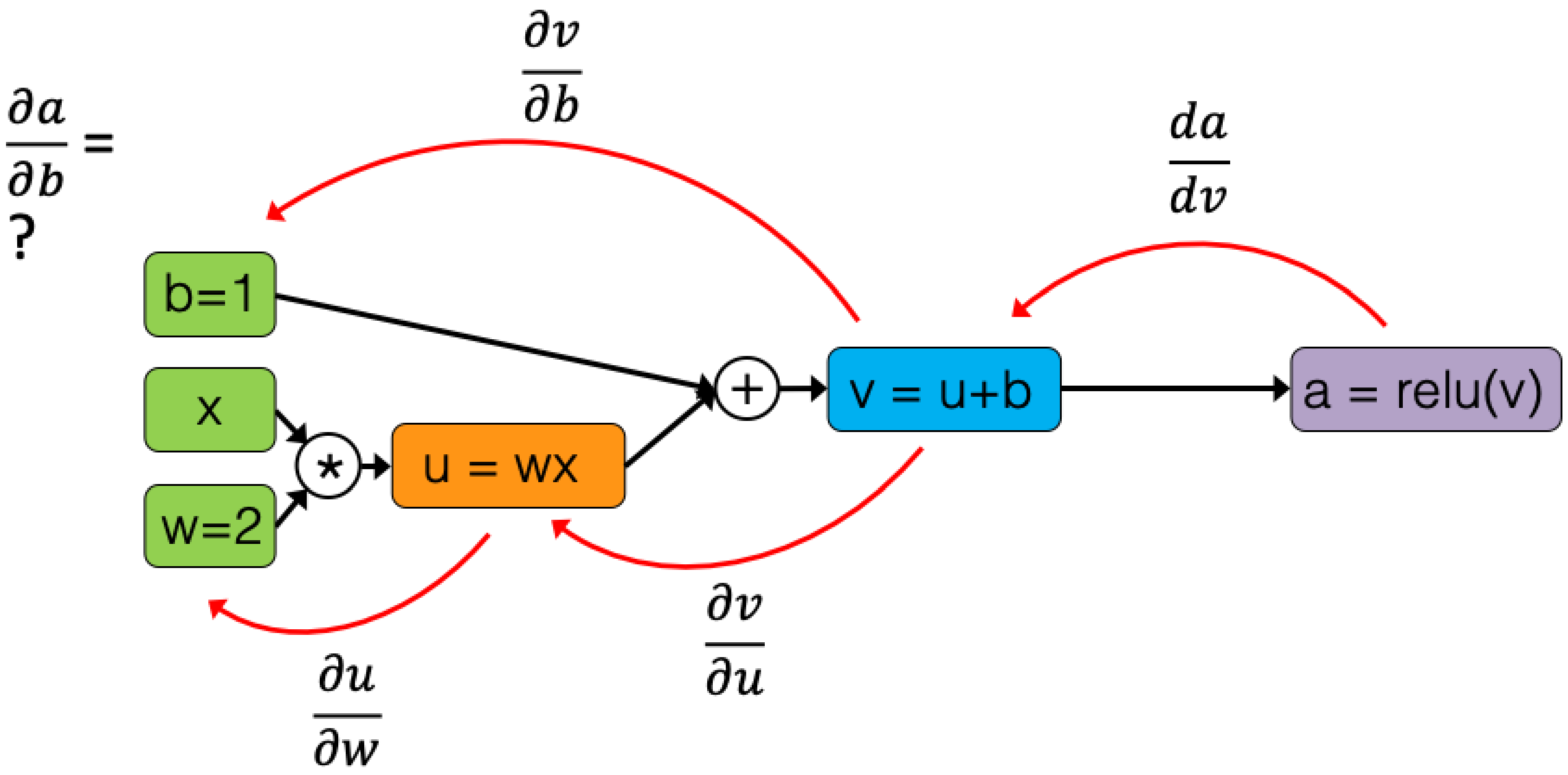
Computation graphs: ReLU



Computation graphs: ReLU

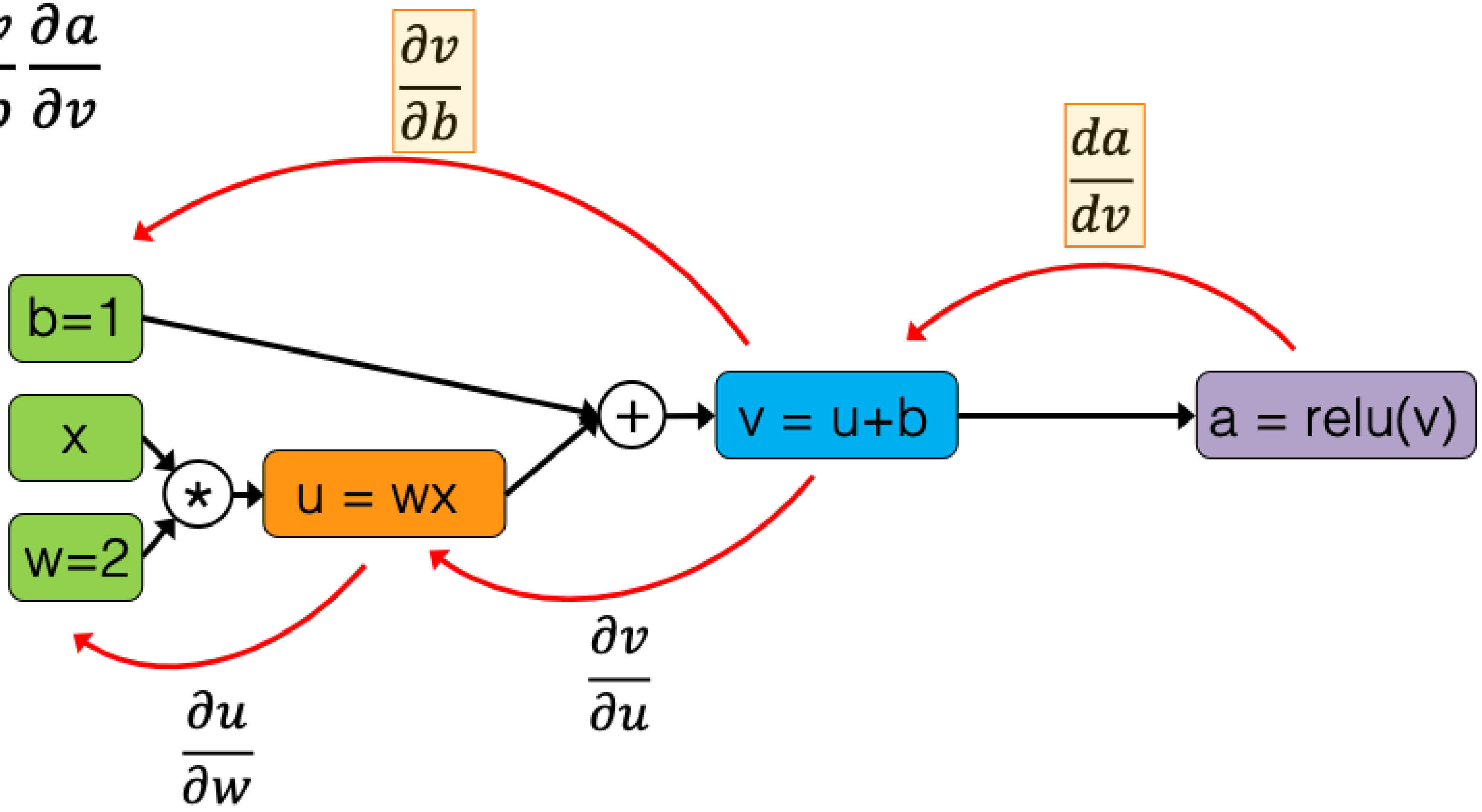


Computation graphs: ReLU



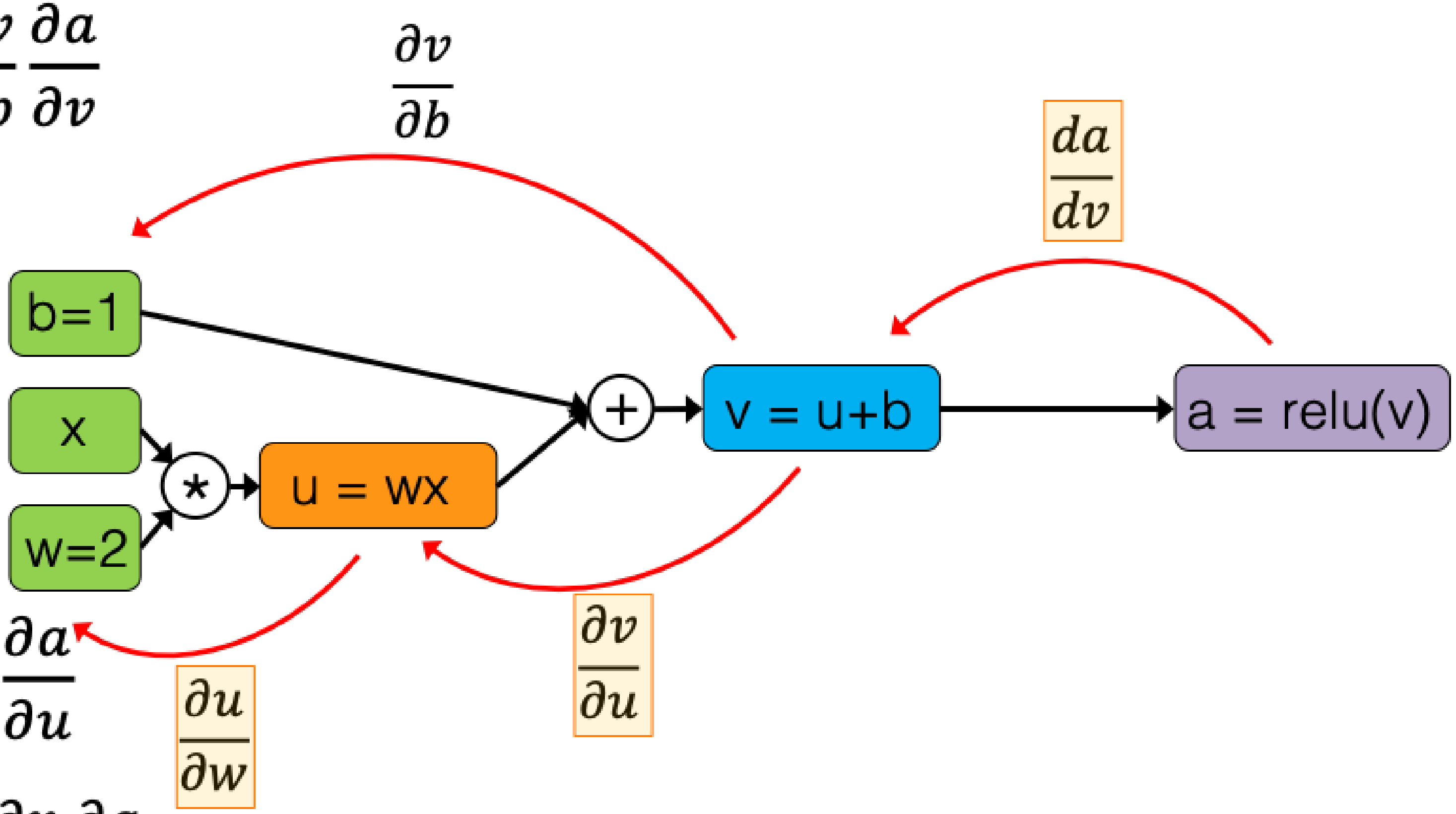
Computation graphs: ReLU

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



Computation graphs: ReLU

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

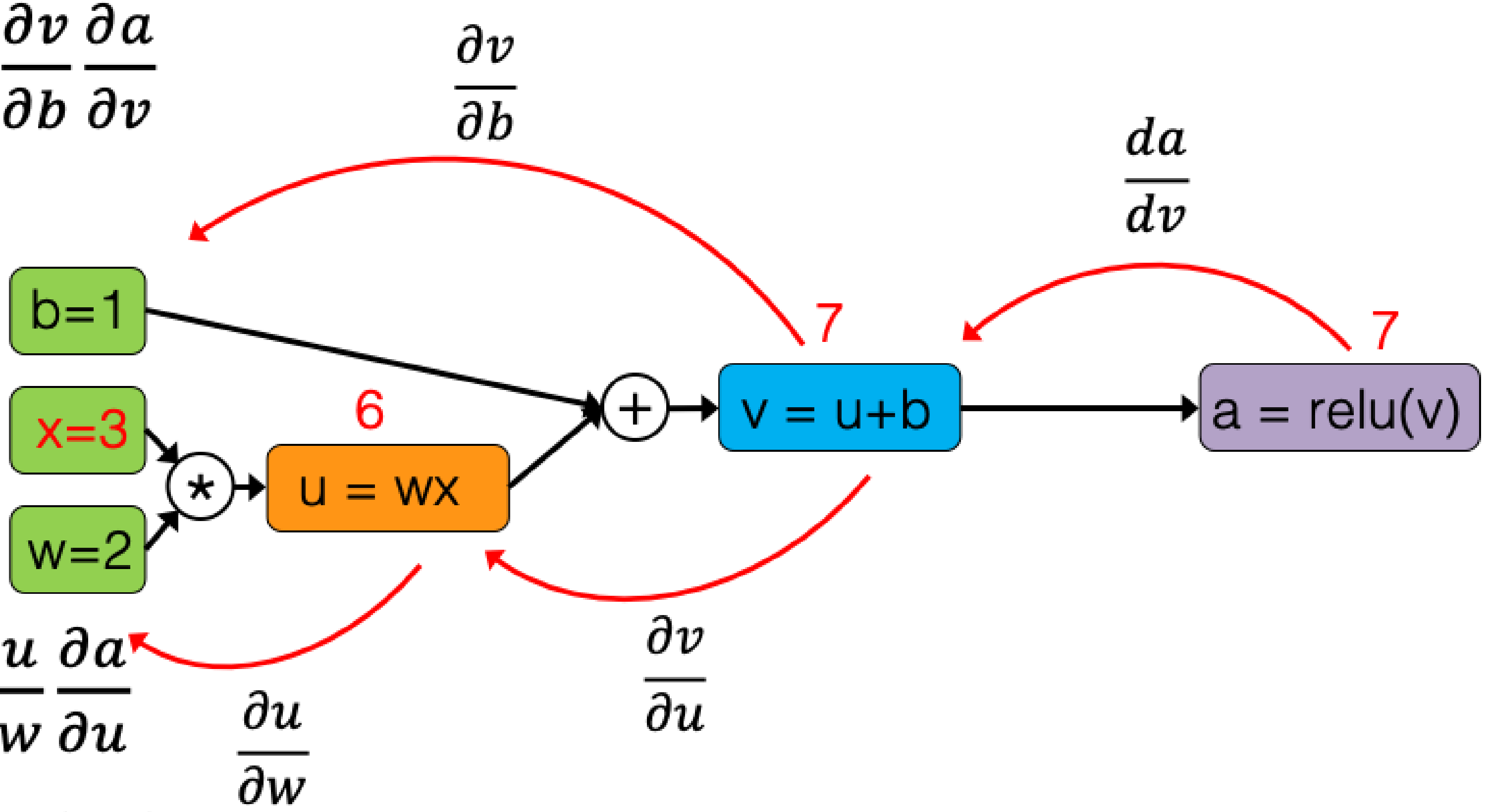


$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

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

Computation graphs: ReLU

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



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

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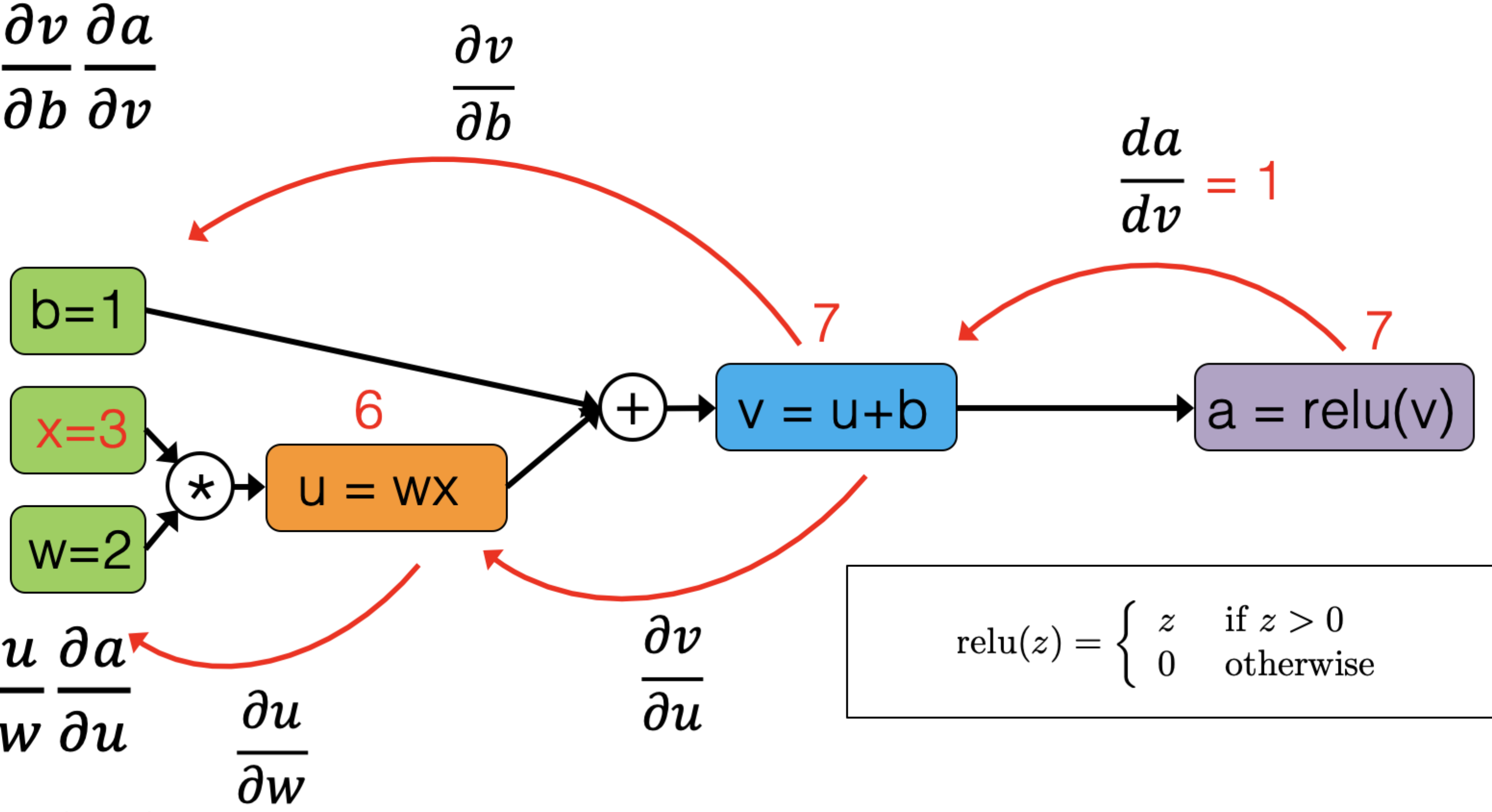
Computation graphs: ReLU

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



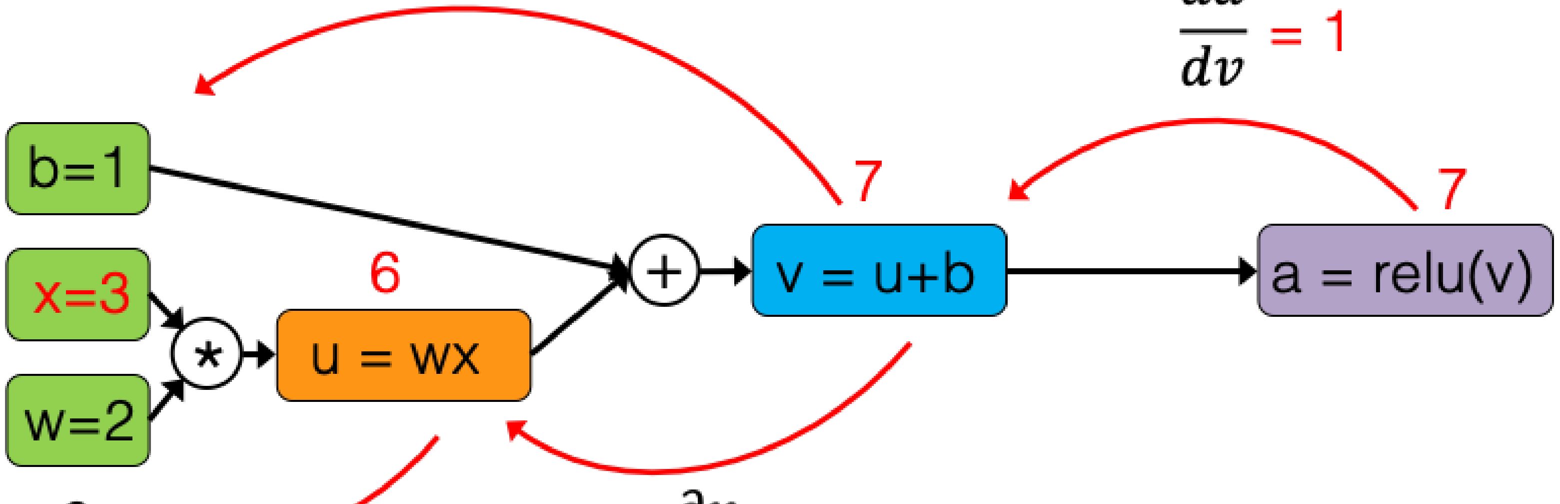
$$\mathrm{relu}(z) = \begin{cases} z & \text{if } z > 0 \\ 0 & \text{otherwise} \end{cases}$$

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

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

Computation graphs: ReLU

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



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

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

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

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

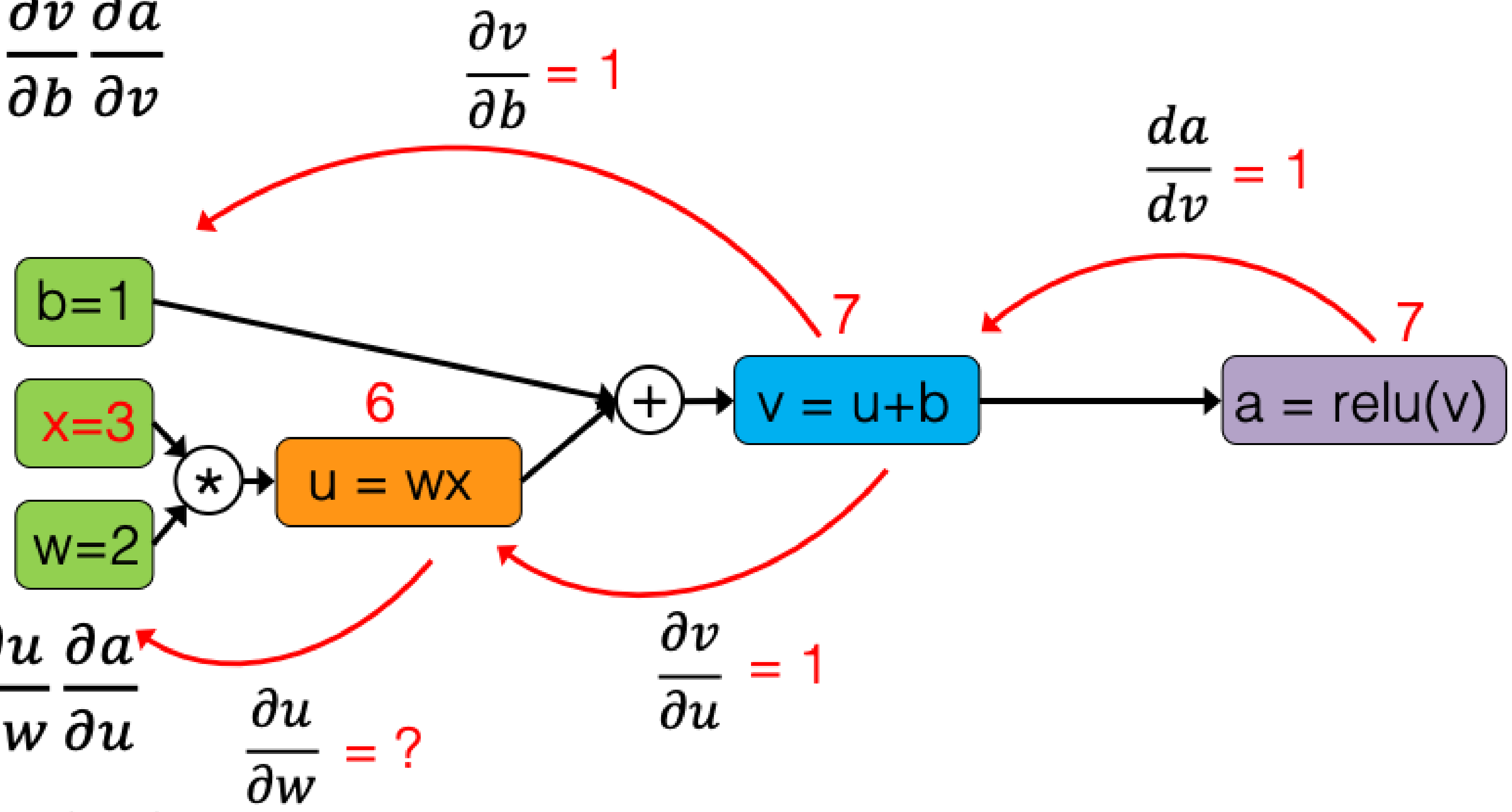
$$= \frac{\partial u}{\partial w}\frac{\partial v}{\partial u}\frac{\partial a}{\partial v}$$

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

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

Computation graphs: ReLU

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

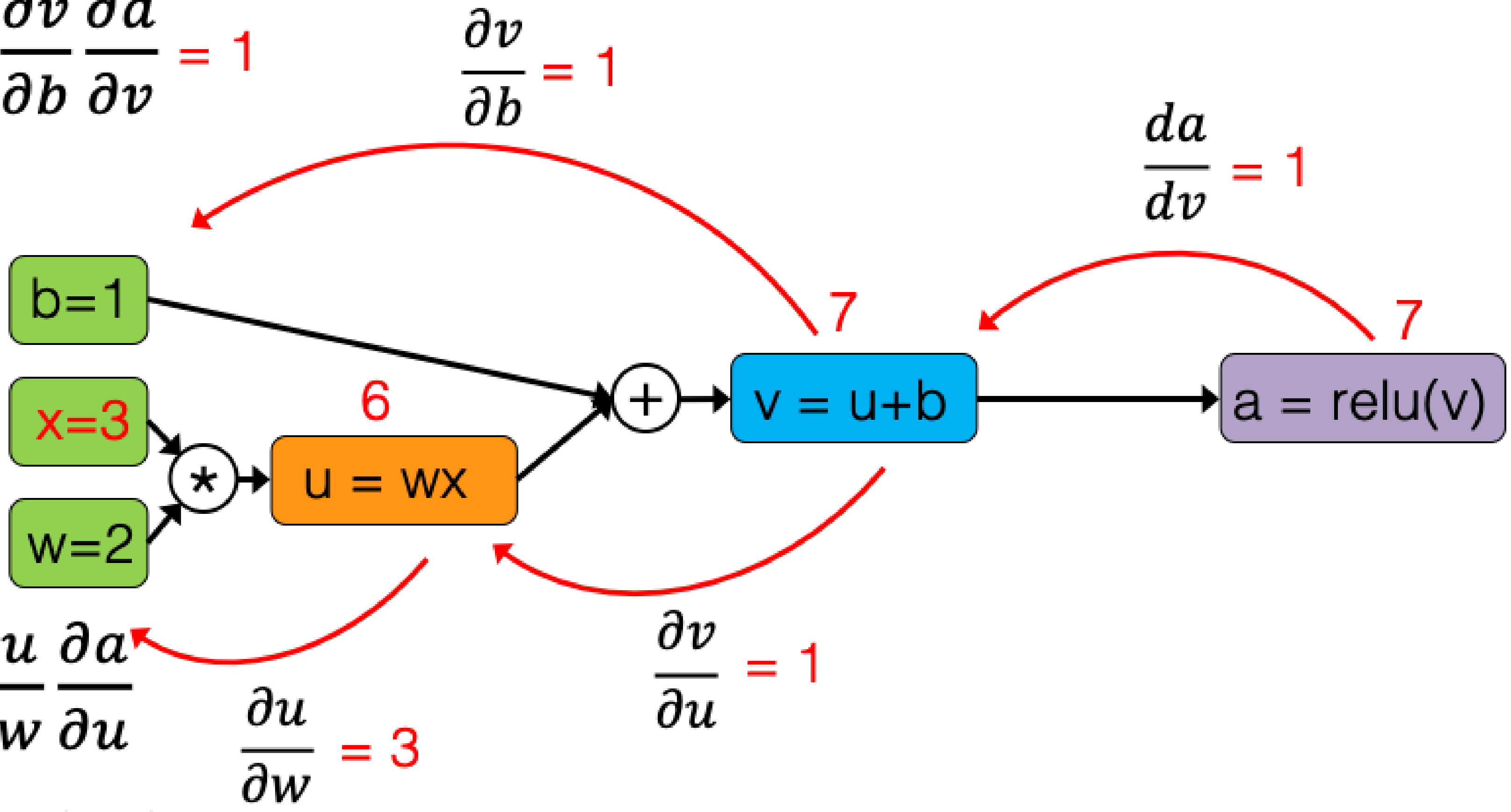


$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

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

Computation graphs: ReLU

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



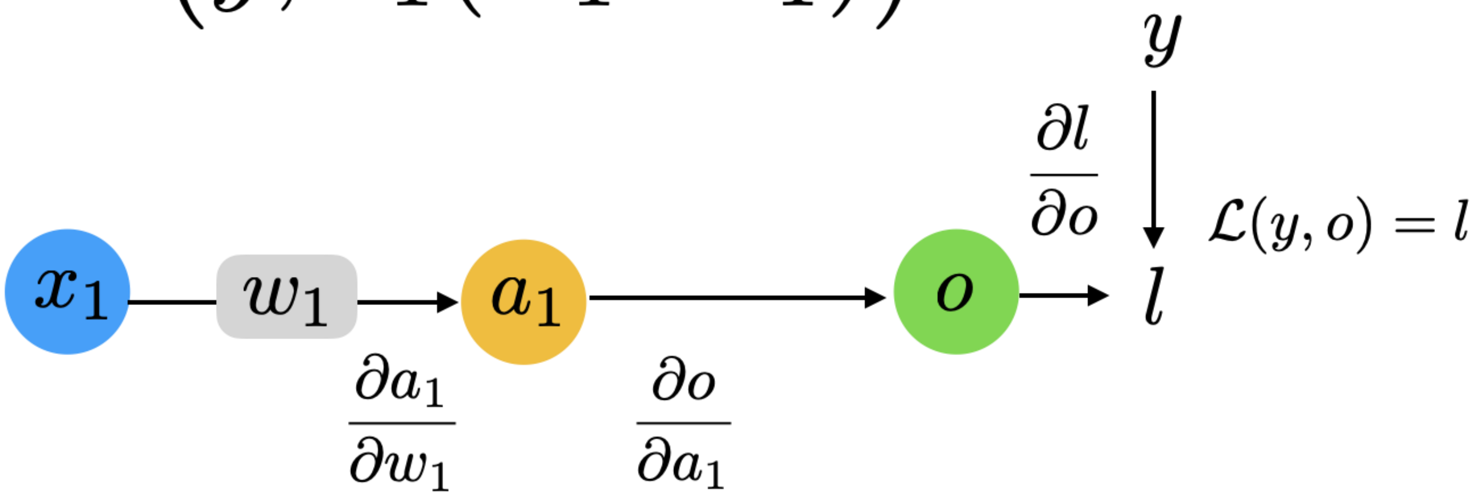
$$\frac{\partial a}{\partial w} = \frac{\partial u}{\partial w}\frac{\partial a}{\partial u}$$

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

- Some more computation graphs

Computation graphs: Single-path

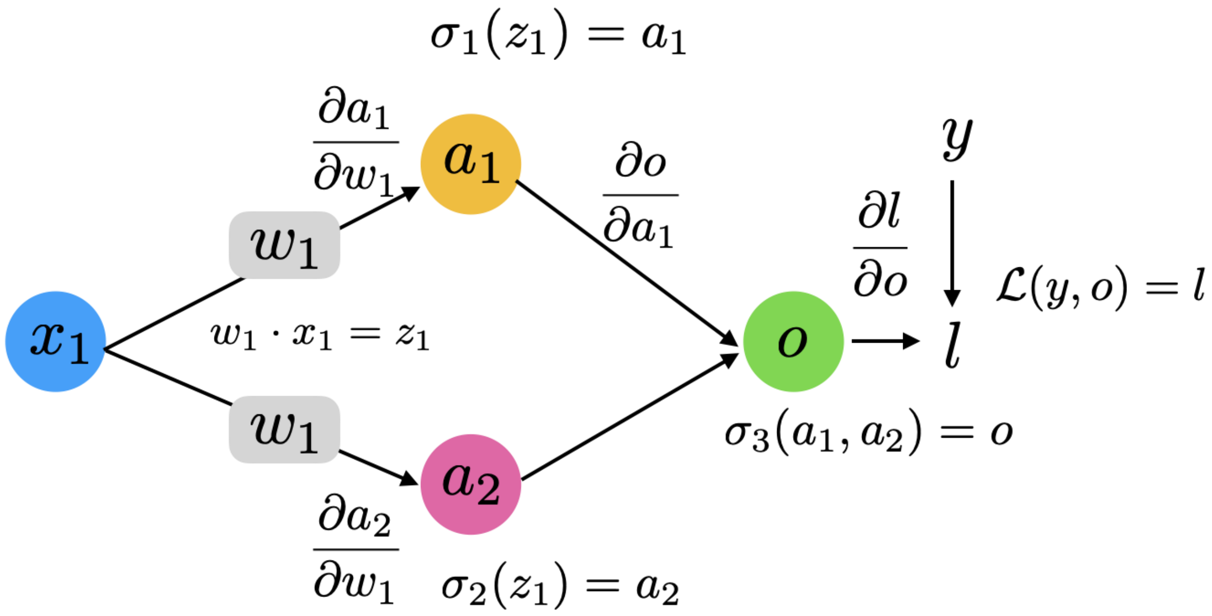
$$\mathcal{L}\left(y, \sigma_1(w_1 \cdot x_1)\right)$$



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

Computation graphs: Weight-Sharing

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

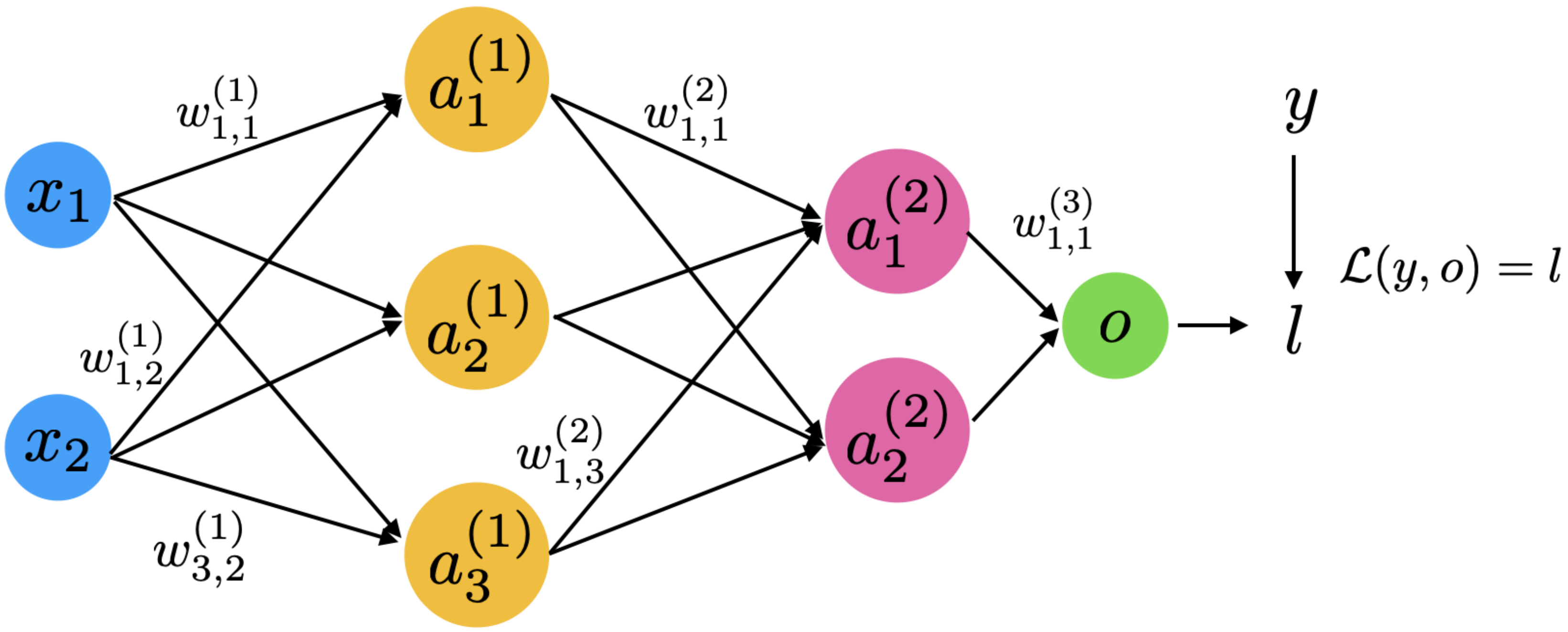


Upper path

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

Lower path

Computation graphs: Fully-Connected Layer



$$\frac{\partial l}{\partial w^{(1)}_{1,1}} = \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a^{(2)}_1} \cdot \frac{\partial a^{(2)}_1}{\partial a^{(1)}_1} \cdot \frac{\partial a^{(1)}_1}{\partial w^{(1)}_{1,1}} + \frac{\partial l}{\partial o} \cdot \frac{\partial o}{\partial a^{(2)}_2} \cdot \frac{\partial a^{(2)}_2}{\partial a^{(1)}_1} \cdot \frac{\partial a^{(1)}_1}{\partial w^{(1)}_{1,1}}$$

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Automatic Differentiation in PyTorch

- An example: https://github.com/rasbt/stat453-deep-learning-ss21/tree/master/L06/code/pytorch-autograd.ipynb

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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 3 (Training)

Run for a specified number of epochs

Iterate over minibatches in epoch

```
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
```

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

y = model(x) calls .__call__ and then .forward(), where some extra stuff is done in __call__;

don't run y = model.forward(x) directly

Gradients at each leaf node are accumulated under the .grad attribute, not just stored. This is why we have to zero them before each backward pass

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)
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        ### 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)
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        ### 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

Simple “print” statements don’t work for debugging

[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>)]
```

Questions?

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