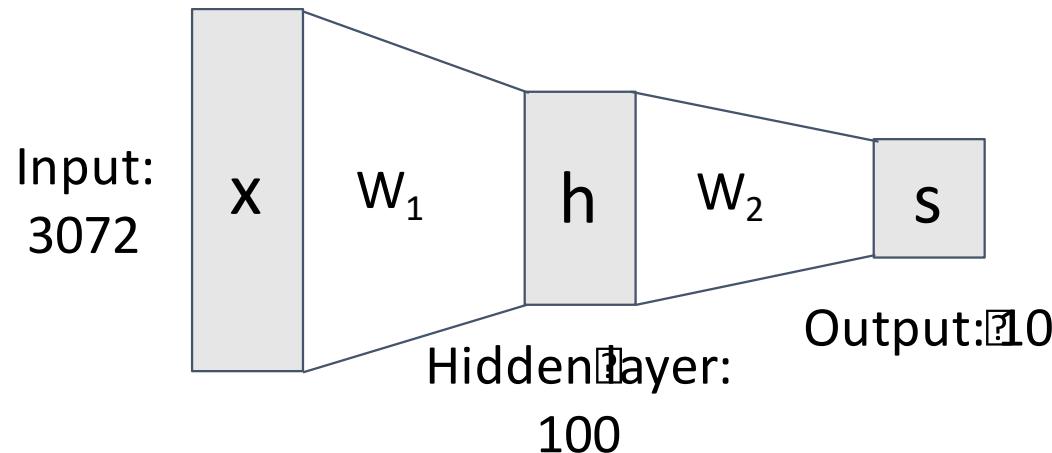


Lecture 6: Backpropagation

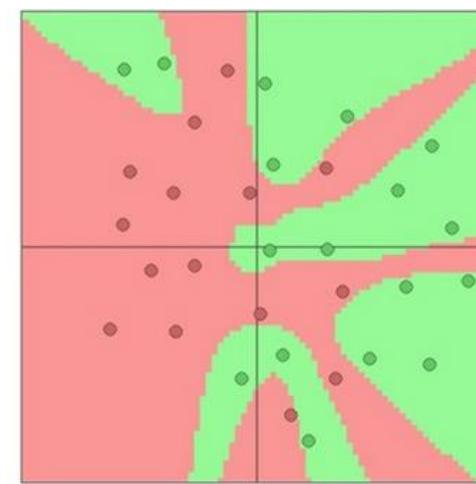
Last time: (Fully-Connected) Neural Networks

From linear classifiers to
fully-connected networks

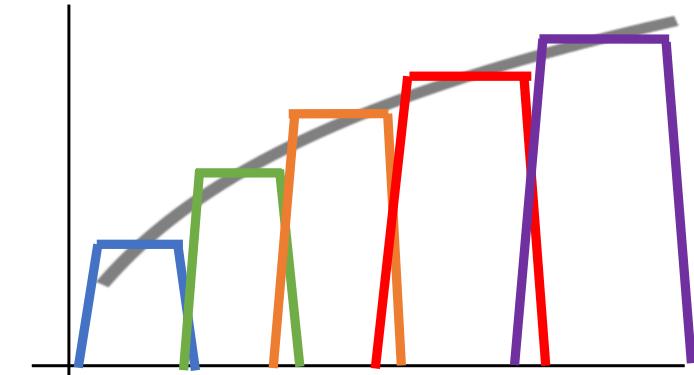
$$f(x) = W_2 \max(0, W_1 x + b_1) + b_2$$



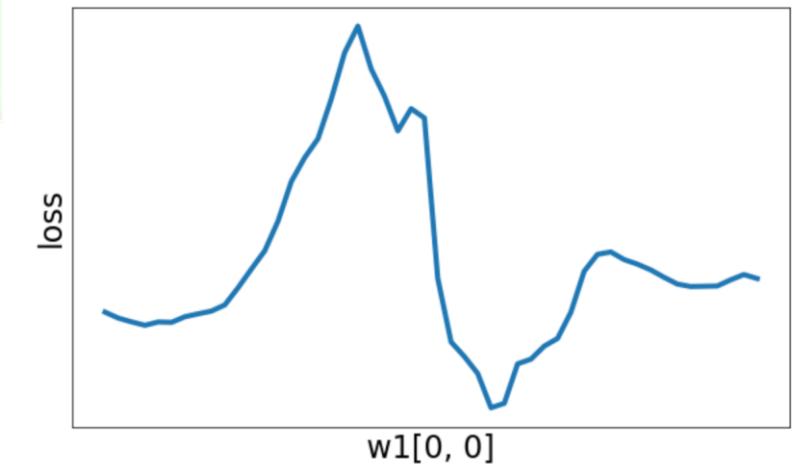
Space Warping



Universal Approximation



Nonconvex



Problem: How to compute gradients?

$$s = W_2 \max(0, W_1 x + b_1) + b_2 \quad \text{Nonlinear score function}$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1) \quad \text{Per-element data loss}$$

$$R(W) = \sum_k W_k^2 \quad \text{L2 Regularization}$$

$$L(W_1, W_2, b_1, b_2) = \frac{1}{N} \sum_{i=1}^N L_i + \lambda R(W_1) + \lambda R(W_2) \quad \text{Total loss}$$

If we can compute $\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial W_2}, \frac{\partial L}{\partial b_1}, \frac{\partial L}{\partial b_2}$ then we can optimize with SGD

(Bad) Idea: Derive $\nabla_W L$ on paper

$$s = f(x; W) = Wx$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

$$= \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1)$$

$$L = \frac{1}{N} \sum_{i=1}^N L_i + \lambda \sum_k W_k^2$$

$$= \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2$$

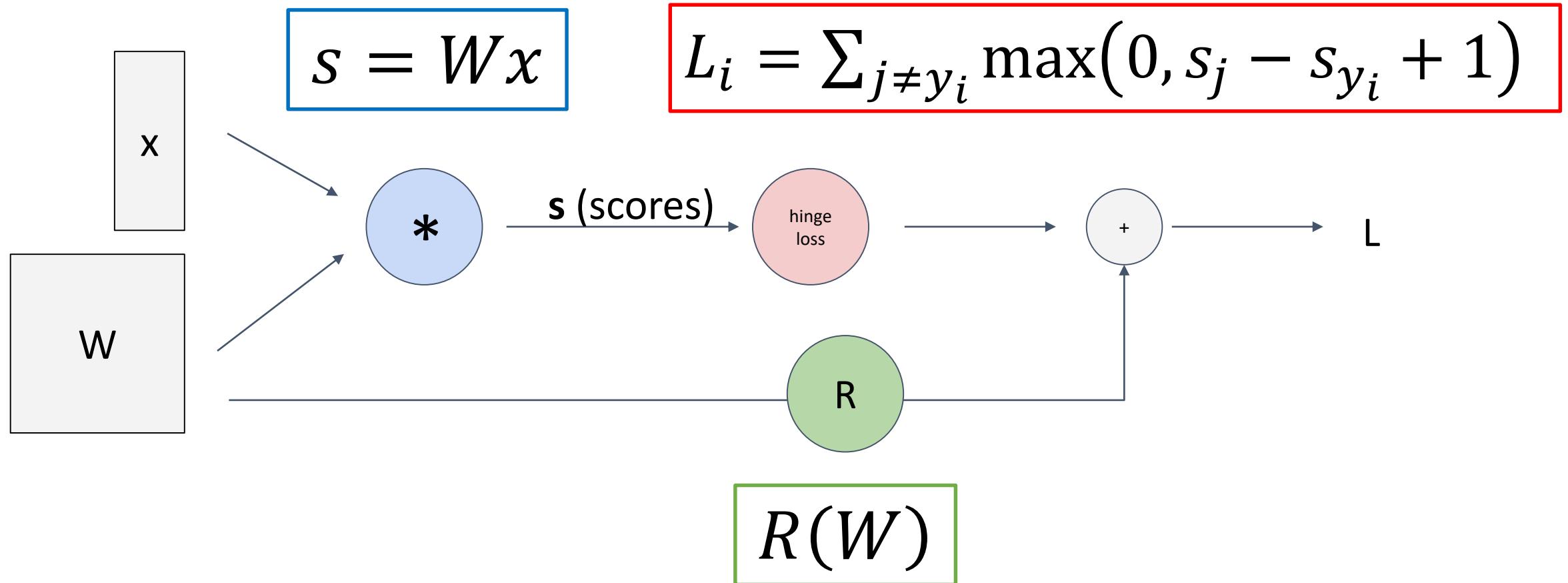
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

Problem: Very tedious: Lots of matrix calculus, need lots of paper

Problem: What if we want to change loss? E.g. use softmax instead of SVM? Need to re-derive from scratch. Not modular!

Problem: Not feasible for very complex models!

Better Idea: Computational Graphs

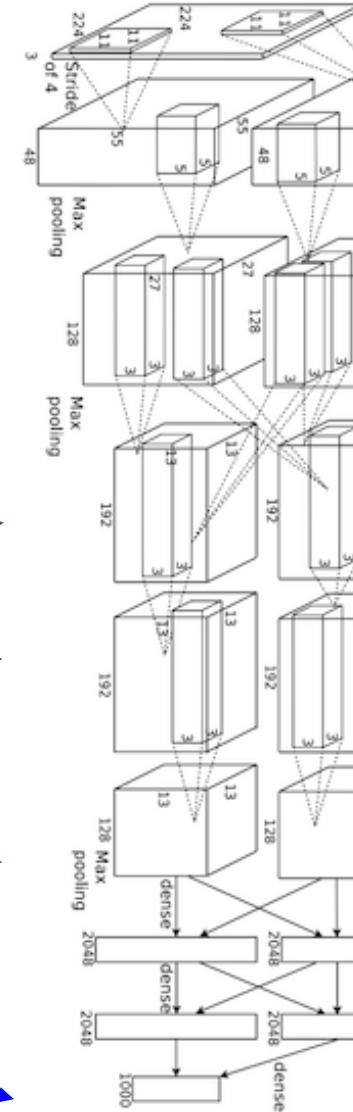


Deep Network (AlexNet)

input image

weights

loss



Neural Turing Machine

input image

loss

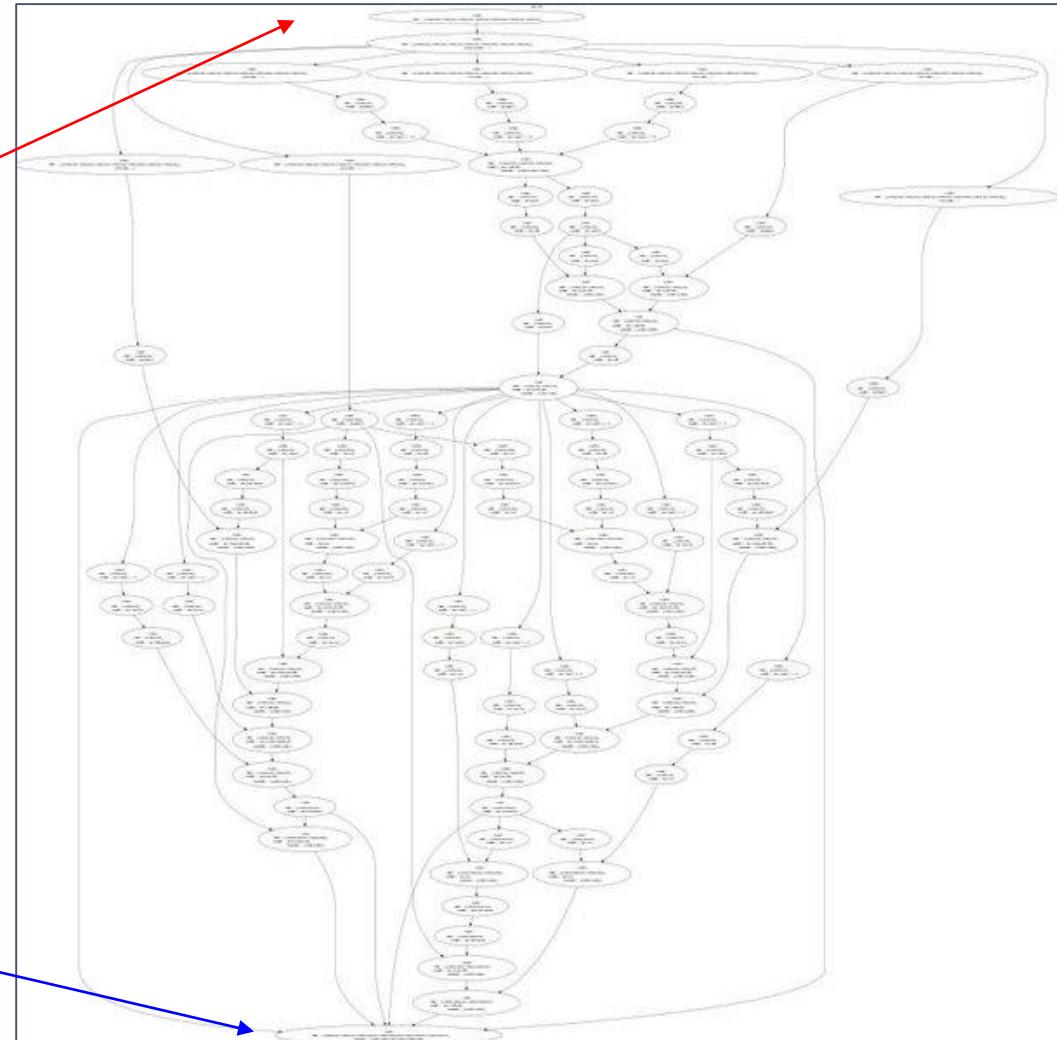
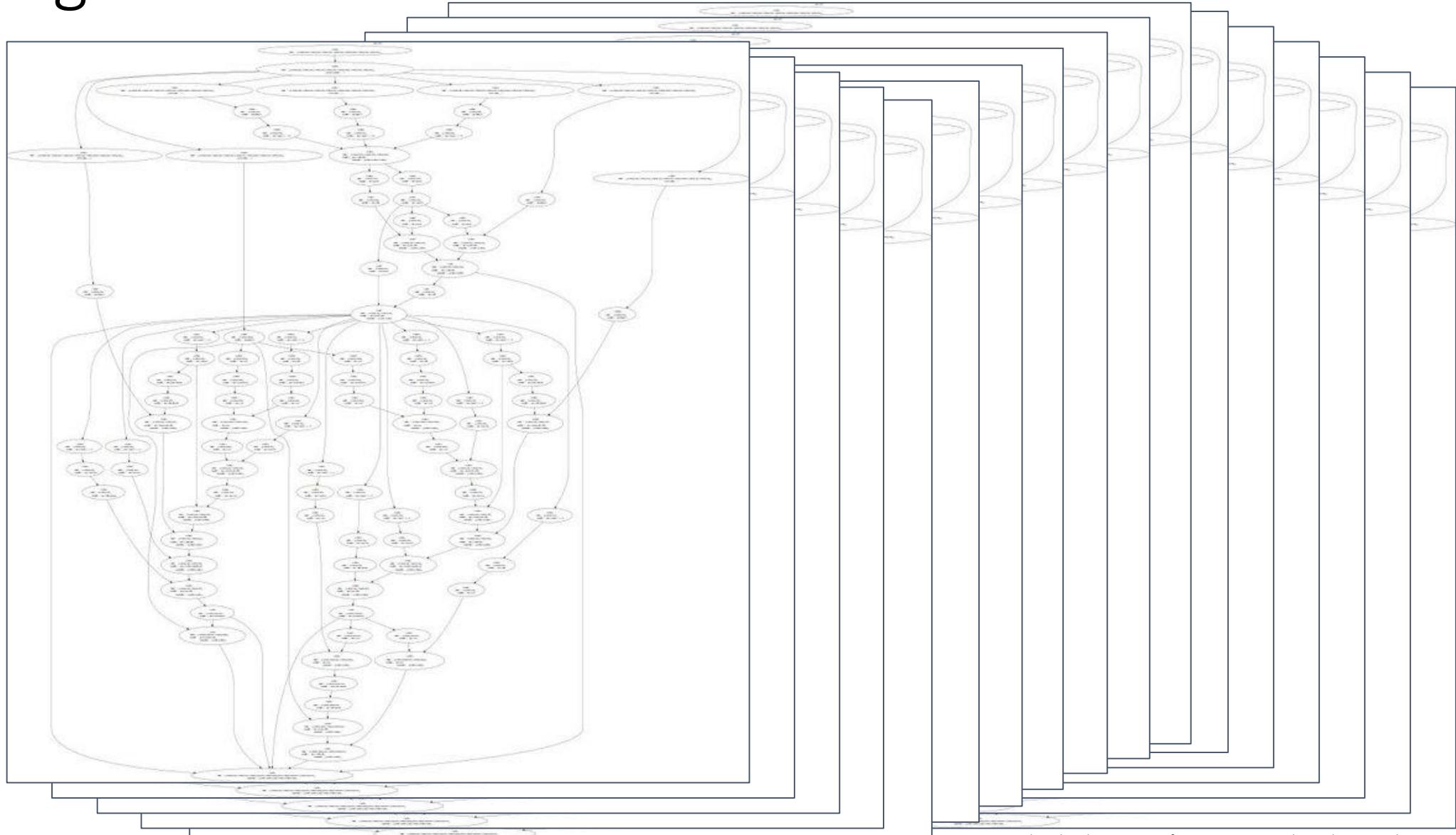


Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

Neural Turing Machine

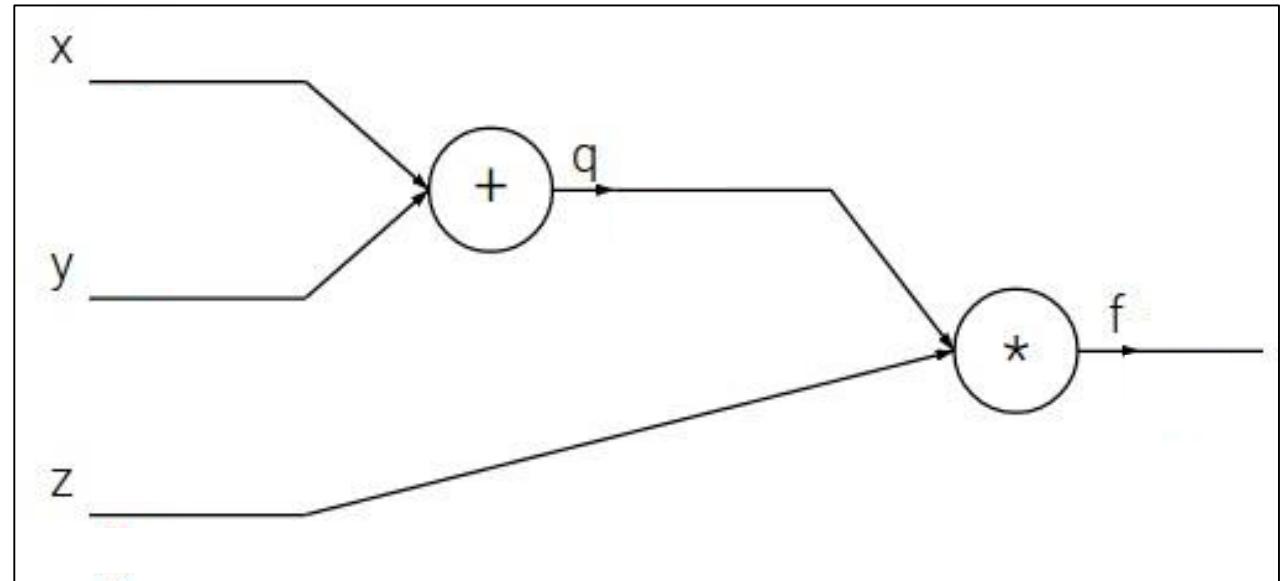


Graves et al, arXiv 2014

Figure reproduced with permission from a [Twitter post](#) by Andrej Karpathy.

Backpropagation: Simple Example

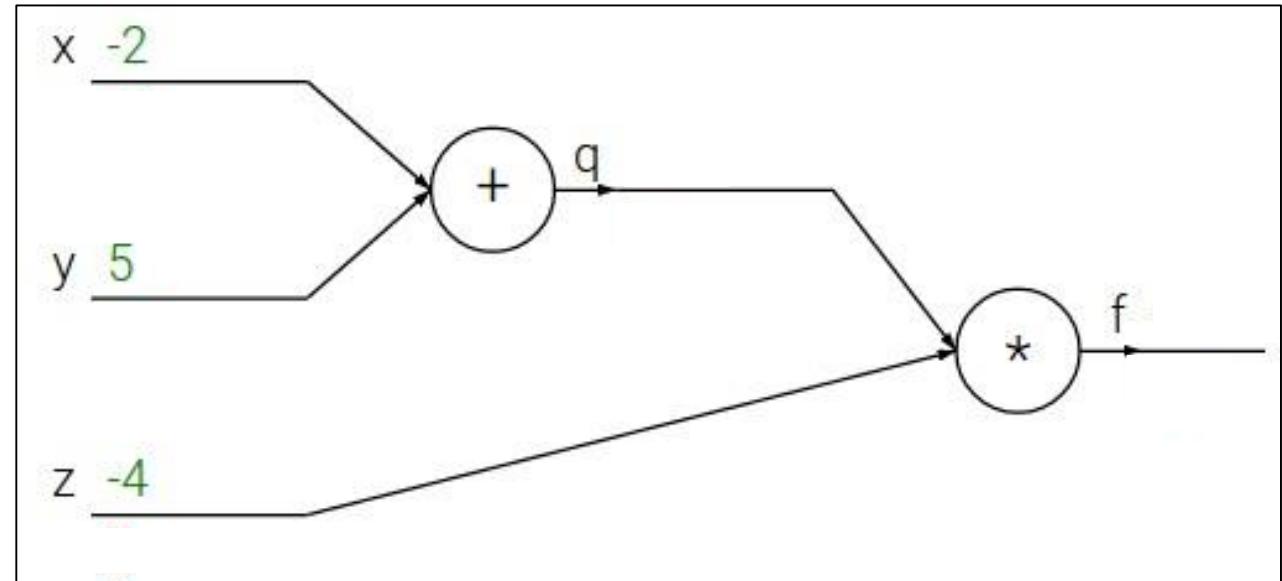
$$f(x, y, z) = (x + y) \cdot z$$



Backpropagation: Simple Example

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

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



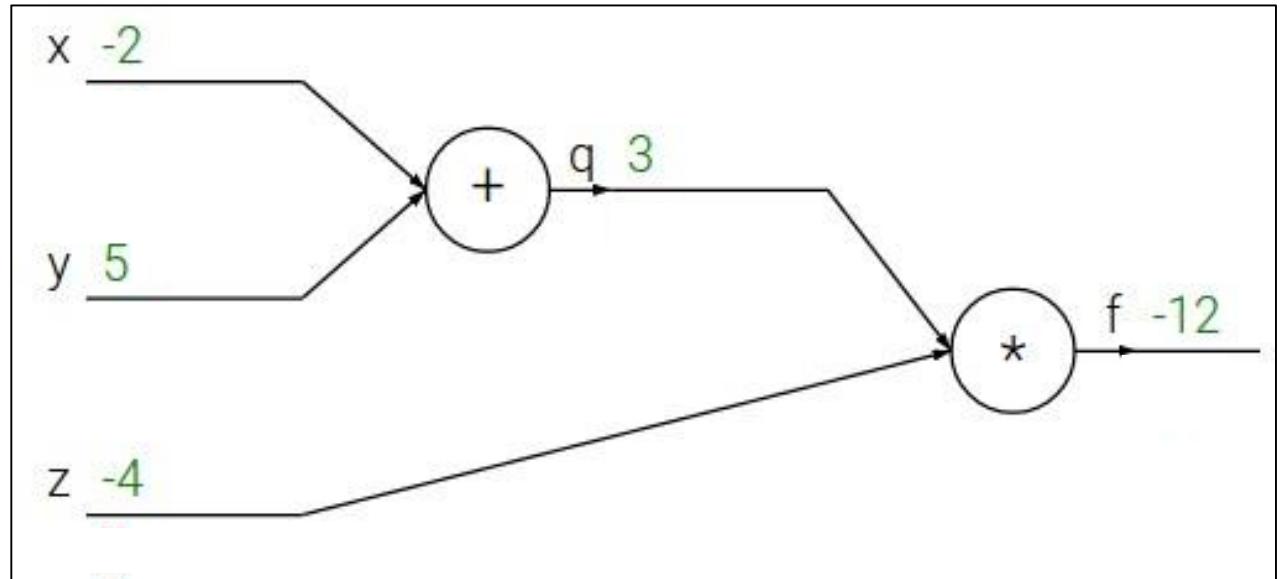
Backpropagation: Simple Example

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

1. Forward pass: Compute outputs

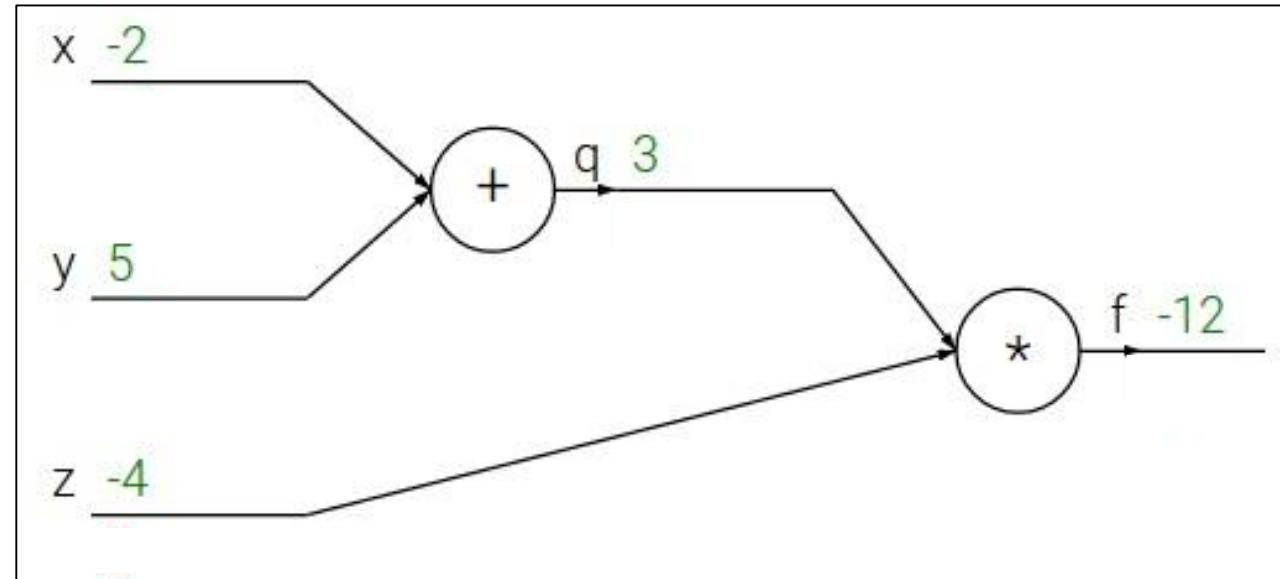
$$q = x + y \quad f = q \cdot z$$



Backpropagation: Simple Example

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

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



1. Forward pass: Compute outputs

$$q = x + y \quad f = q \cdot z$$

2. Backward pass: Compute derivatives

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

Backpropagation: Simple Example

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

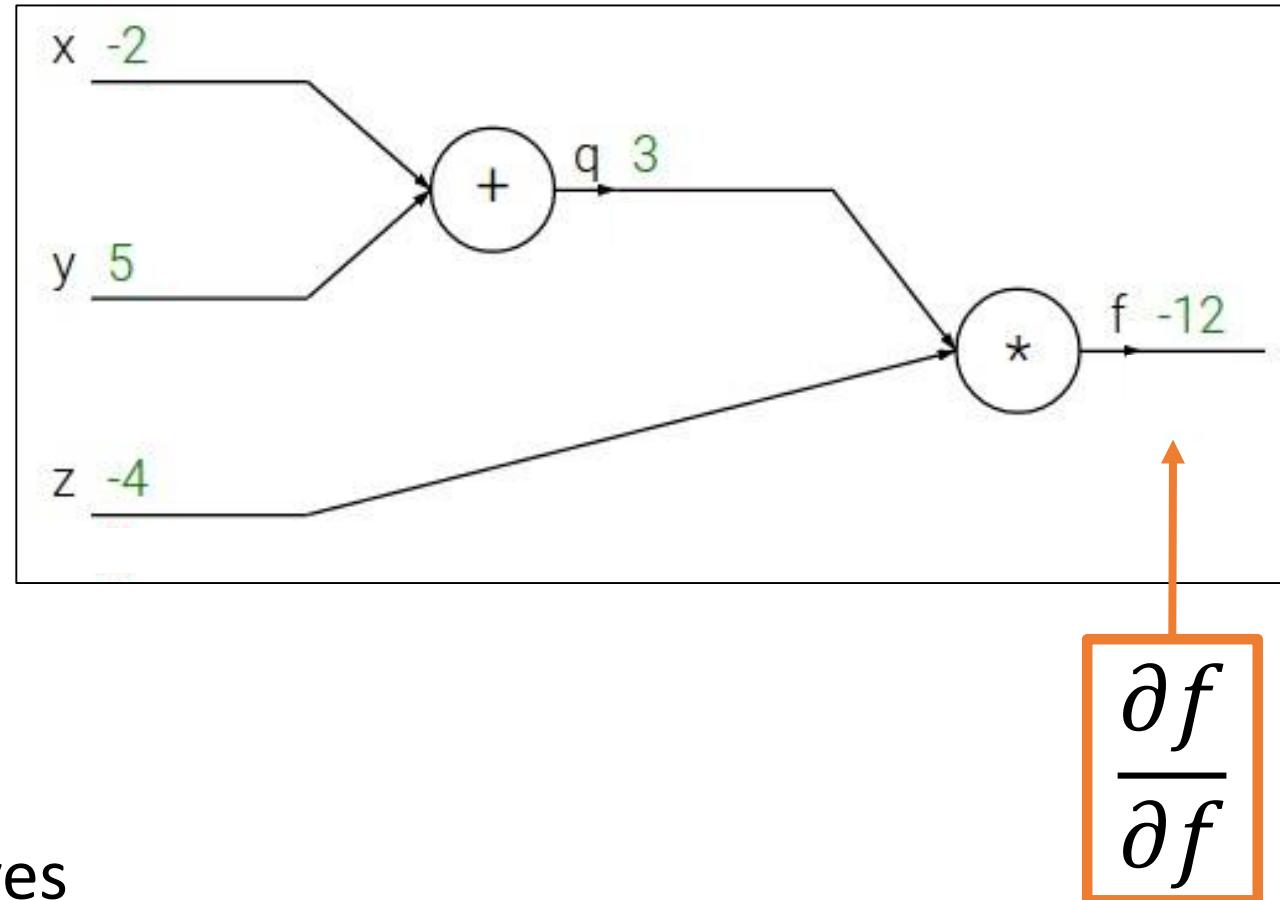
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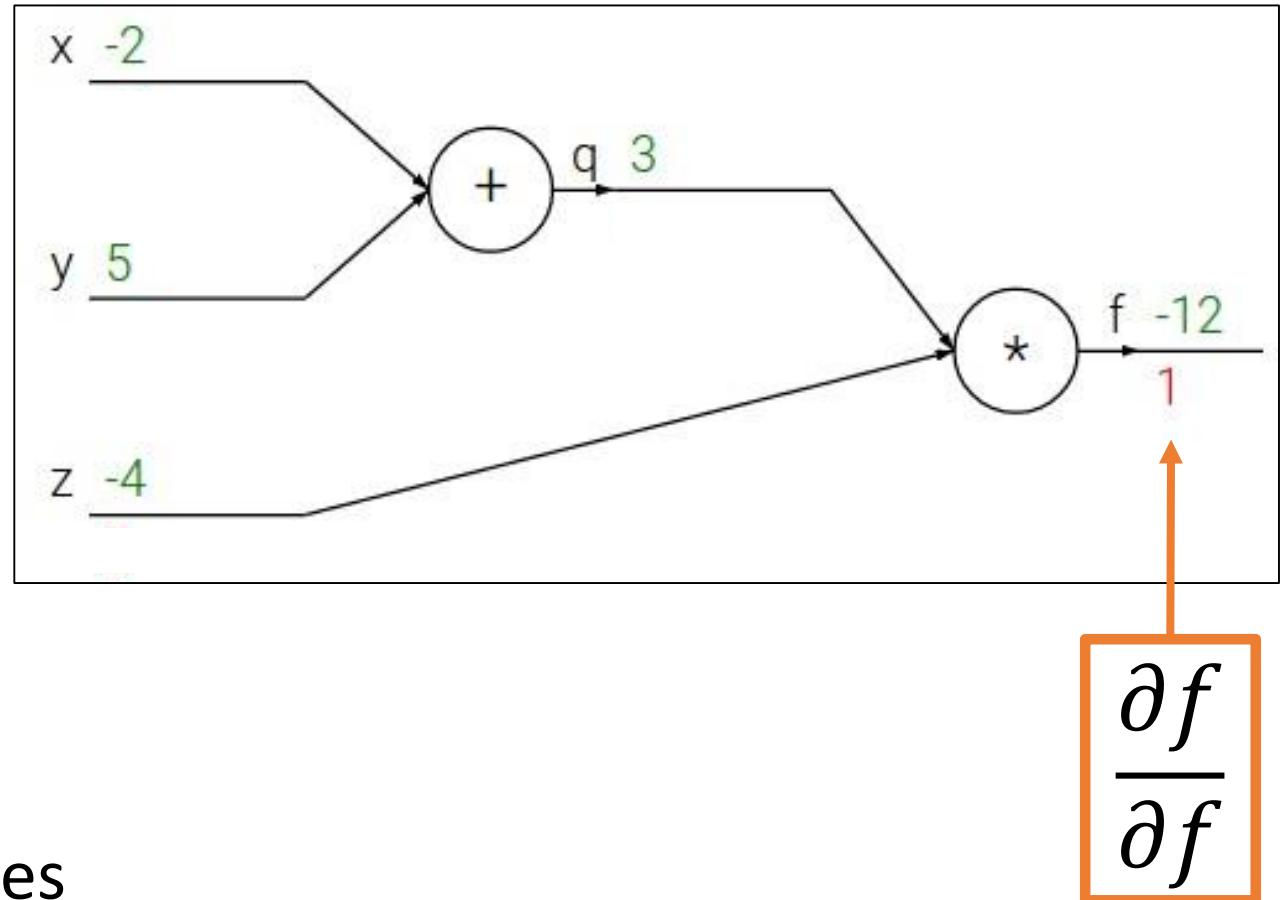
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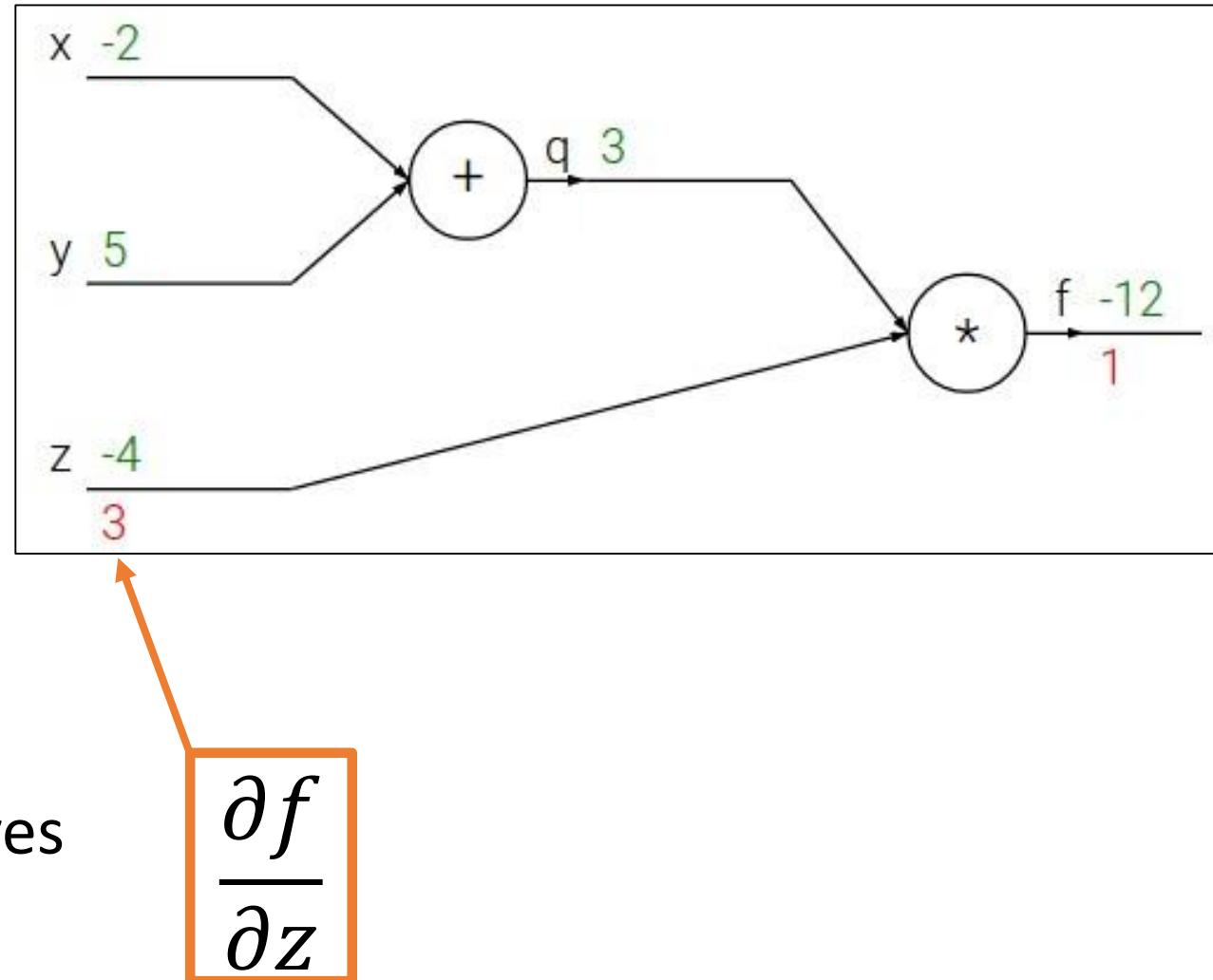
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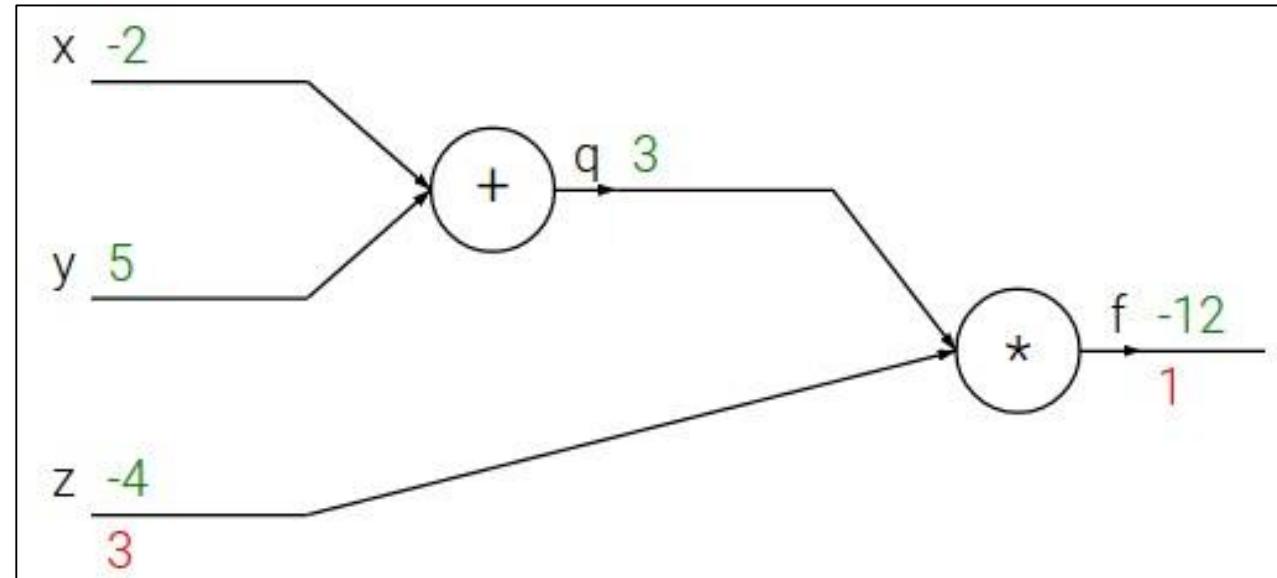
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$$q = x + y \quad f = q \cdot z$$

2. Backward pass: Compute derivatives

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



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

Backpropagation: Simple Example

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

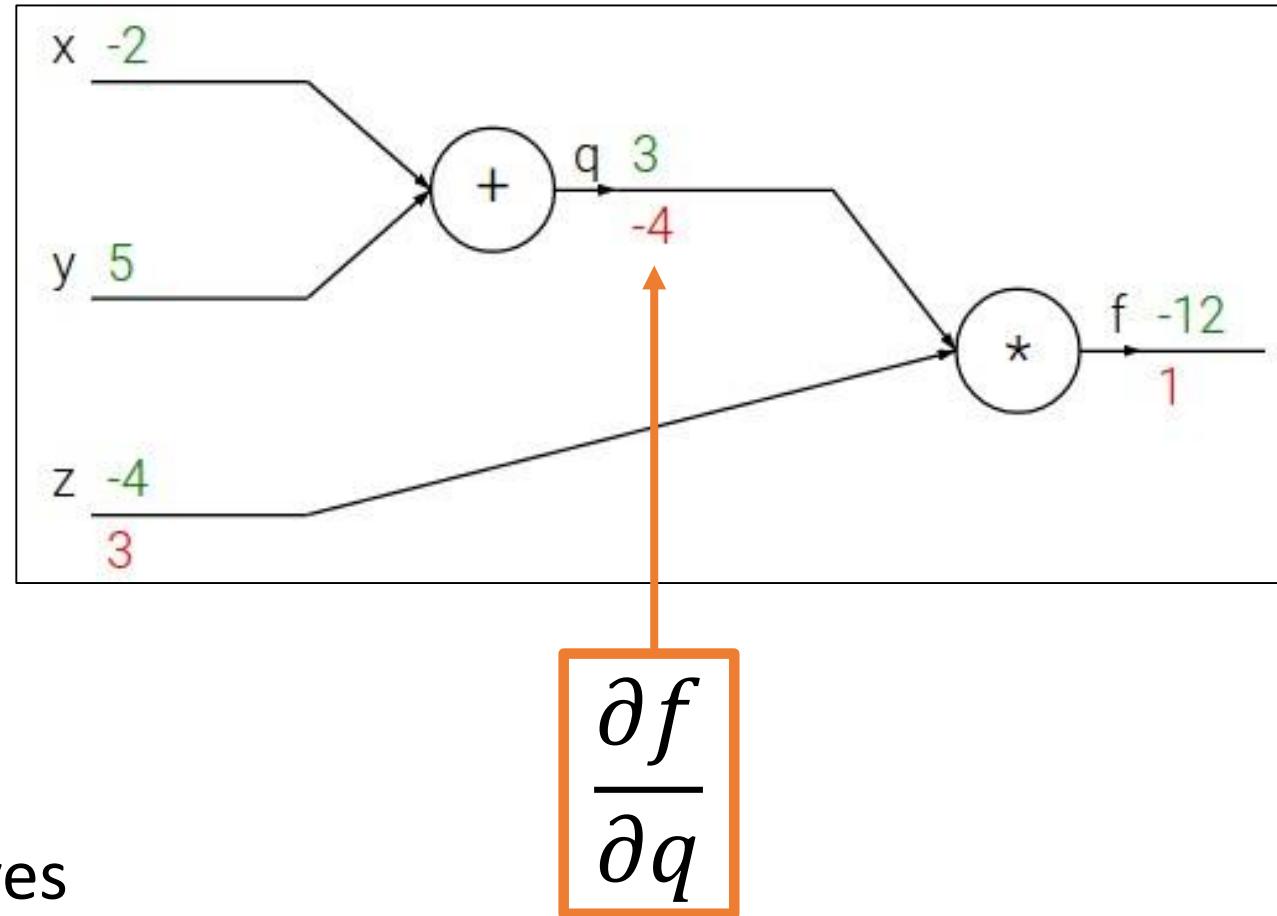
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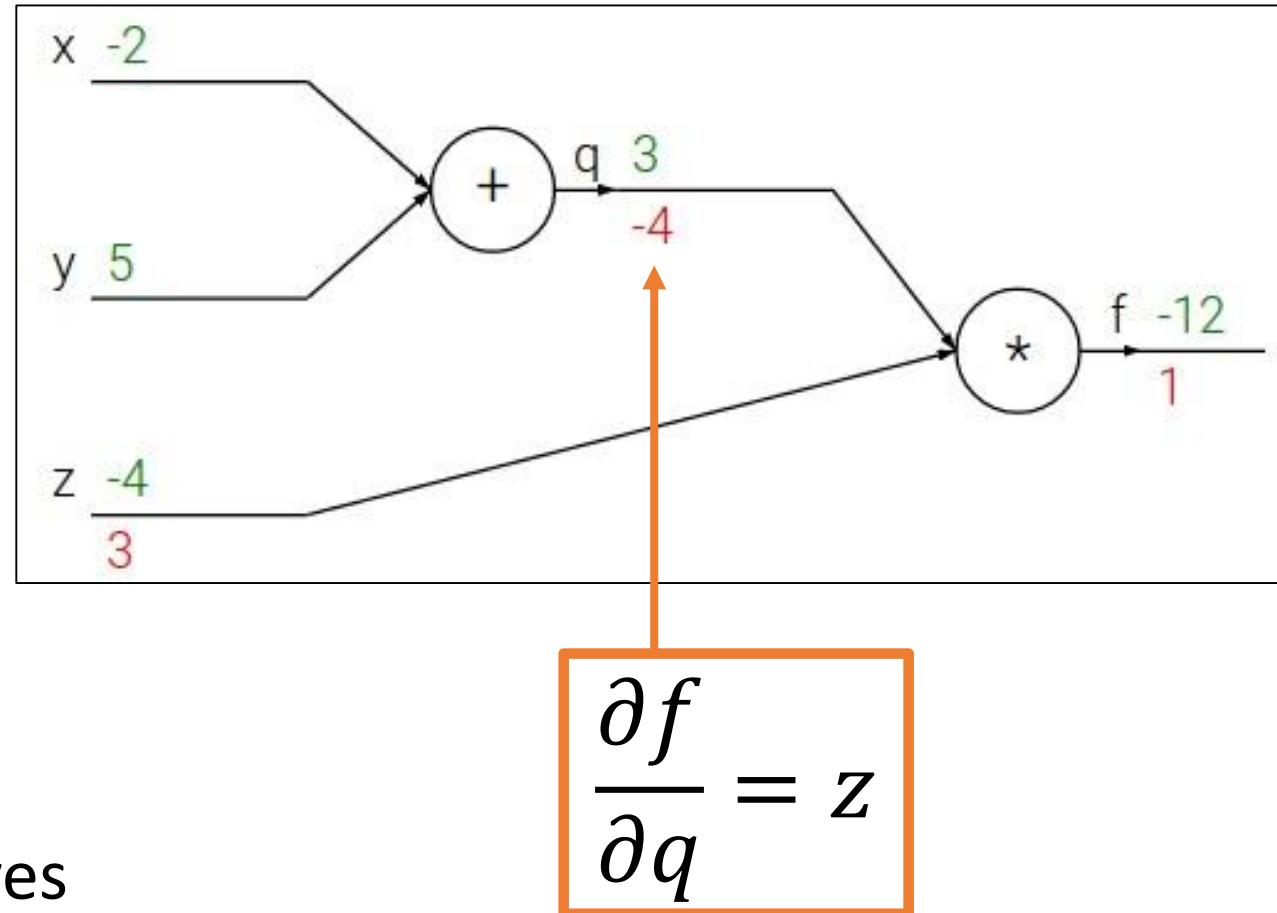
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Backpropagation: Simple Example

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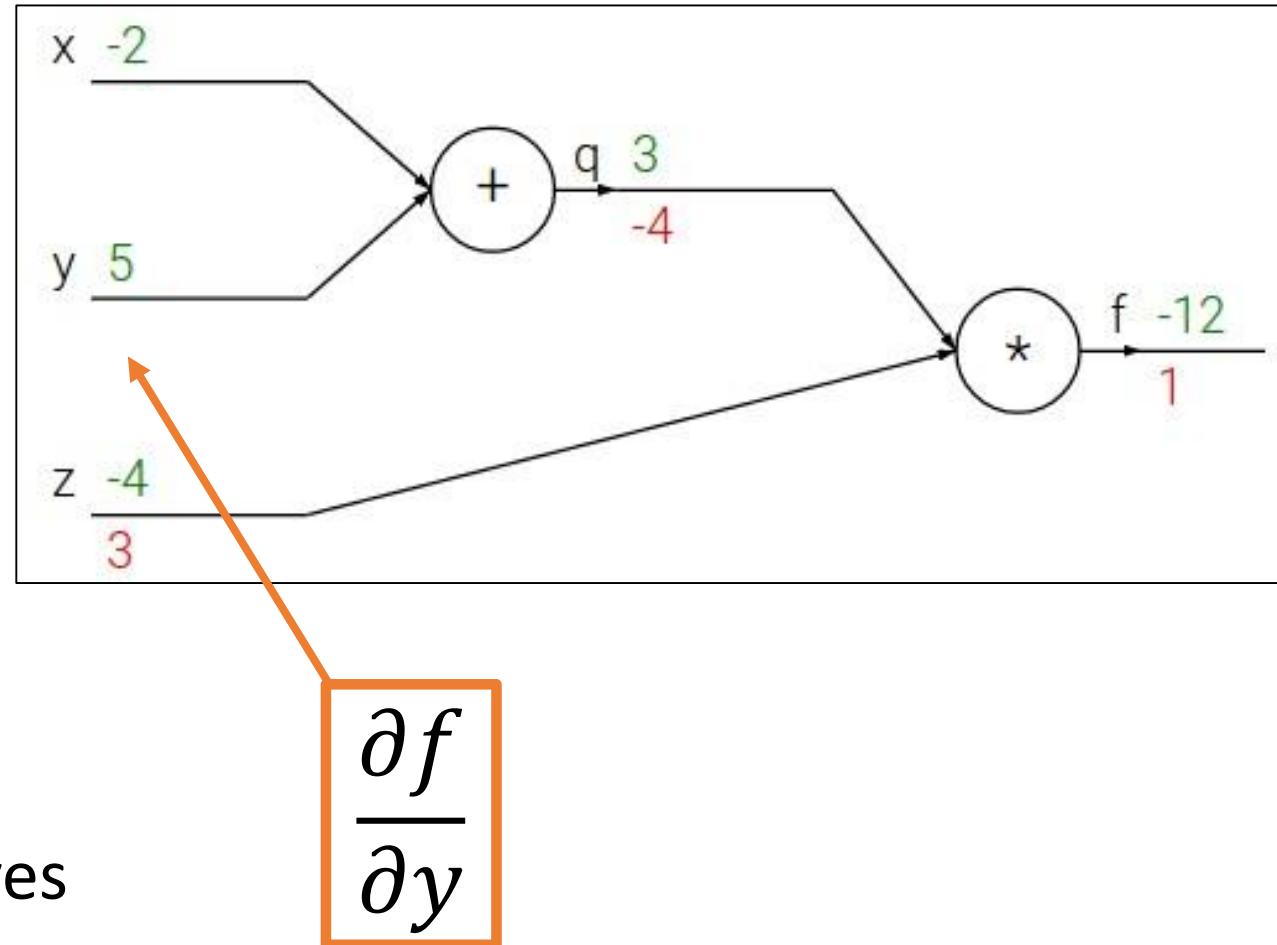
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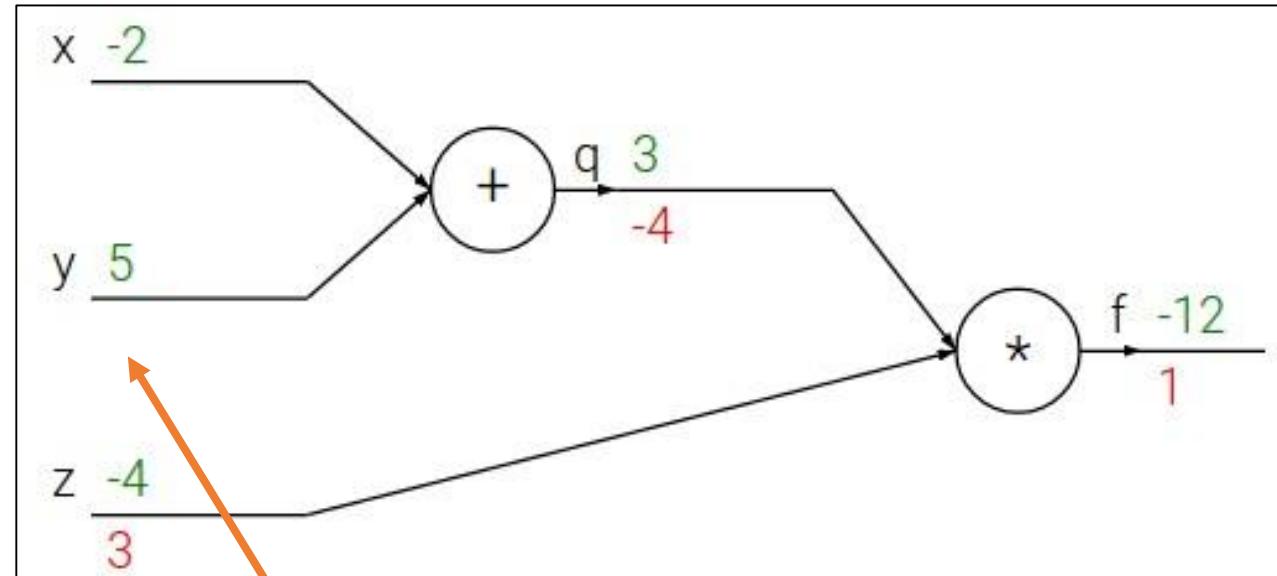
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2. Backward pass: Compute derivatives

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



Chain Rule

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

Backpropagation: Simple Example

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

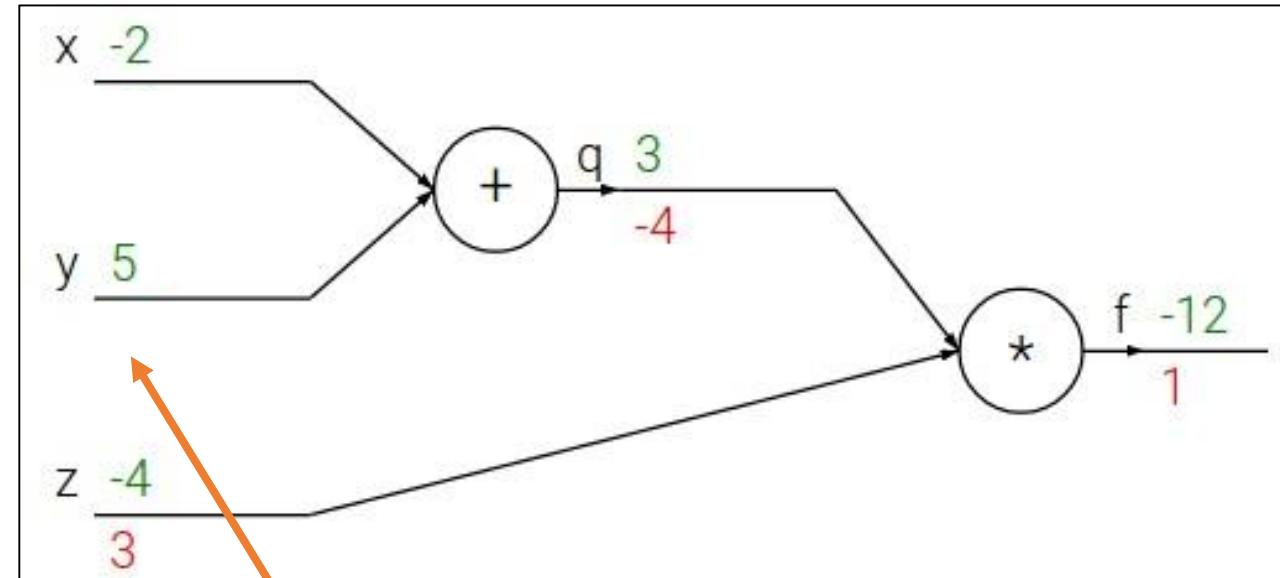
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Chain Rule

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

Downstream
Gradient

Local
Gradient

Upstream
Gradient

$$\frac{\partial q}{\partial y} = 1$$

Backpropagation: Simple Example

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

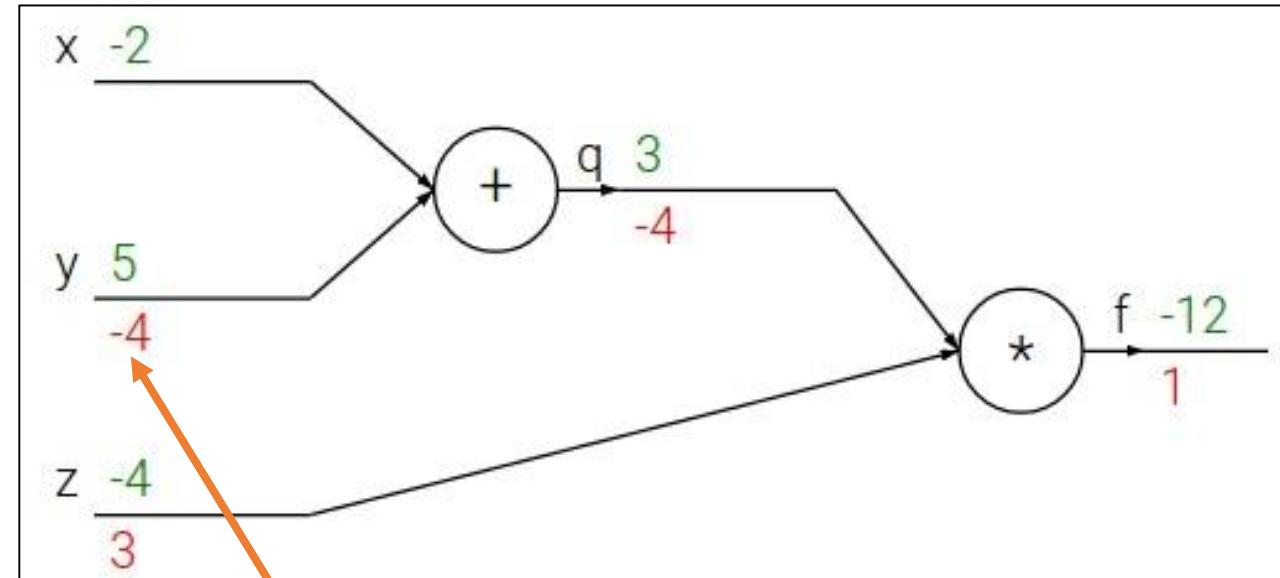
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$$\frac{\partial f}{\partial y} = \frac{\partial q}{\partial y} \frac{\partial f}{\partial q}$$

Downstream
Gradient

Local
Gradient

Upstream
Gradient

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Backpropagation: Simple Example

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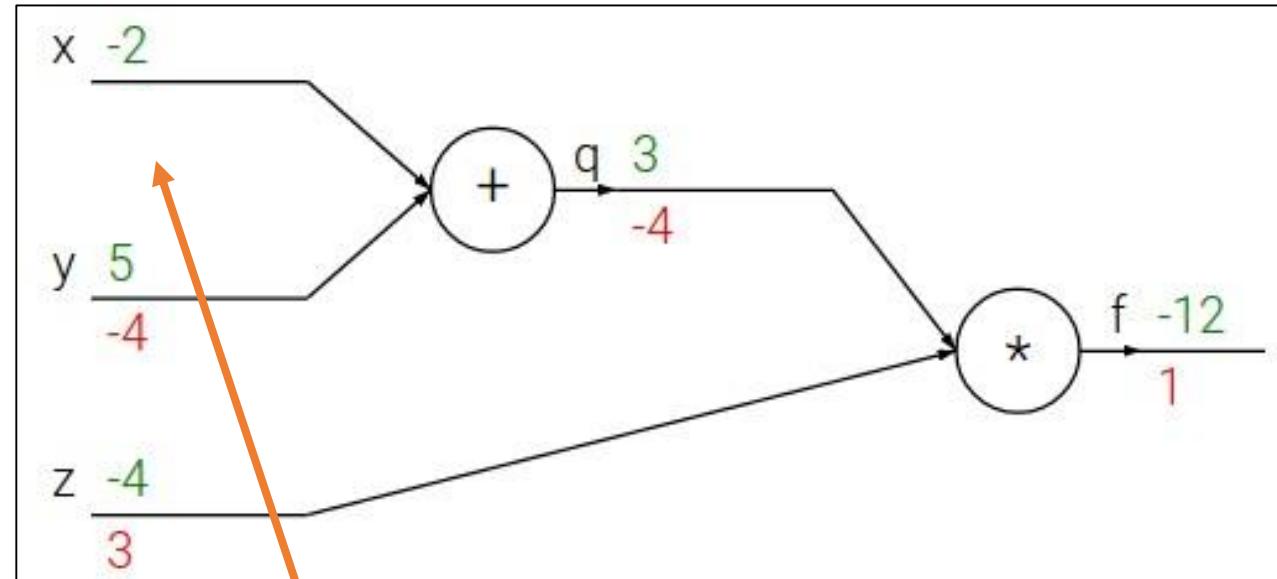
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Gradient

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Gradient

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Backpropagation: Simple Example

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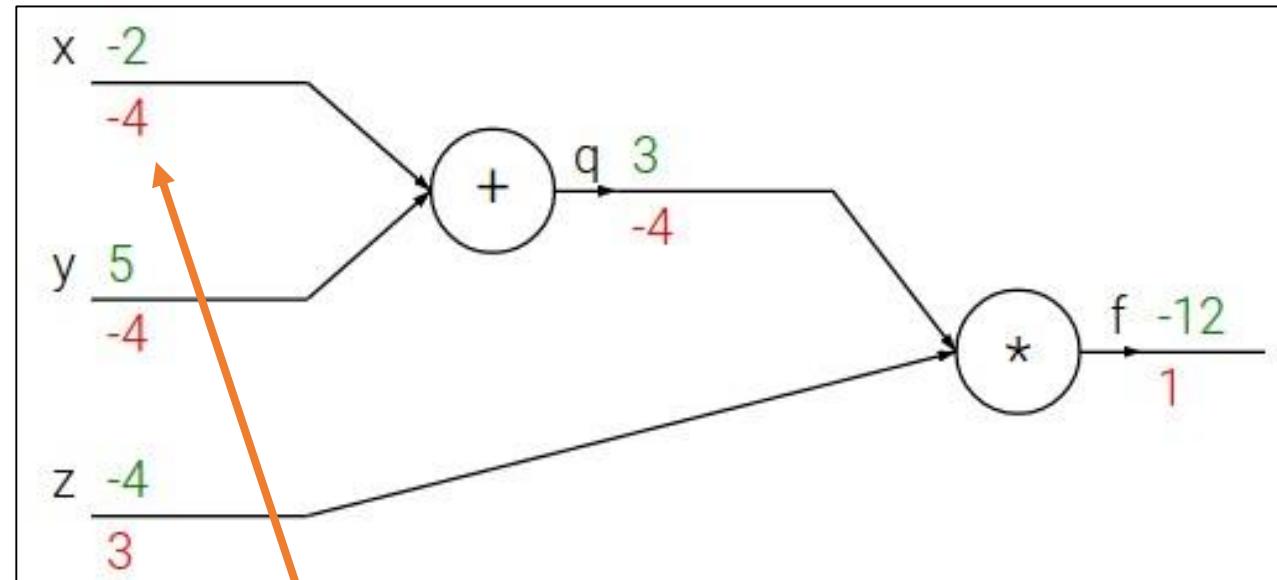
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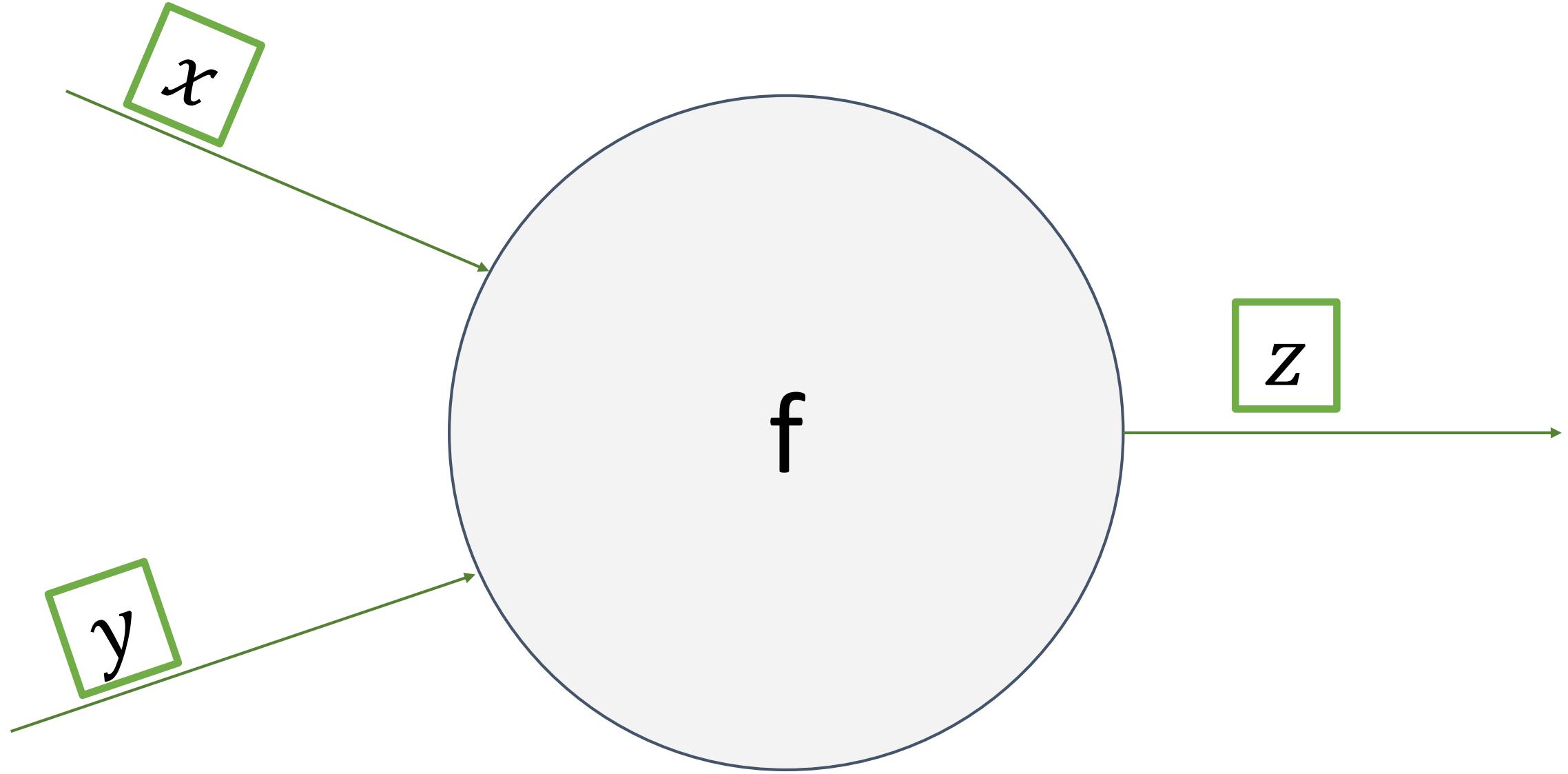
Chain Rule

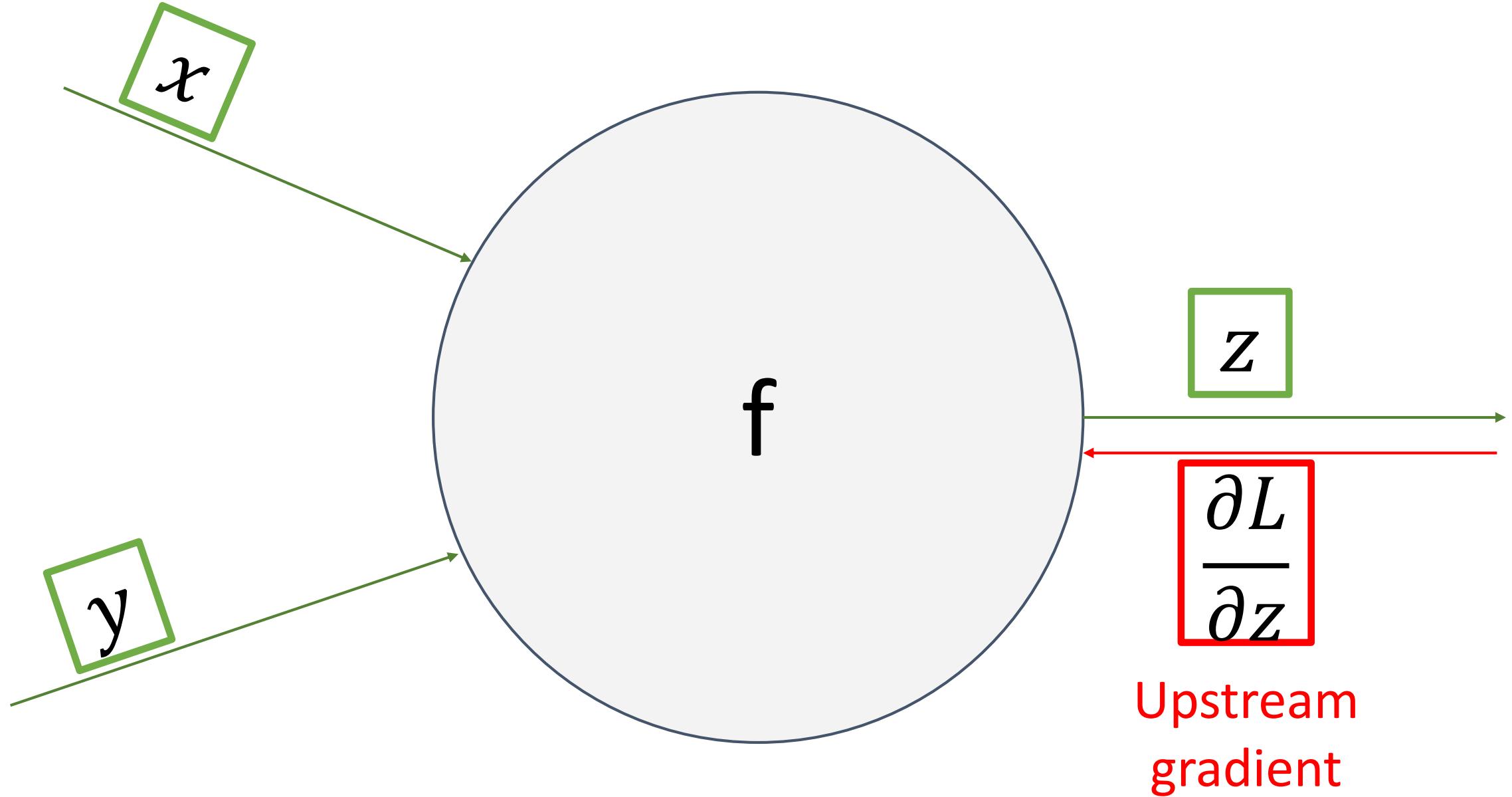
$$\frac{\partial f}{\partial x} = \frac{\partial q}{\partial x} \frac{\partial f}{\partial q}$$

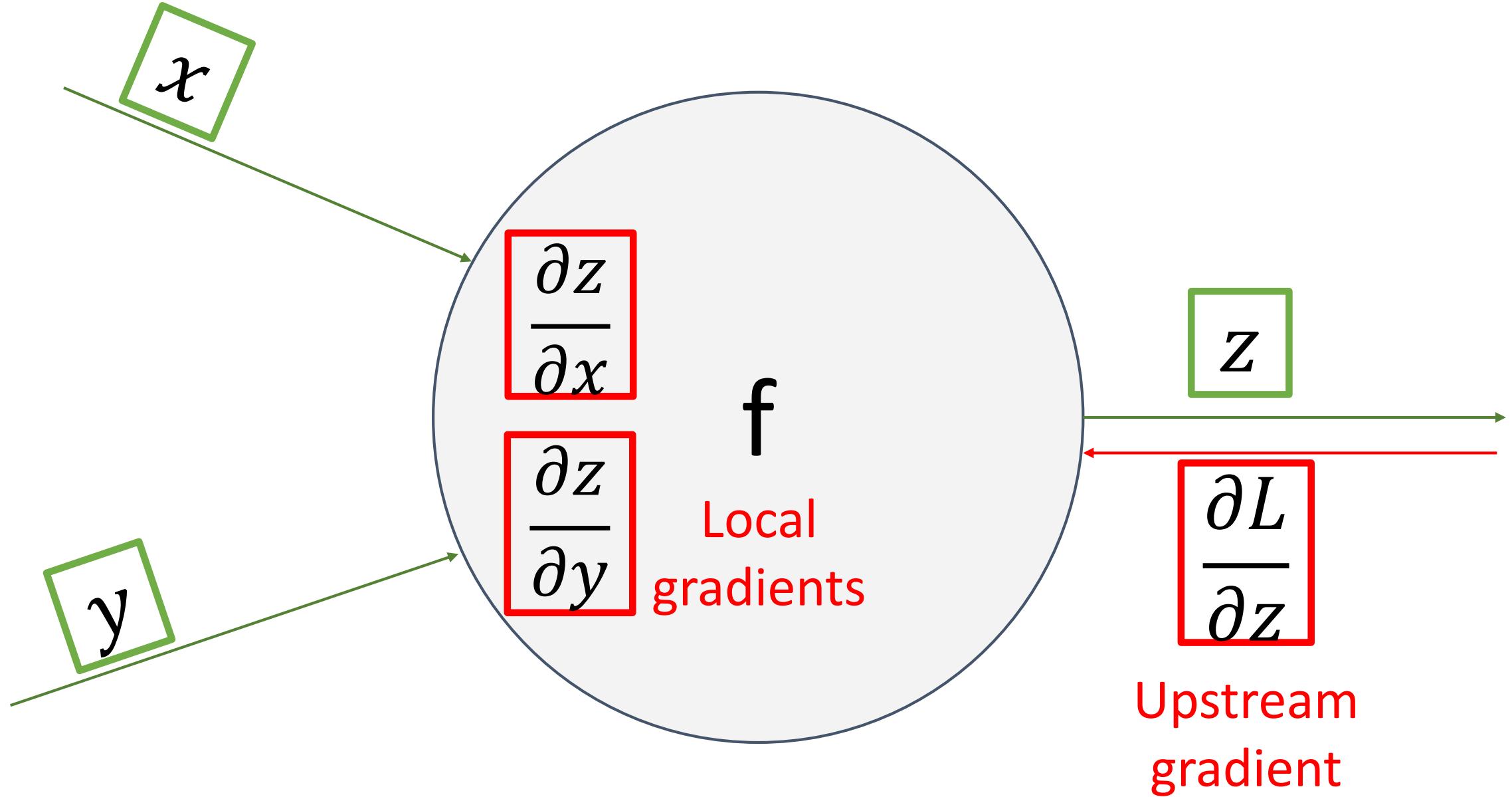
Downstream
Gradient

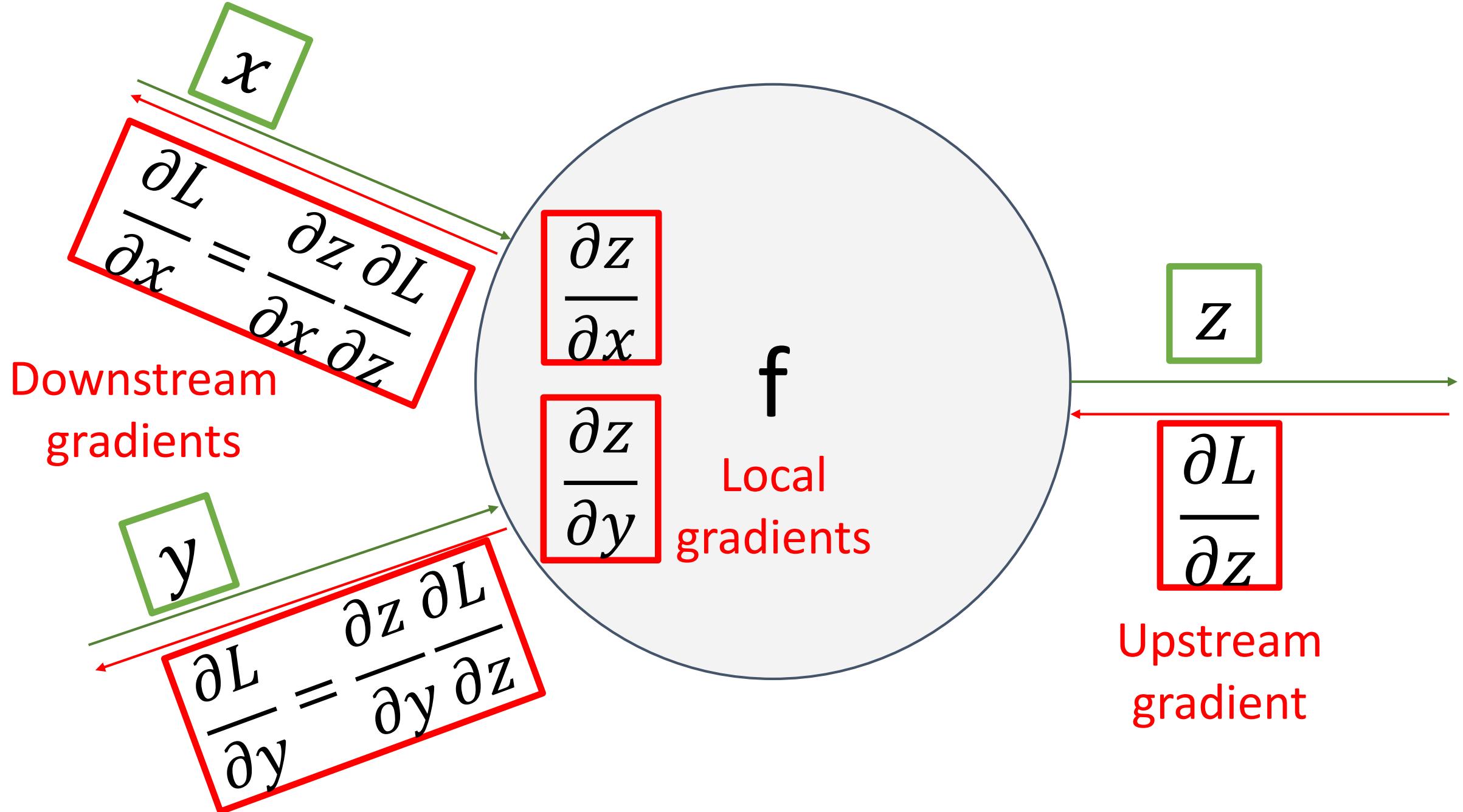
Local
Gradient

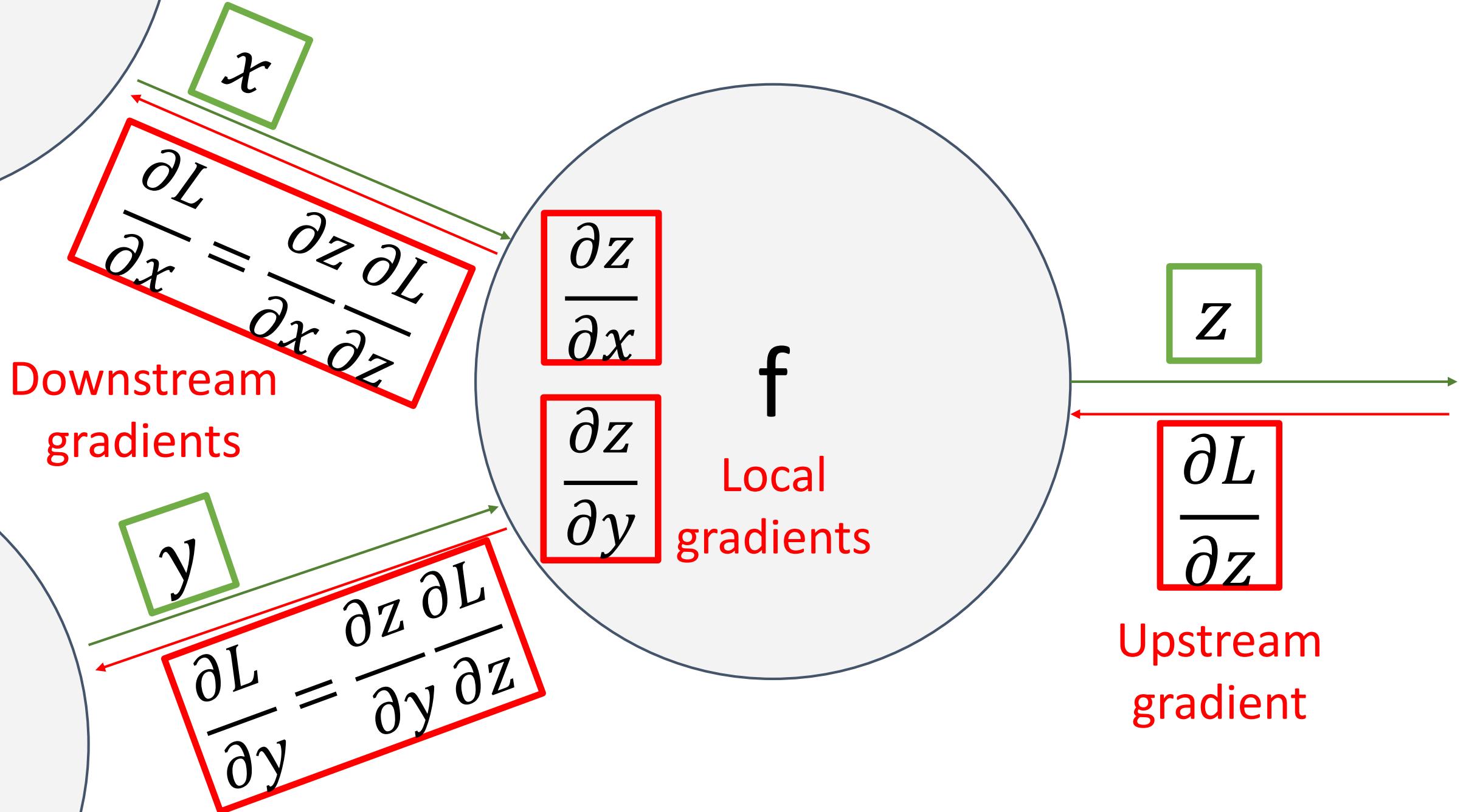
Upstream
Gradient



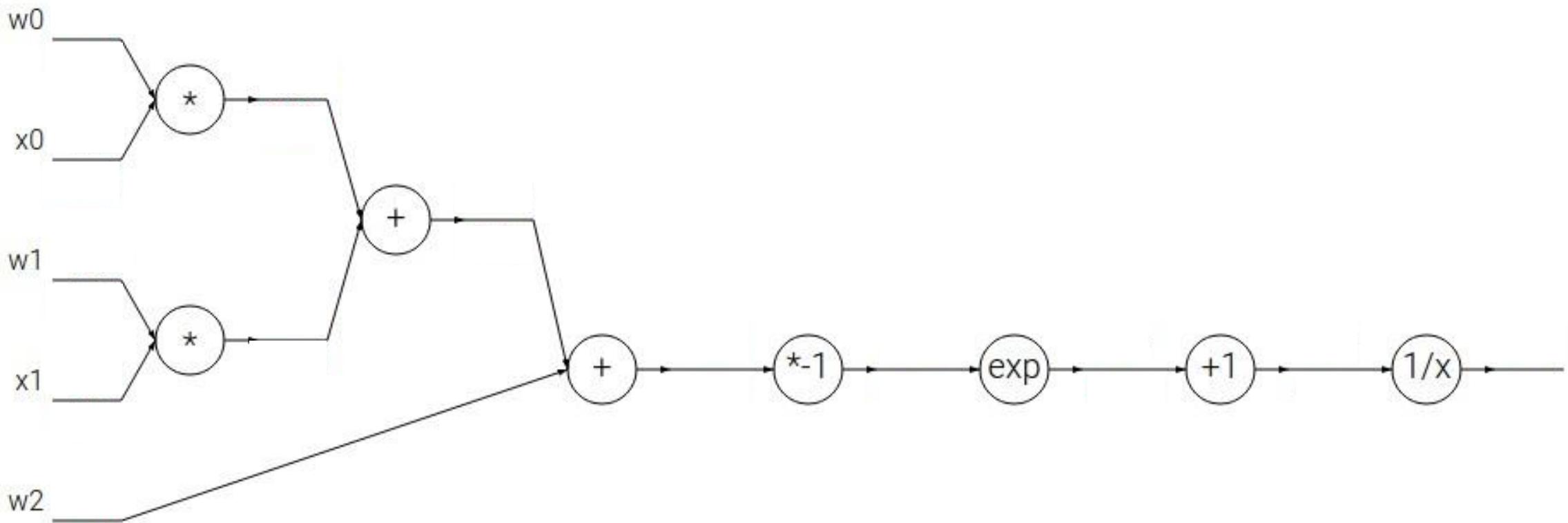








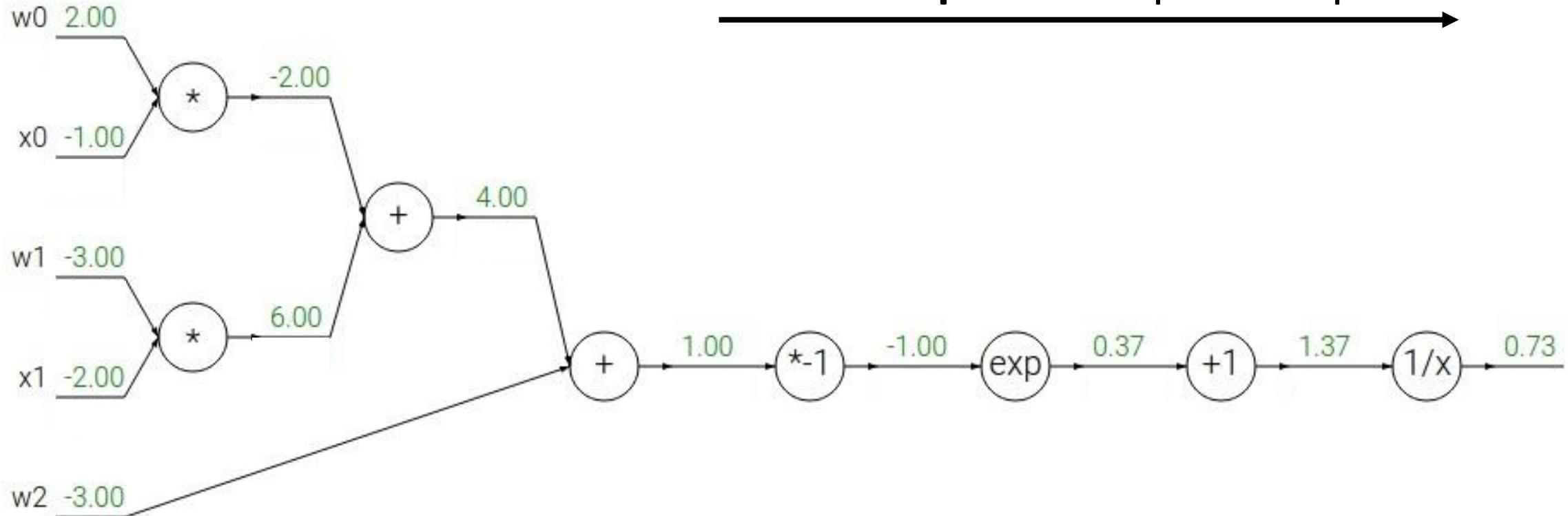
Another Example $f(x, w) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}}$



Another Example

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

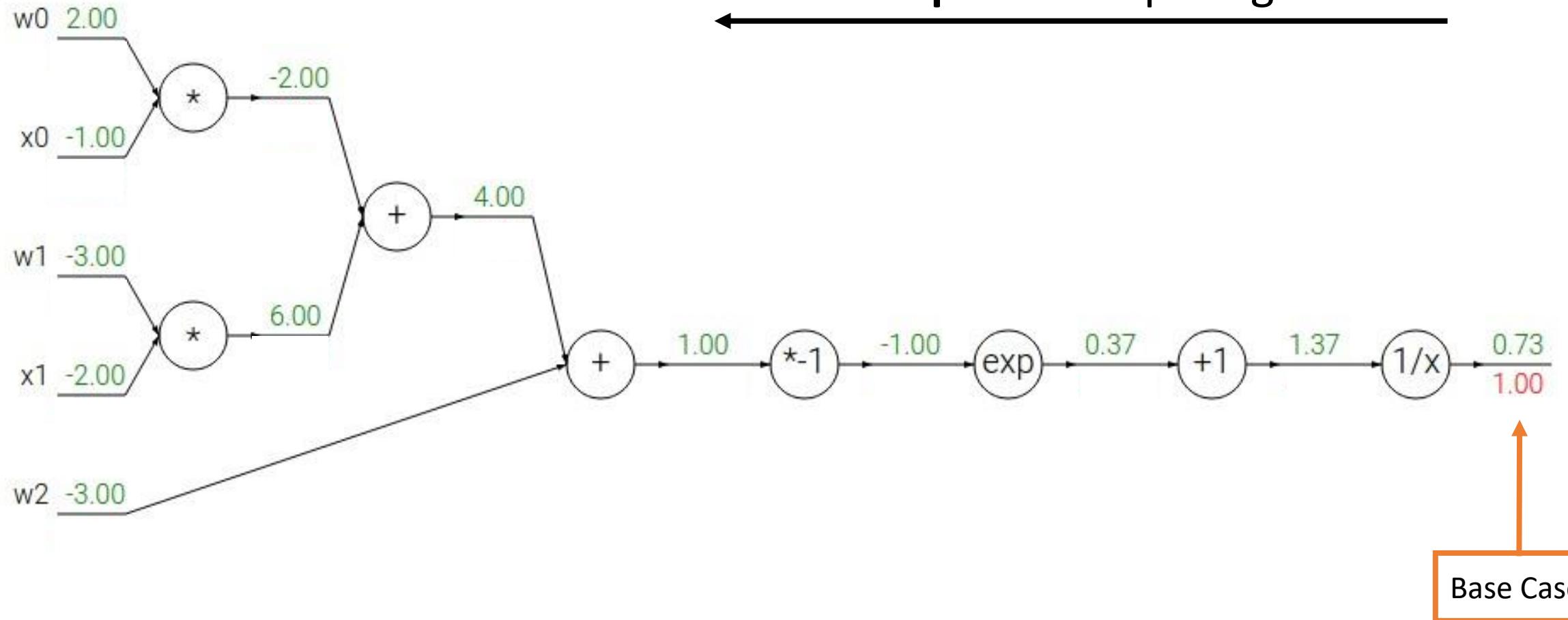
Forward pass: Compute outputs



Another Example

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

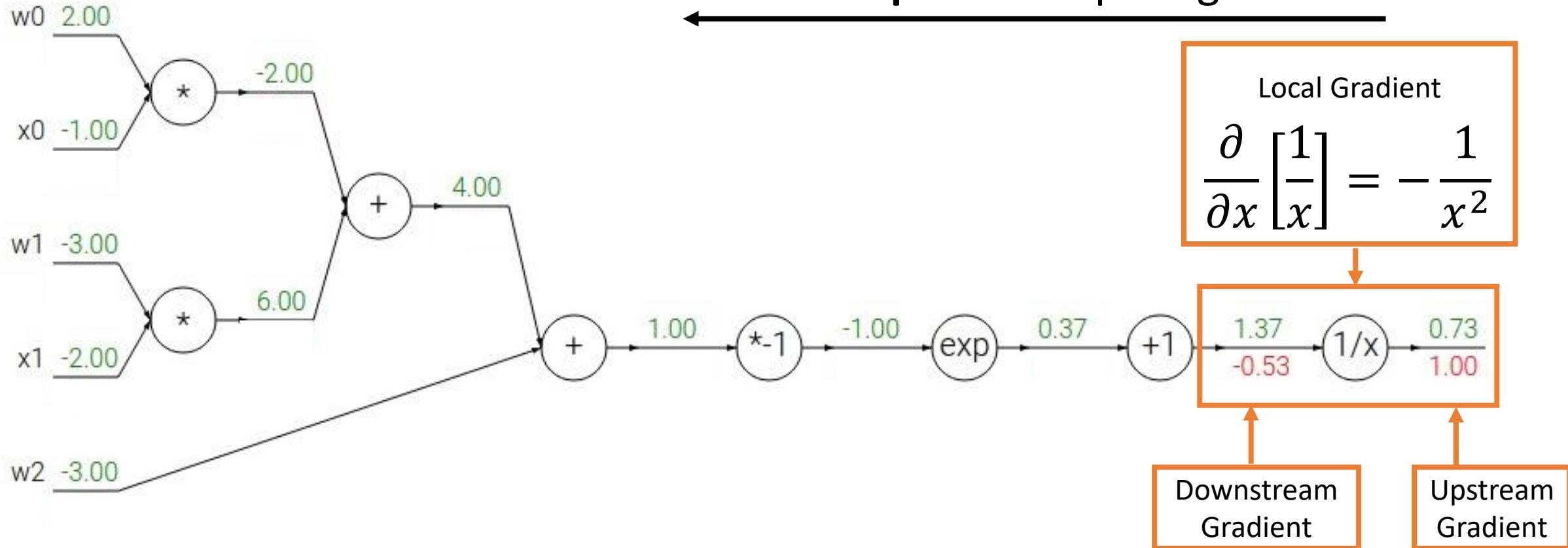
Backward pass: Compute gradients



Another Example

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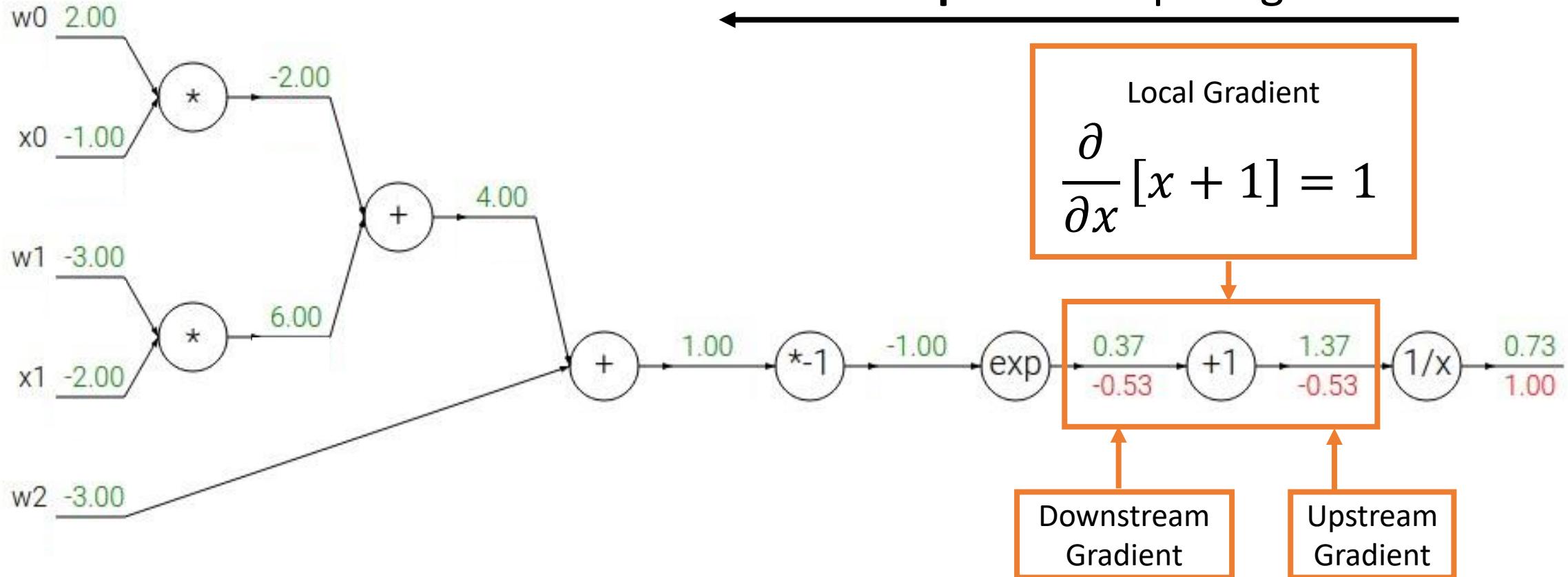
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Another Example

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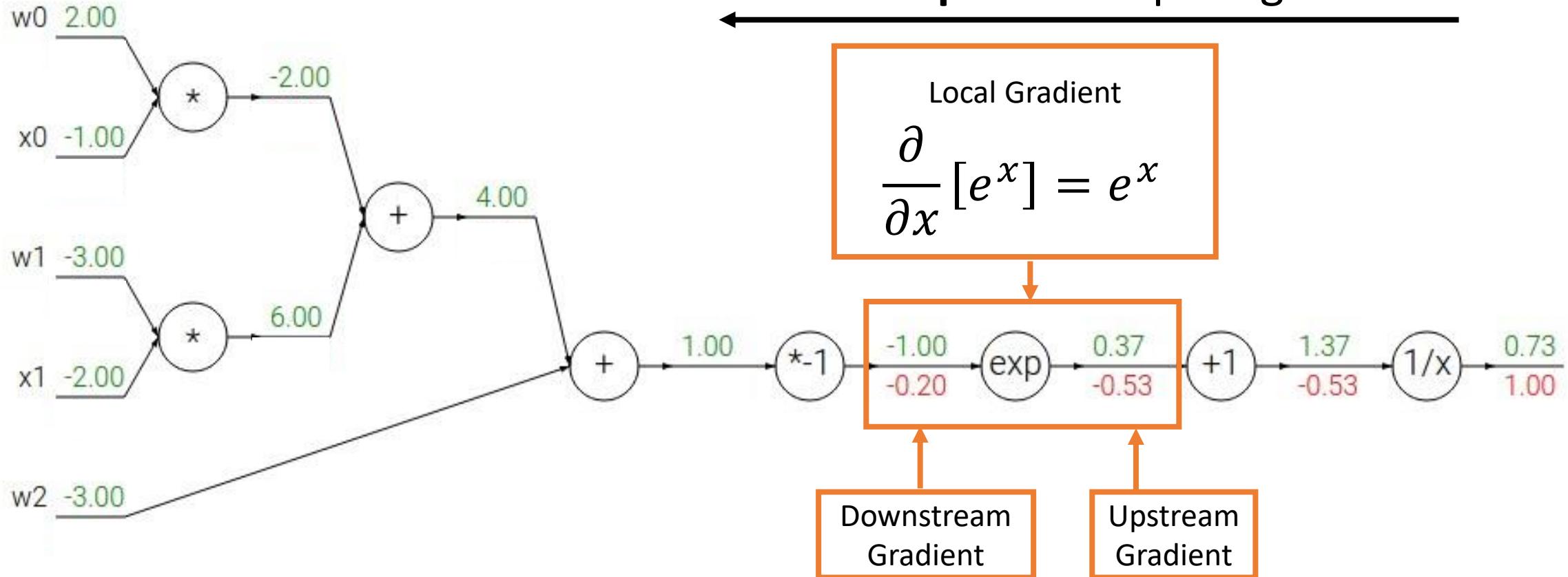
Backward pass: Compute gradients



Another Example

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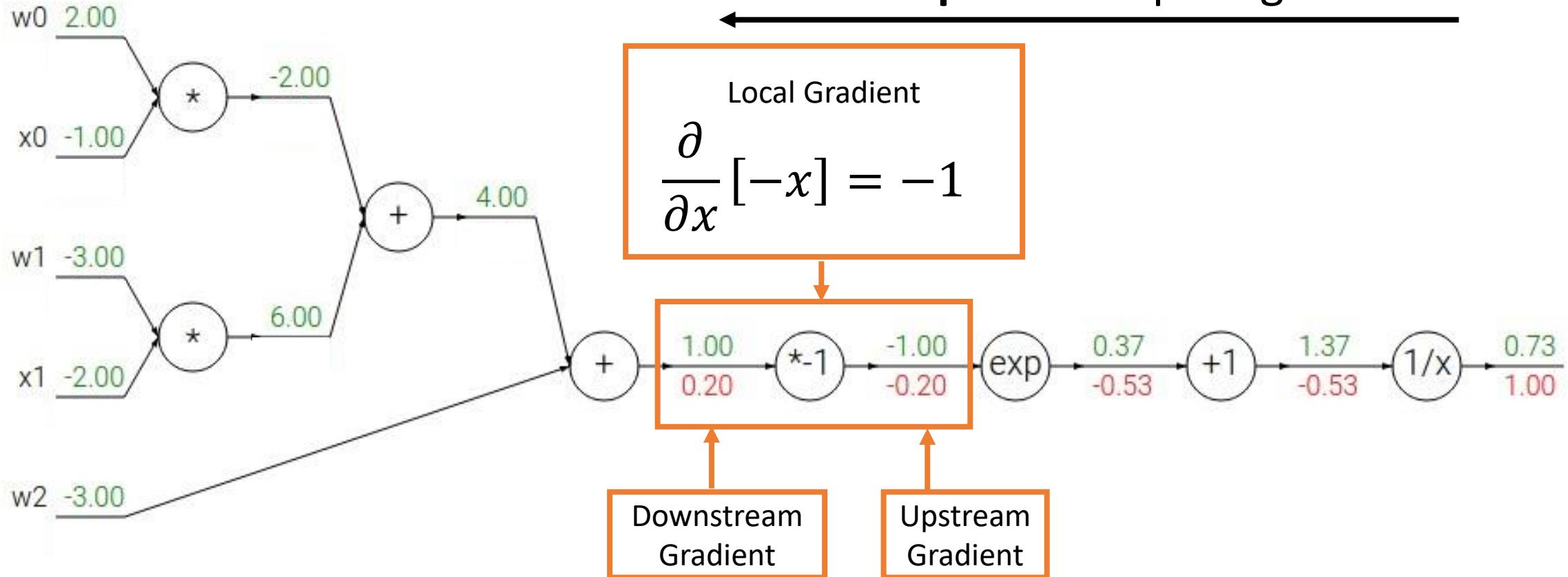
Backward pass: Compute gradients



Another Example

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

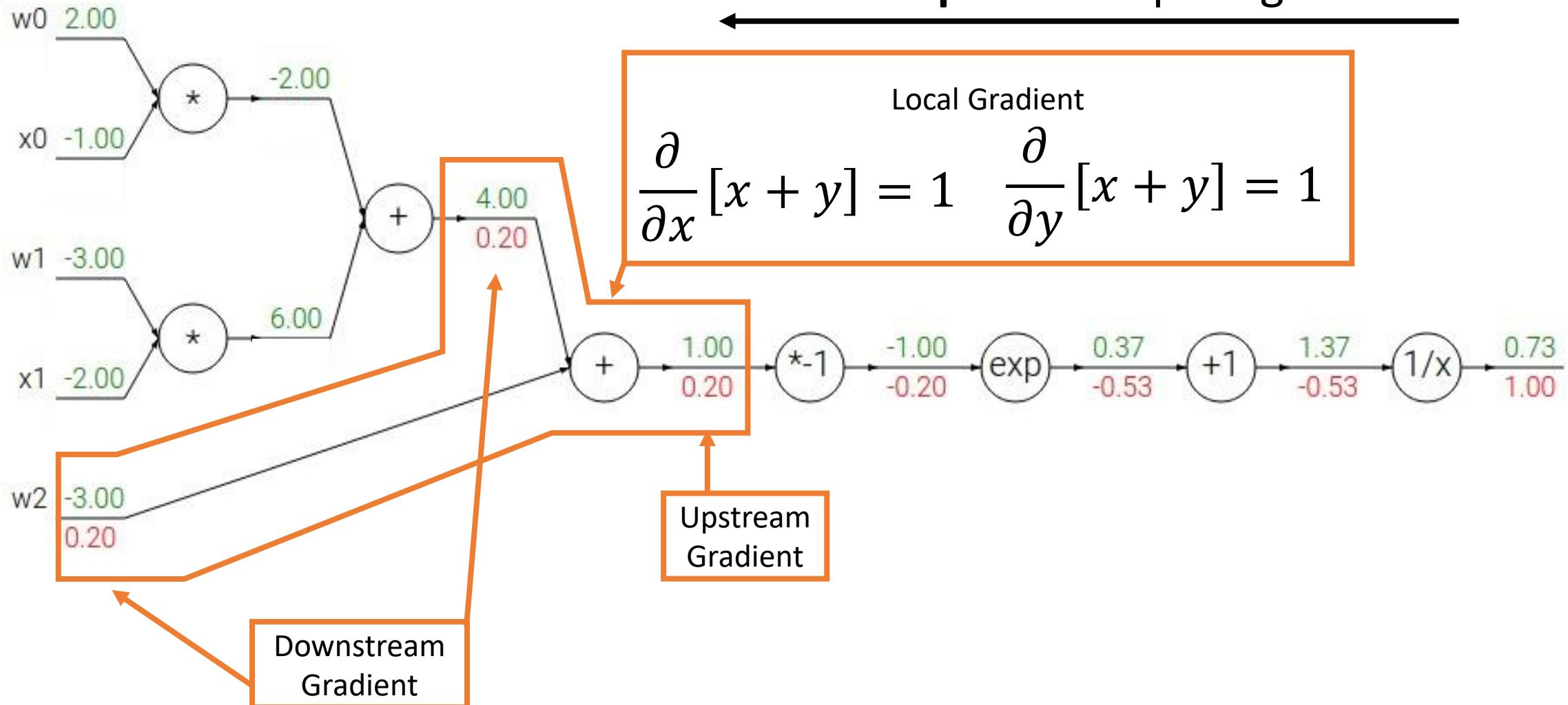
Backward pass: Compute gradients



Another Example

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

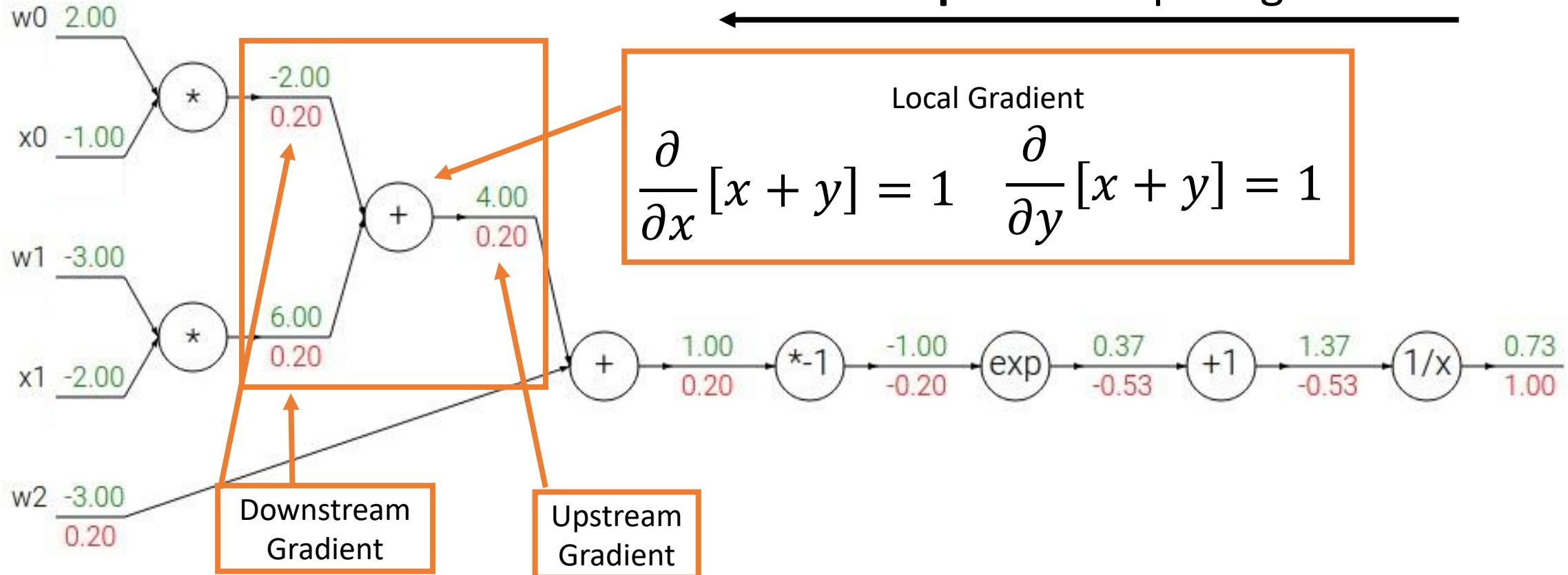
Backward pass: Compute gradients



Another Example

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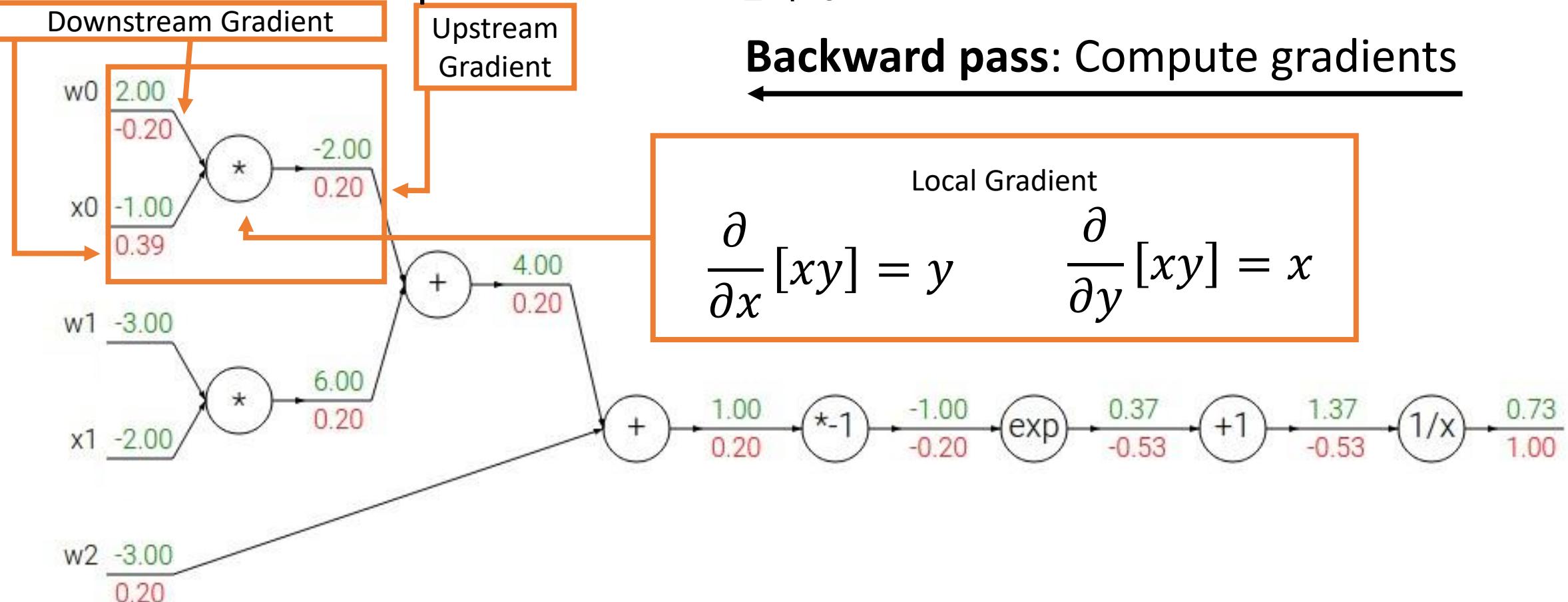
Backward pass: Compute gradients



Another Example

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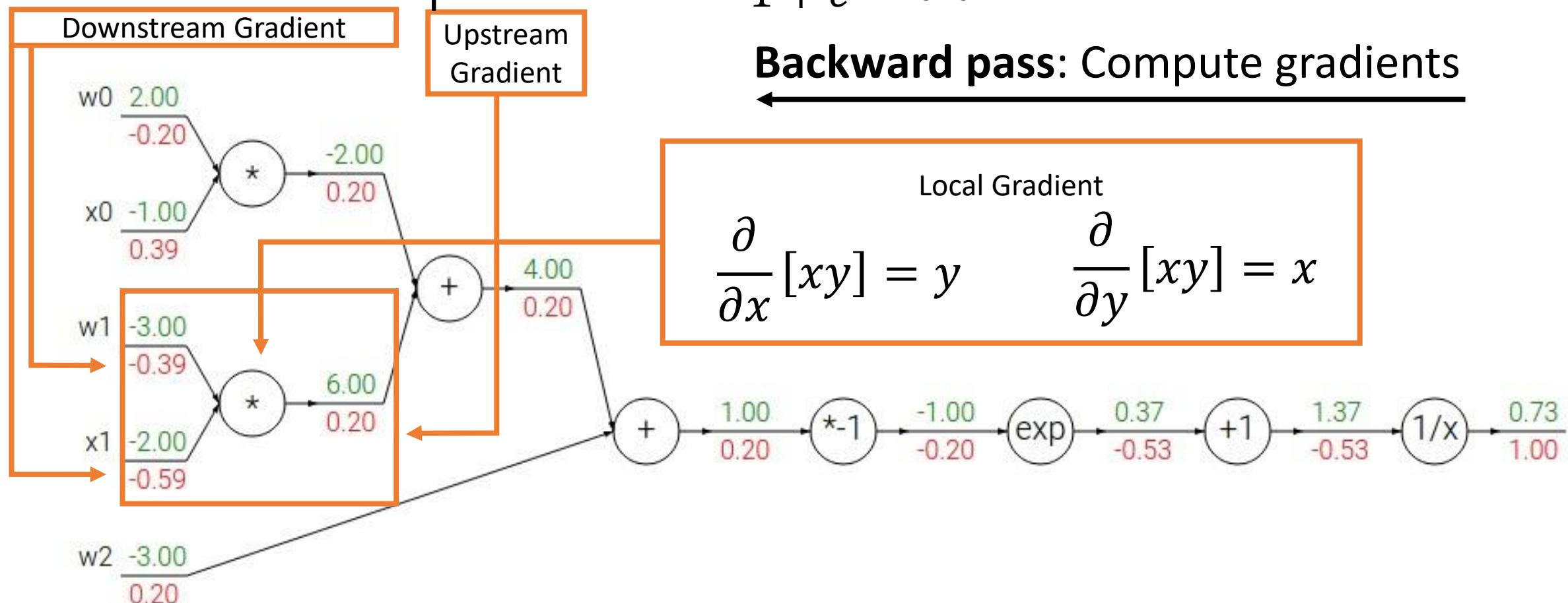
Backward pass: Compute gradients



Another Example

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

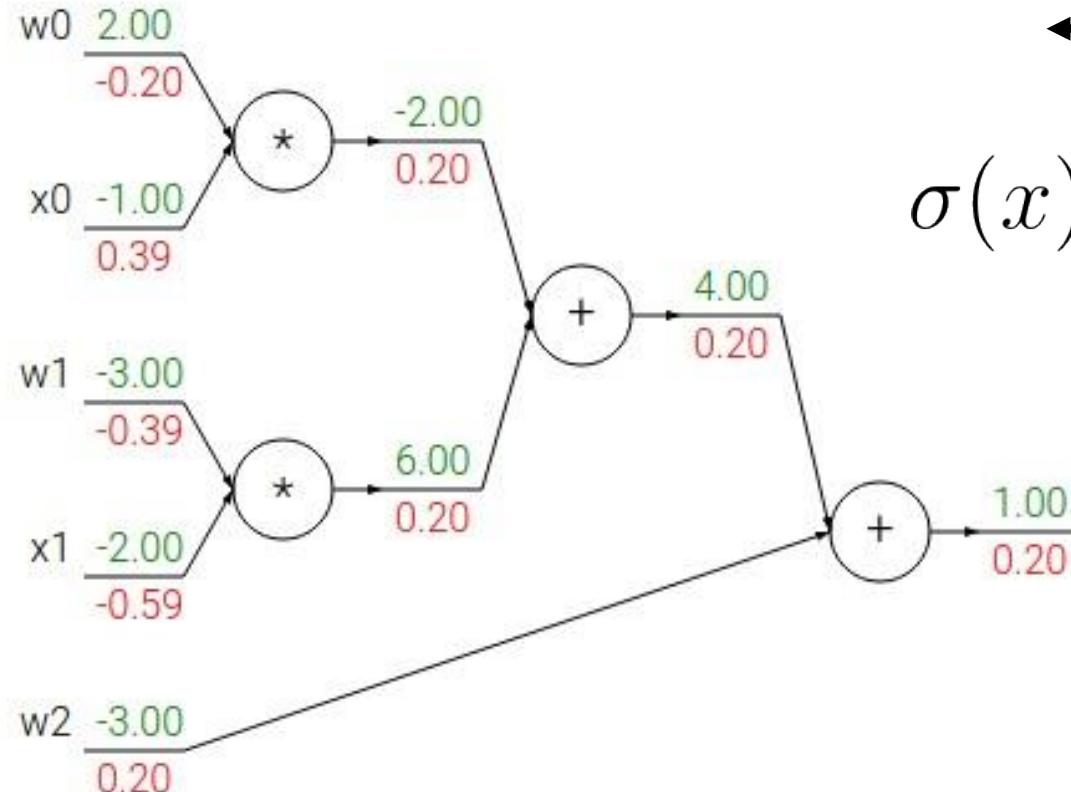
Backward pass: Compute gradients



Another Example

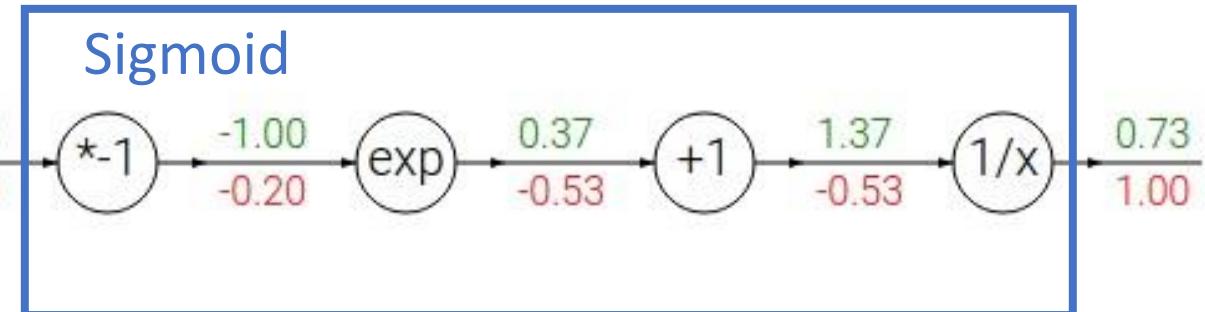
$$f(x, w) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}} = \sigma(w_0x_0 + w_1x_1 + w_2)$$

Backward pass: Compute gradients



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

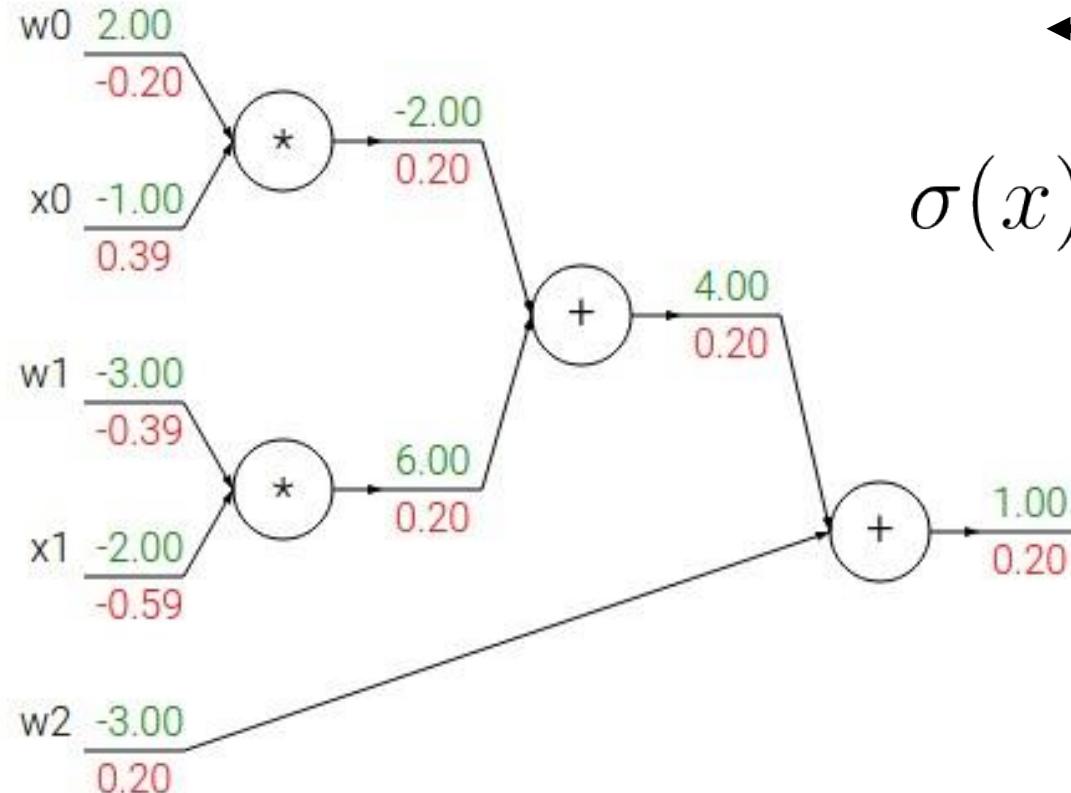
Computational graph is not unique: we can use primitives that have simple local gradients



Another Example

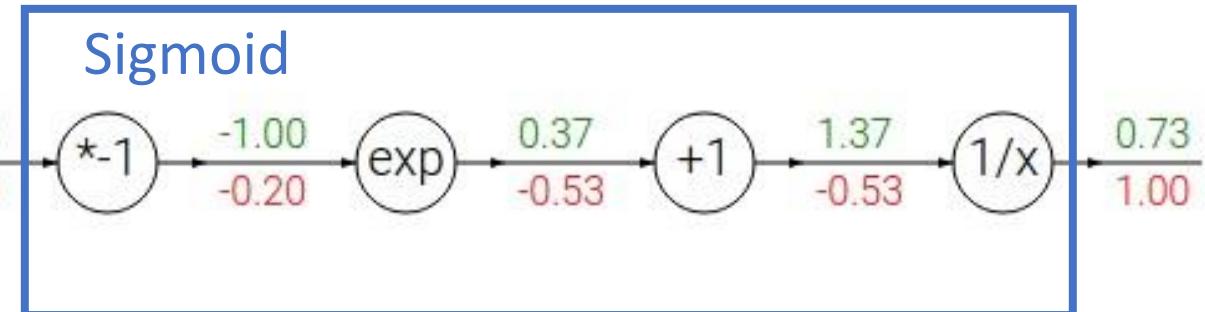
$$f(x, w) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}} = \sigma(w_0x_0 + w_1x_1 + w_2)$$

Backward pass: Compute gradients



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

Computational graph is not unique: we can use primitives that have simple local gradients

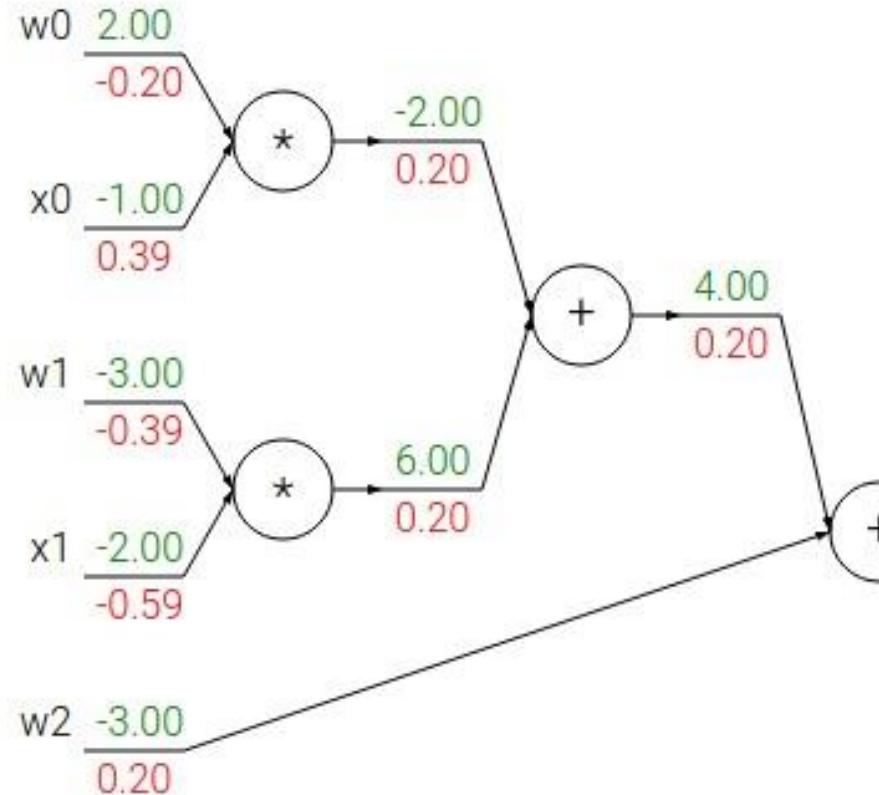


Sigmoid local gradient: $\frac{\partial}{\partial x} [\sigma(x)] = \frac{e^{-x}}{(1 + e^{-x})^2} = \left(\frac{1 + e^{-x} - 1}{1 + e^{-x}} \right) \left(\frac{1}{1 + e^{-x}} \right) = (1 - \sigma(x))\sigma(x)$

Another Example

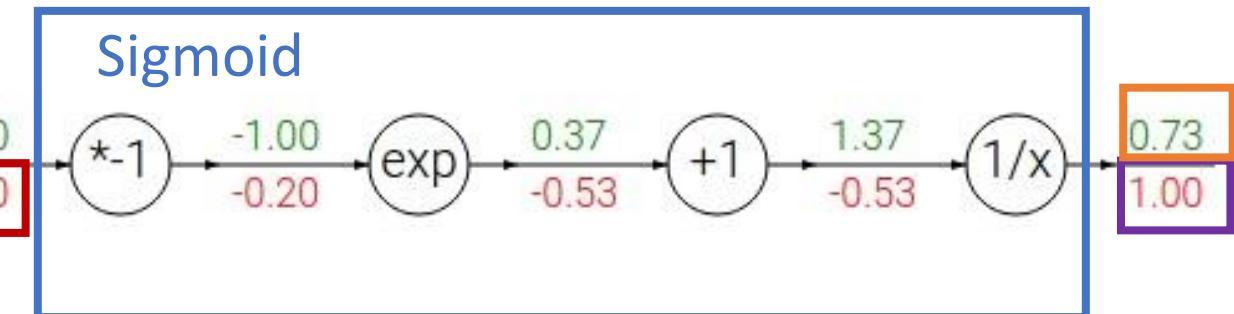
$$f(x, w) = \frac{1}{1 + e^{-(w_0x_0 + w_1x_1 + w_2)}} = \sigma(w_0x_0 + w_1x_1 + w_2)$$

Backward pass: Compute gradients



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

Computational graph is not unique: we can use primitives that have simple local gradients

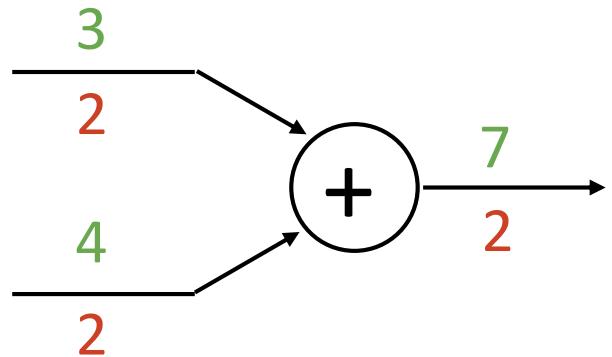


$$\begin{aligned} [\text{Downstream}] &= [\text{Local}] * [\text{Upstream}] \\ &= (1 - 0.73) * 0.73 * 1.0 = 0.2 \end{aligned}$$

Sigmoid local gradient: $\frac{\partial}{\partial x} [\sigma(x)] = \frac{e^{-x}}{(1 + e^{-x})^2} = \left(\frac{1 + e^{-x} - 1}{1 + e^{-x}} \right) \left(\frac{1}{1 + e^{-x}} \right) = (1 - \sigma(x))\sigma(x)$

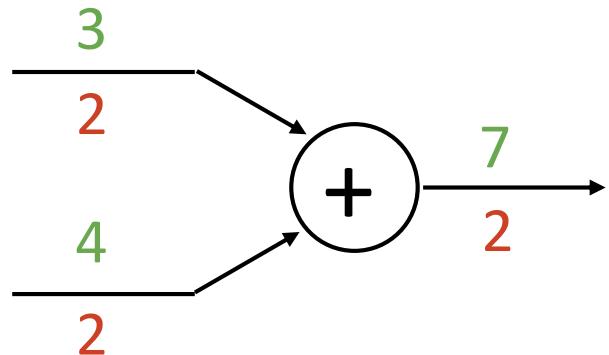
Patterns in Gradient Flow

add gate: gradient distributor

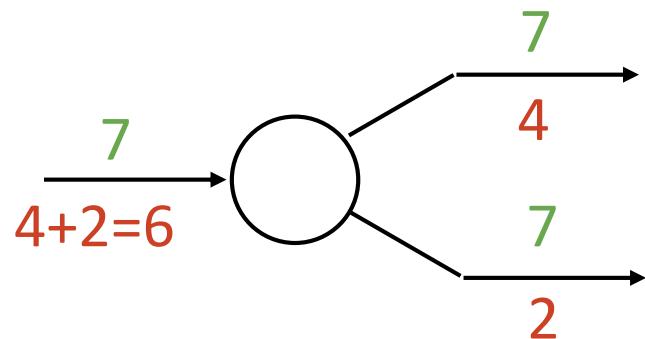


Patterns in Gradient Flow

add gate: gradient distributor

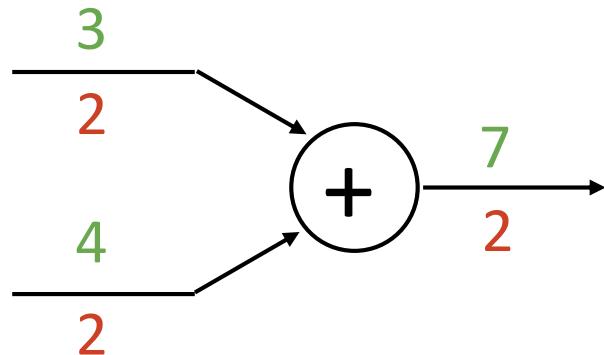


copy gate: gradient adder

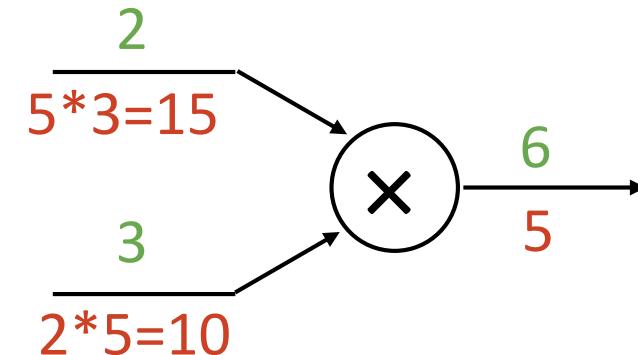


Patterns in Gradient Flow

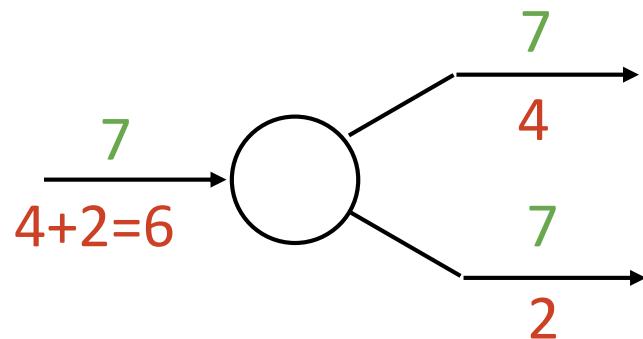
add gate: gradient distributor



mul gate: “swap multiplier”

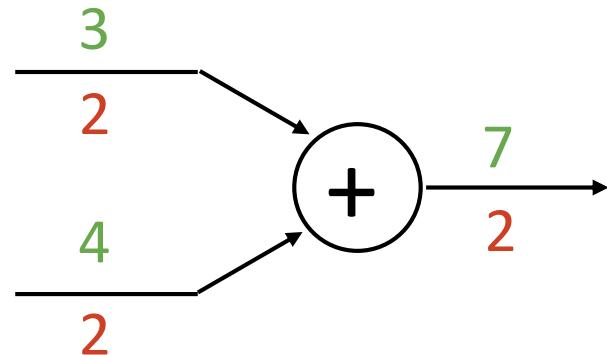


copy gate: gradient adder

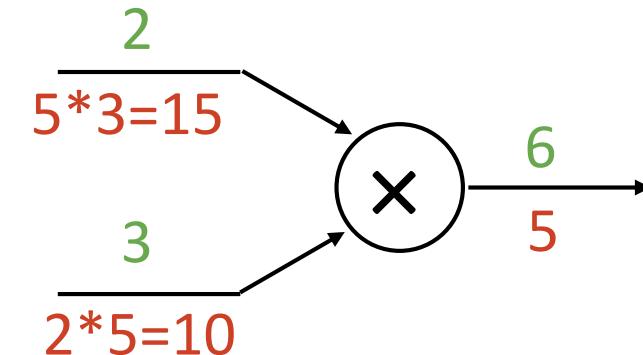


Patterns in Gradient Flow

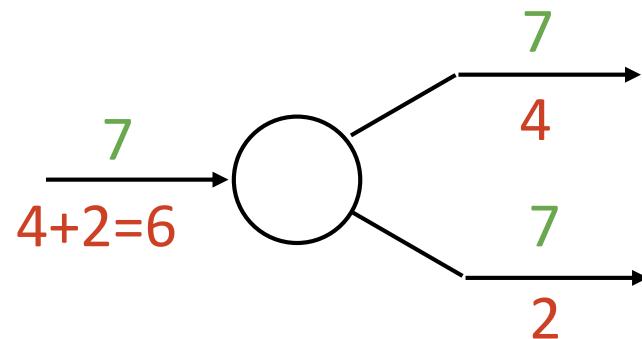
add gate: gradient distributor



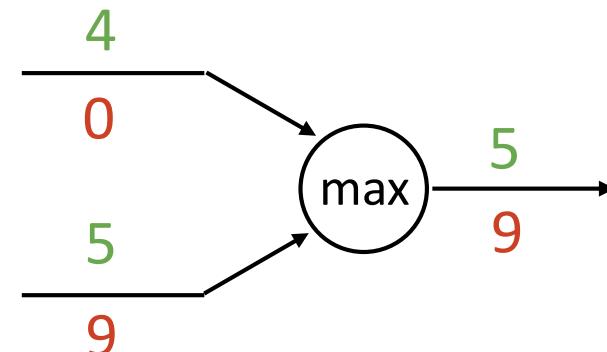
mul gate: “swap multiplier”



copy gate: gradient adder

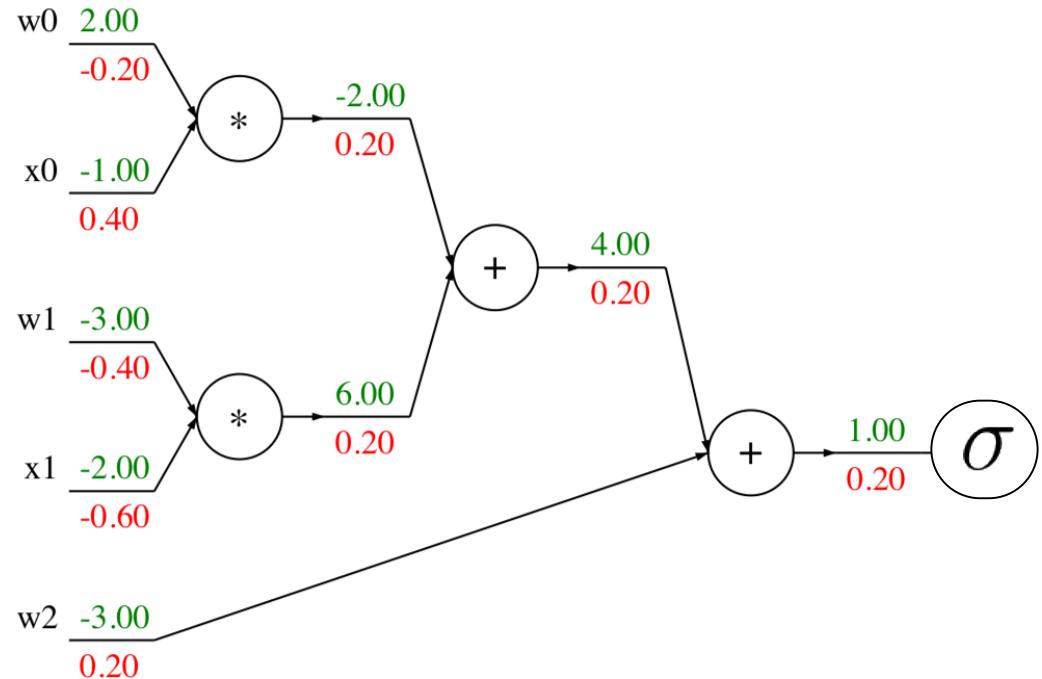


max gate: gradient router



Backprop Implementation: "Flat" gradient code:

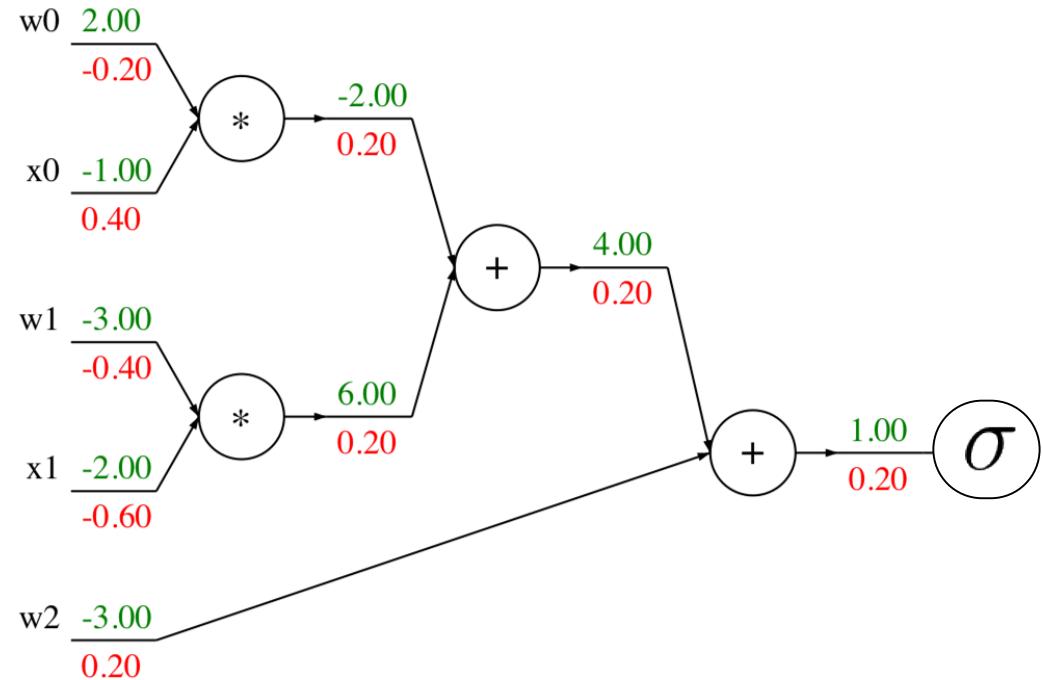
Forward pass:
Compute output



```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output



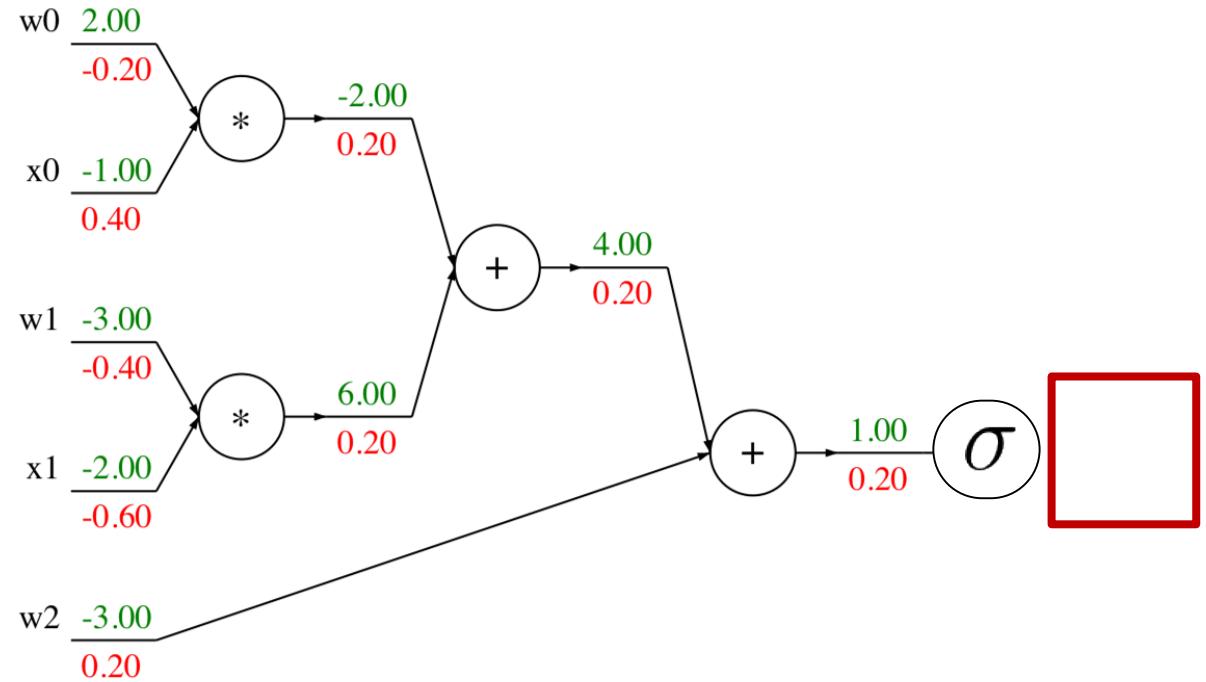
Backward pass:
Compute grads

```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output



Base case

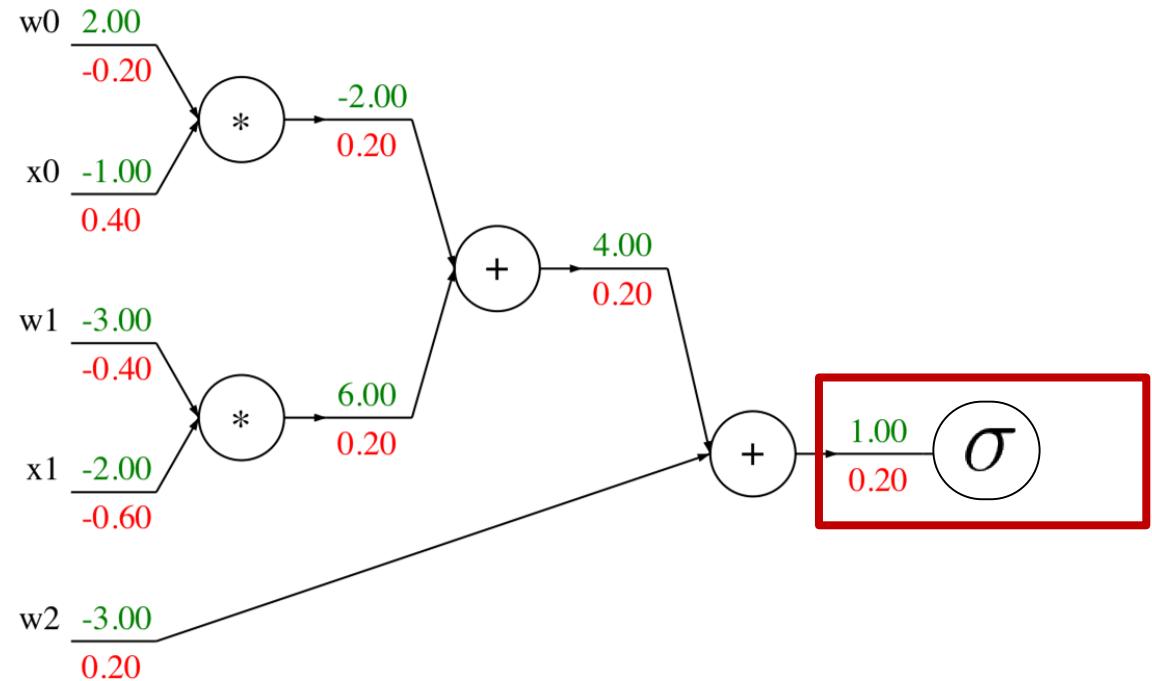
```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

grad_L = 1.0

```
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output



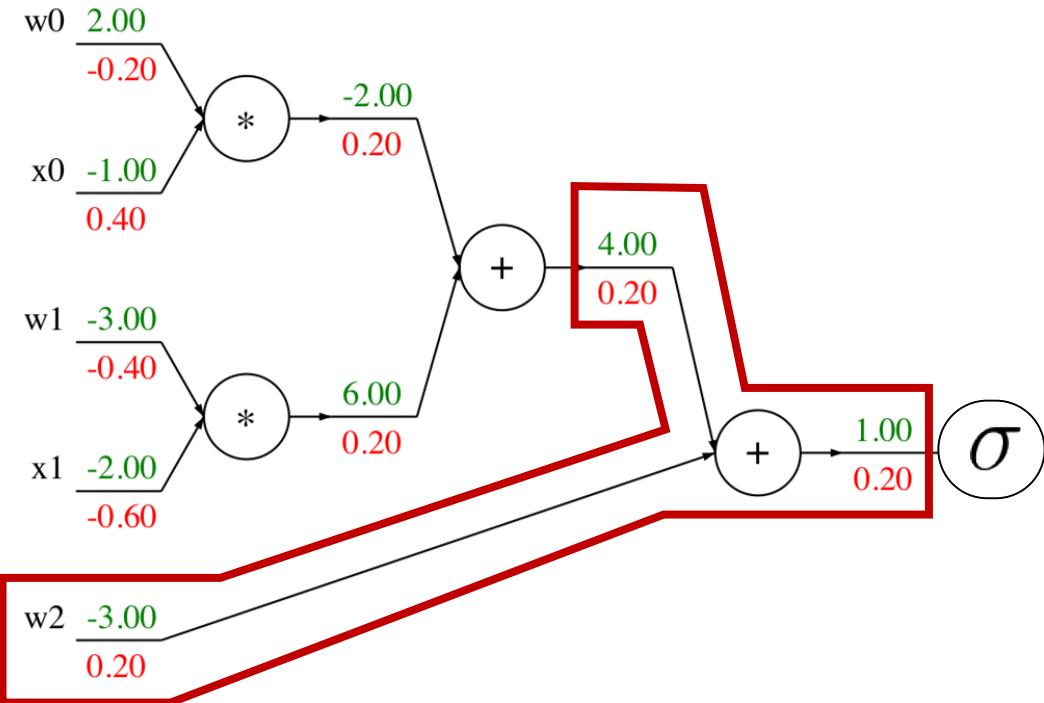
Sigmoid

```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output



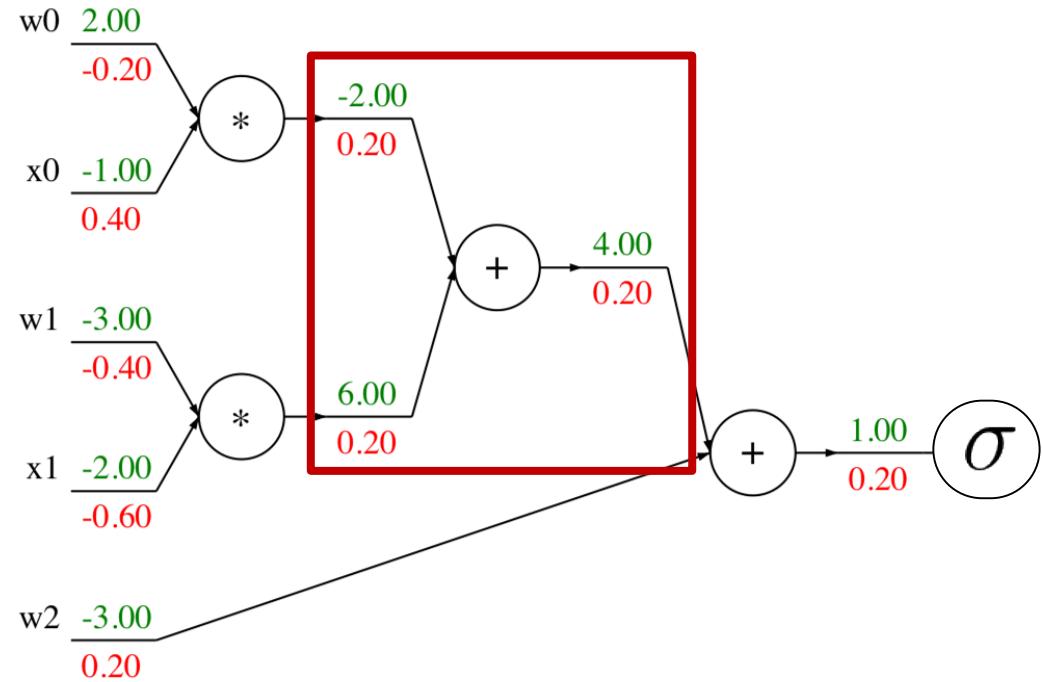
Add

```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output



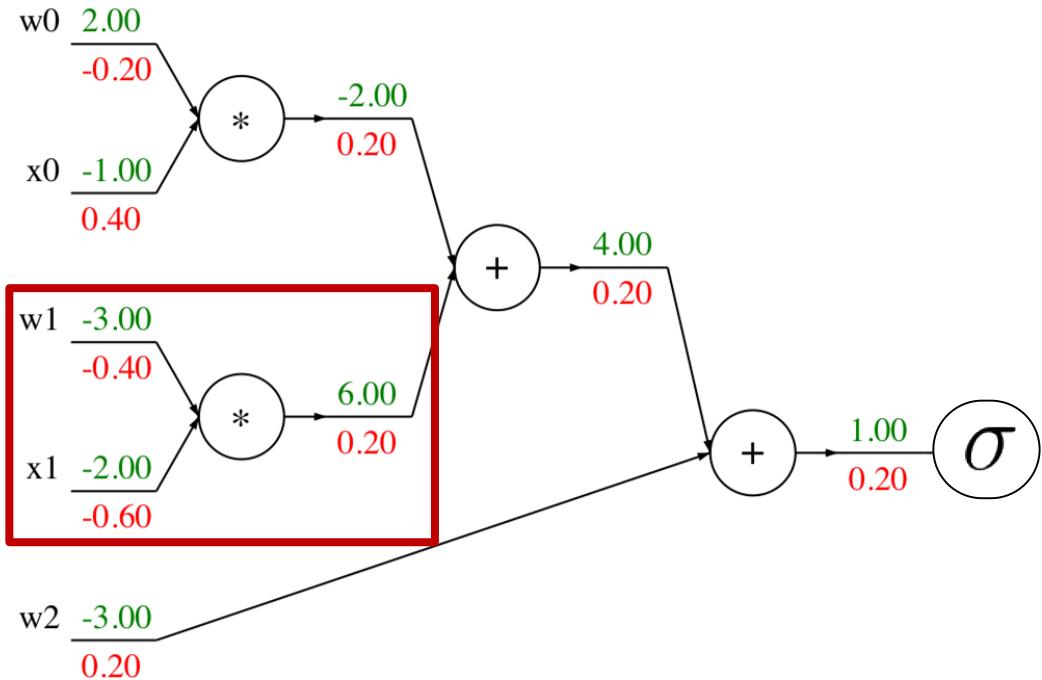
Add

```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output



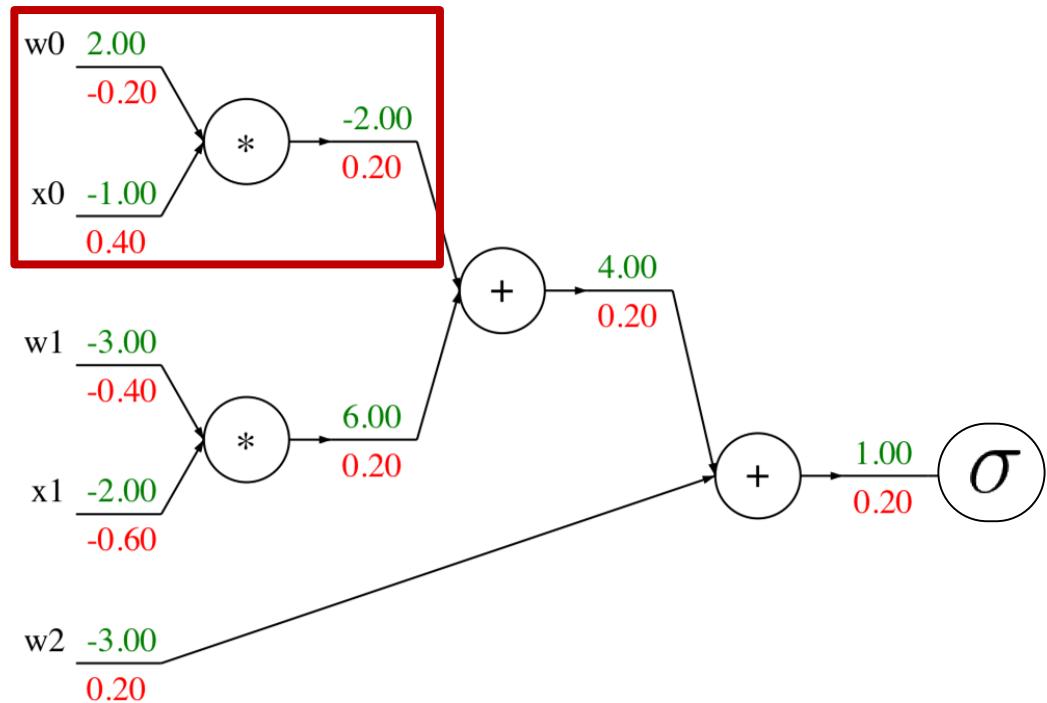
Multiply

```
def f(w0, x0, w1, x1, w2):  
    s0 = w0 * x0  
    s1 = w1 * x1  
    s2 = s0 + s1  
    s3 = s2 + w2  
    L = sigmoid(s3)
```

```
grad_L = 1.0  
grad_s3 = grad_L * (1 - L) * L  
grad_w2 = grad_s3  
grad_s2 = grad_s3  
grad_s0 = grad_s2  
grad_s1 = grad_s2  
grad_w1 = grad_s1 * x1  
grad_x1 = grad_s1 * w1  
grad_w0 = grad_s0 * x0  
grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output



Multiply

```
def f(w0, x0, w1, x1, w2):
```

```
s0 = w0 * x0
```

```
s1 = w1 * x1
```

```
s2 = s0 + s1
```

```
s3 = s2 + w2
```

```
L = sigmoid(s3)
```

```
grad_L = 1.0
```

```
grad_s3 = grad_L * (1 - L) * L
```

```
grad_w2 = grad_s3
```

```
grad_s2 = grad_s3
```

```
grad_s0 = grad_s2
```

```
grad_s1 = grad_s2
```

```
grad_w1 = grad_s1 * x1
```

```
grad_x1 = grad_s1 * w1
```

```
grad_w0 = grad_s0 * x0
```

```
grad_x0 = grad_s0 * w0
```

“Flat” Backprop: Do this for Assignment 2!

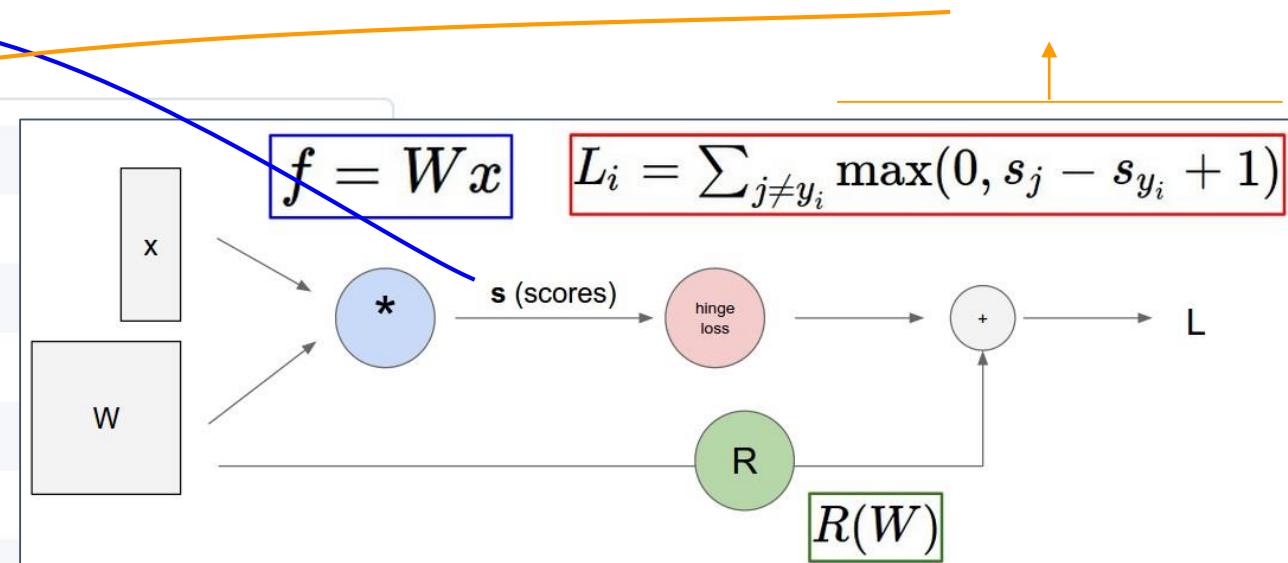
Your gradient code should look like a “reversed version” of your forward pass!

E.g. for the SVM:

```
# receive W (weights), X (data)
# forward pass (we have 8 lines)

scores = ...
margins = ...
data_loss = ...
reg_loss = ...
loss = data_loss + reg_loss

# backward pass (we have 5 lines)
dmargins = ... (optionally, we go direct to dscores)
dscores = ...
dW = ...
```



“Flat” Backprop: Do this for Assignment 2!

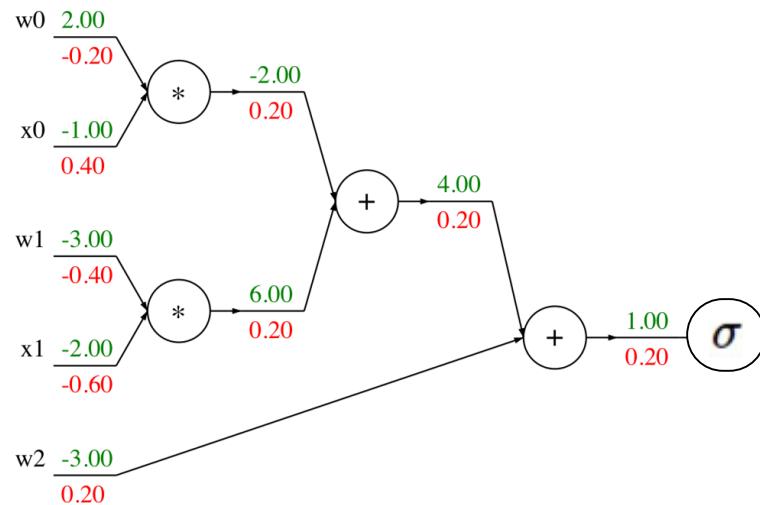
Your gradient code should look like a “reversed version” of your forward pass!

E.g. for two-layer neural net:

```
# receive W1,W2,b1,b2 (weights/biases), X (data)
# forward pass:
h1 = #... function of X,W1,b1
scores = #... function of h1,W2,b2
loss = #... (several lines of code to evaluate Softmax loss)
# backward pass:
dscores = #...
dh1,dW2,db2 = #...
dW1,db1 = #...
```

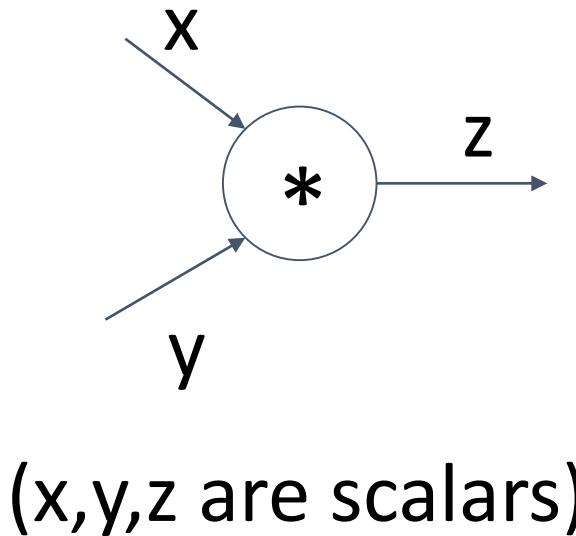
Backprop Implementation: Modular API

Graph (or Net) object (*rough pseudo code*)



```
class ComputationalGraph(object):  
    #...  
    def forward(inputs):  
        # 1. [pass inputs to input gates...]  
        # 2. forward the computational graph:  
        for gate in self.graph.nodes_topologically_sorted():  
            gate.forward()  
        return loss # the final gate in the graph outputs the loss  
    def backward():  
        for gate in reversed(self.graph.nodes_topologically_sorted()):  
            gate.backward() # little piece of backprop (chain rule applied)  
        return inputs_gradients
```

Example: PyTorch Autograd Functions



```
class Multiply(torch.autograd.Function):  
    @staticmethod  
    def forward(ctx, x, y):  
        ctx.save_for_backward(x, y) ← Need to stash some values for use in backward  
        z = x * y  
        return z  
  
    @staticmethod  
    def backward(ctx, grad_z): ← Upstream gradient  
        x, y = ctx.saved_tensors  
        grad_x = y * grad_z # dz/dx * dL/dz  
        grad_y = x * grad_z # dz/dy * dL/dz  
        return grad_x, grad_y
```

Need to stash some values for use in backward

Upstream gradient

Multiply upstream and local gradients

Example: PyTorch operators

pytorch / pytorch		
Code	Issues 2,286	Pull requests 561
Tree: 517c7c9861	pytorch / aten / src / THNN / generic /	Create new file Upload files Find file History
 ezyang and facebook-github-bot Canonicalize all includes in PyTorch. (#14849) ...	Latest commit 517c7c9 on Dec 8, 2018	
..		
AbsCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
BCECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ClassNLLCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Col2Im.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ELU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
FeatureLPPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
GatedLinearUnit.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
HardTanh.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Im2Col.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
IndexLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LeakyReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LogSigmoid.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MSECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MultiLabelMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MultiMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
RReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Sigmoid.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SmoothL1Criterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SoftMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SoftPlus.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SoftShrink.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SparseLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialAdaptiveAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialAdaptiveMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialClassNLLCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialConvolutionMM.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialDilatedMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialFractionalMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialMaxUnpooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialReflectionPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialUpSamplingBilinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
SpatialUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
THNN.h	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Tanh.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalReflectionPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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TemporalUpSamplingLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
TemporalUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricAdaptiveAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricAdaptiveMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricAveragePooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricConvolutionMM.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricDilatedMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricFractionalMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricMaxUnpooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricReplicationPadding.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricUpSamplingNearest.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
VolumetricUpSamplingTrilinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
linear_upsampling.h	Implement nn.functional.interpolate based on upsample. (#8591)	9 months ago
pooling_shape.h	Use integer math to compute output size of pooling operations (#14405)	4 months ago
unfold.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago

PyTorch sigmoid layer

```
1 #ifndef TH_GENERIC_FILE
2 #define TH_GENERIC_FILE "THNN/generic/Sigmoid.c"
3 #else
4
5 void THNN_(Sigmoid_updateOutput)(
6     THNNState *state,
7     THTensor *input,
8     THTensor *output)
9 {
10    THTensor_(sigmoid)(output, input);
11 }
12
13 void THNN_(Sigmoid_updateGradInput)(
14     THNNState *state,
15     THTensor *gradOutput,
16     THTensor *gradInput,
17     THTensor *output)
18 {
19    THNN_CHECK_NELEMENT(output, gradOutput);
20    THTensor_(resizeAs)(gradInput, output);
21    TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
22        scalar_t z = *output_data;
23        *gradInput_data = *gradOutput_data * (1. - z) * z;
24    );
25 }
26
27 #endif
```

[Source](#)

PyTorch sigmoid layer

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1 #ifndef TH_GENERIC_FILE
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22        scalar_t z = *output_data;
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```

Forward

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

[Source](#)

PyTorch sigmoid layer

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22        scalar_t z = *output_data;
23        *gradInput_data = *gradOutput_data * (1. - z) * z;
24    );
25 }
26
27 #endif
```

Forward

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

```
static void sigmoid_kernel(TensorIterator& iter) {
    AT_DISPATCH_FLOATING_TYPES(iter.dtype(), "sigmoid_cpu", [&]() {
        unary_kernel_vec(
            iter,
            [=](scalar_t a) -> scalar_t {return (1 / (1 + std::exp((-a))));},
            [=](Vec256<scalar_t> a) {
                a = Vec256<scalar_t>((scalar_t)(0)) - a;
                a = a.exp();
                a = Vec256<scalar_t>((scalar_t)(1)) + a;
                a = a.reciprocal();
                return a;
            });
    });
}
```

Forward actually defined [elsewhere...](#)

return (1 / (1 + std::exp((-a))));

PyTorch sigmoid layer

```
1 #ifndef TH_GENERIC_FILE
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3 #else
4
5 void THNN_(Sigmoid_updateOutput)(
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15     THTensor *gradOutput,
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20     THTensor_(resizeAs)(gradInput, output);
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22         scalar_t z = *output_data;
23         *gradInput_data = *gradOutput_data * (1. - z) * z;
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27 #endif
```

Forward

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

Backward

$$(1 - \sigma(x)) \sigma'(x)$$

[Source](#)

So far: backprop with scalars

What about vector-valued functions?

Recap: Vector Derivatives

$$x \in \mathbb{R}, y \in \mathbb{R}$$

Regular derivative:

$$\frac{\partial y}{\partial x} \in \mathbb{R}$$

If x changes by a small amount, how much will y change?

Recap: Vector Derivatives

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If x changes by a small amount, how much will y change?

$$x \in \mathbb{R}^N, y \in \mathbb{R}$$

Derivative is **Gradient**:

$$\begin{aligned}\frac{\partial y}{\partial x} &\in \mathbb{R}^N, \\ \left(\frac{\partial y}{\partial x}\right)_i &= \frac{\partial y}{\partial x_i}\end{aligned}$$

For each element of x , if it changes by a small amount then how much will y change?

Recap: Vector Derivatives

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$$x \in \mathbb{R}^N, y \in \mathbb{R}$$

Derivative is **Gradient**:

$$\begin{aligned}\frac{\partial y}{\partial x} &\in \mathbb{R}^N, \\ \left(\frac{\partial y}{\partial x}\right)_i &= \frac{\partial y}{\partial x_i}\end{aligned}$$

For each element of x , if it changes by a small amount then how much will y change?

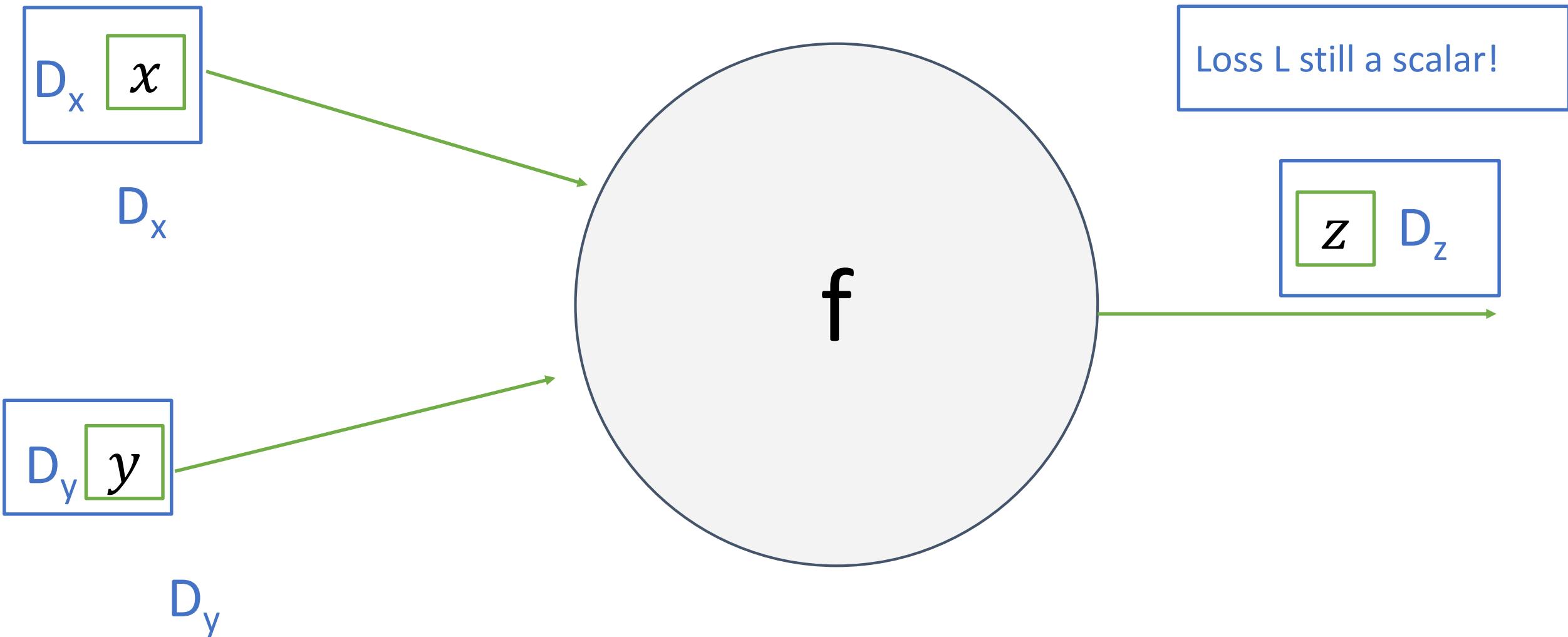
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

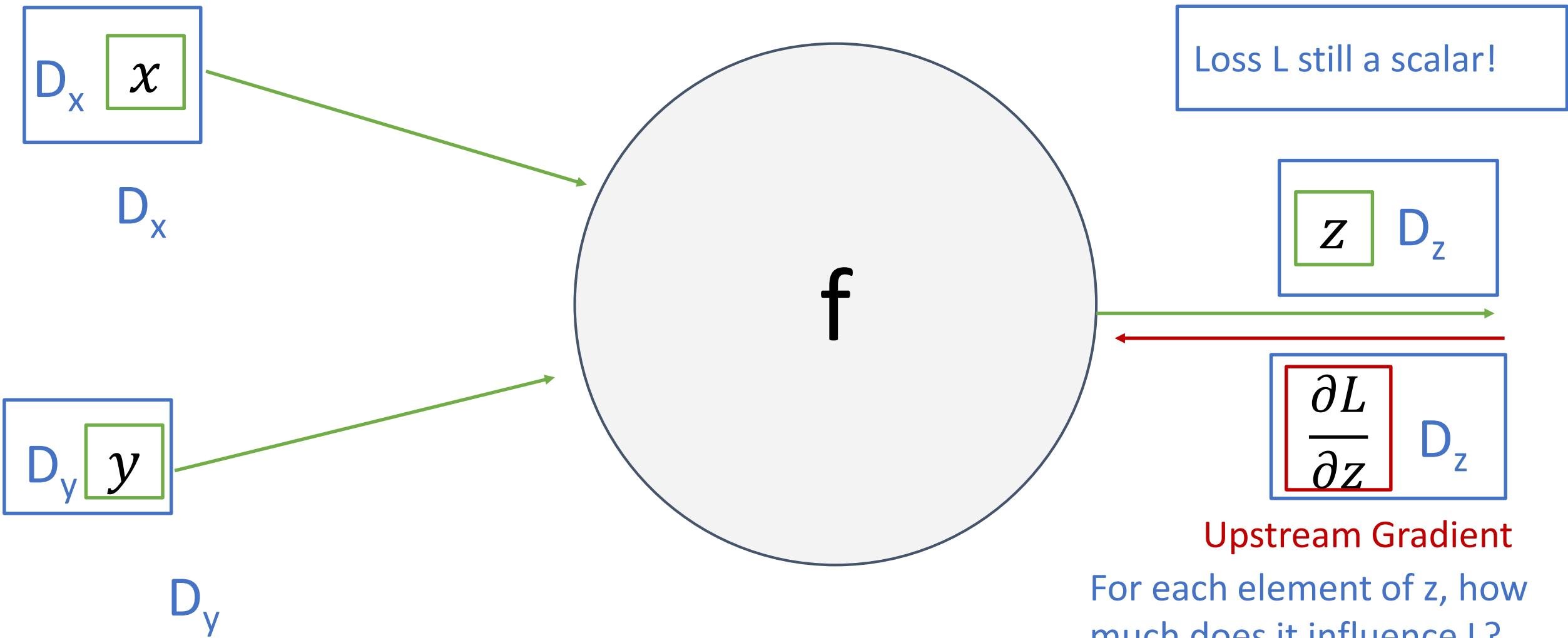
$$\begin{aligned}\frac{\partial y}{\partial x} &\in \mathbb{R}^{N \times M} \\ \left(\frac{\partial y}{\partial x}\right)_{i,j} &= \frac{\partial y_j}{\partial x_i}\end{aligned}$$

For each element of x , if it changes by a small amount then how much will each element of y change?

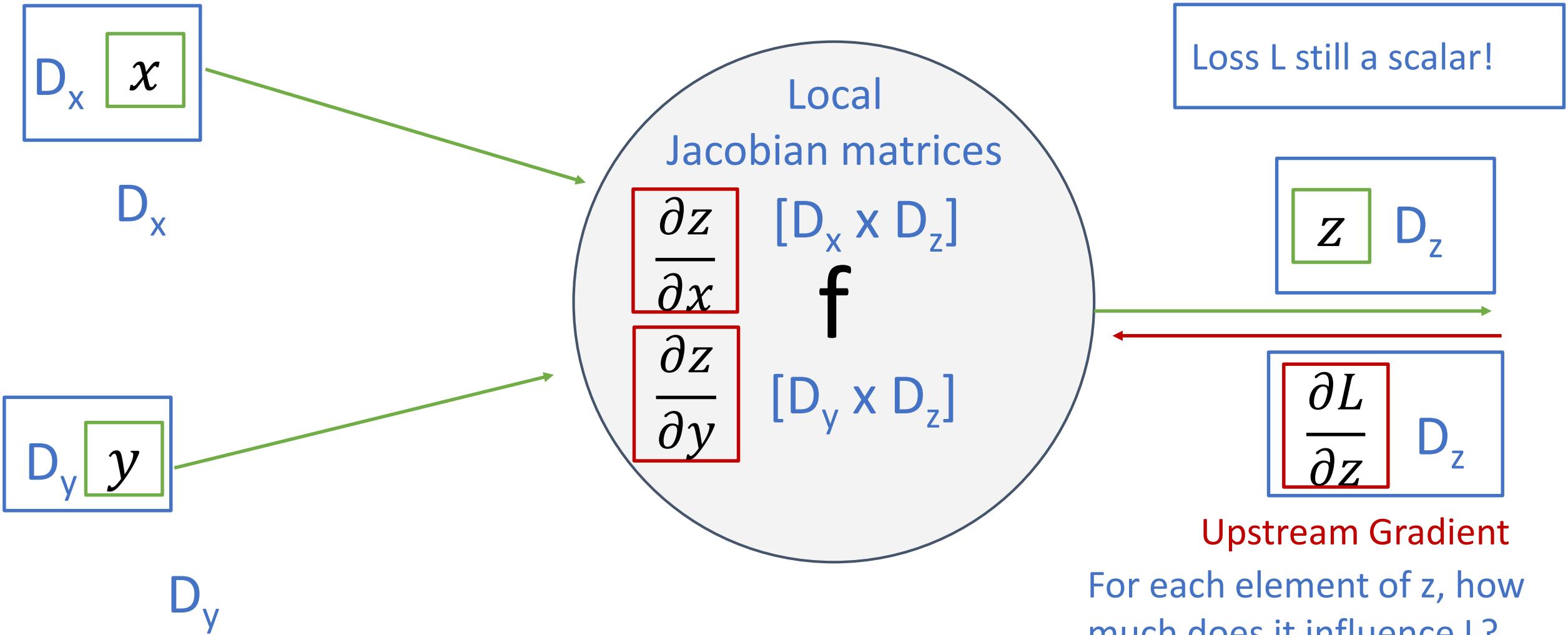
Backprop with Vectors



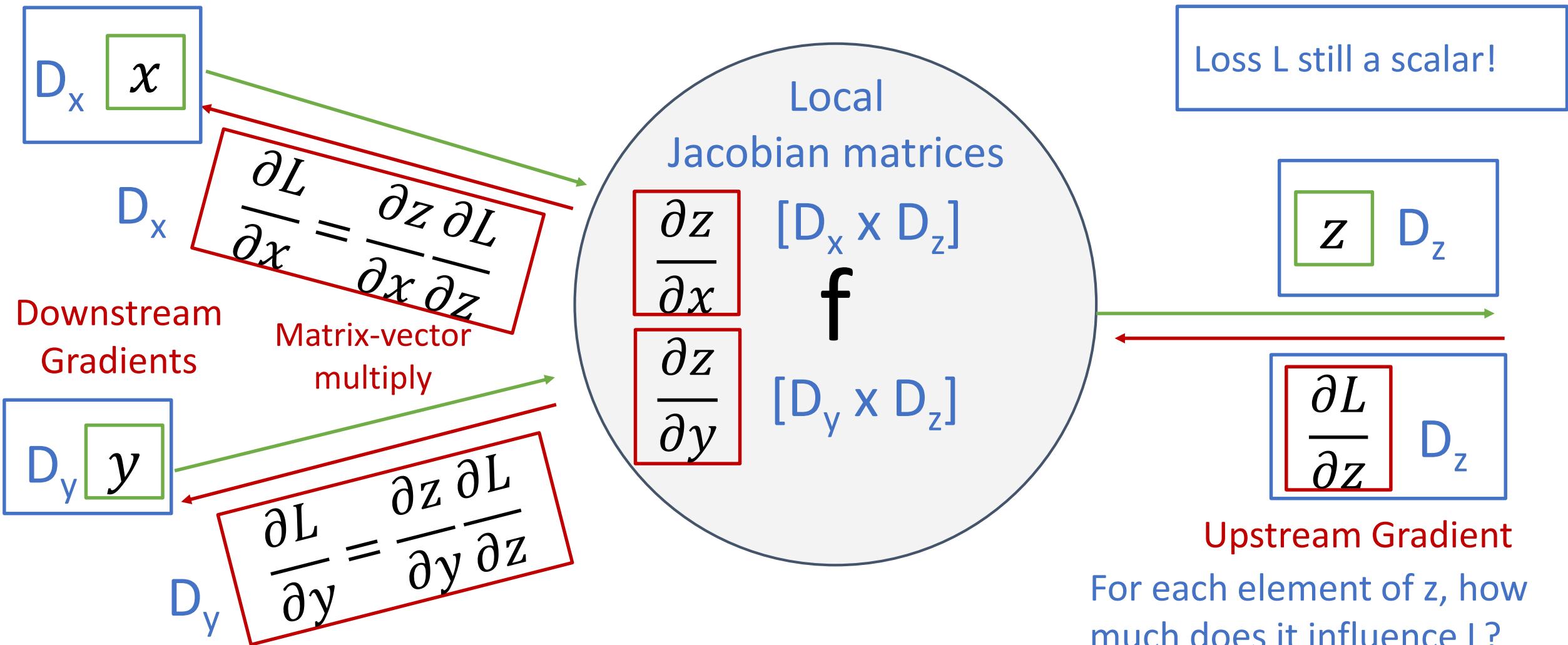
Backprop with Vectors



Backprop with Vectors



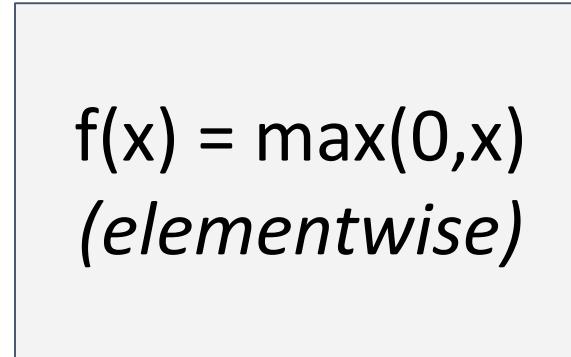
Backprop with Vectors



Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \longrightarrow$$



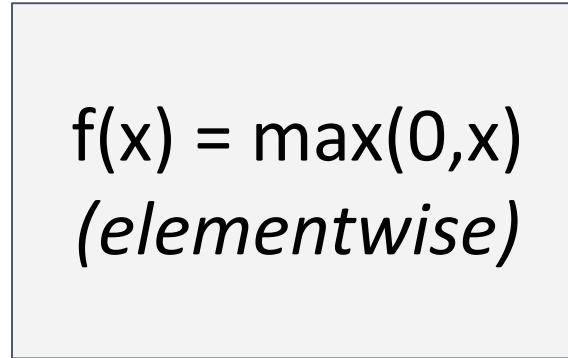
4D output y:

$$\longrightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \xrightarrow{\quad}$$



4D output y:

$$\xrightarrow{\quad} \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D dL/dy:

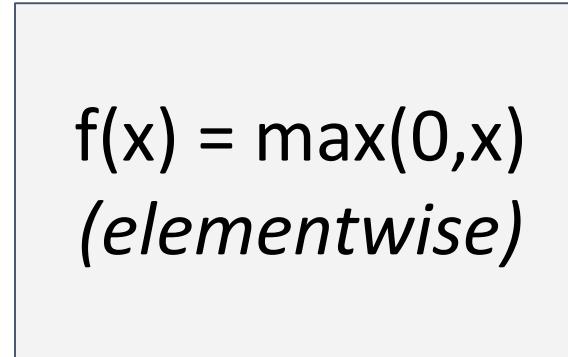
$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \xleftarrow{\quad}$$

Upstream
gradient

Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \longrightarrow$$



4D output y:

$$\longrightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

Jacobian $\frac{\partial y}{\partial x}$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

4D $\frac{\partial L}{\partial y}$:

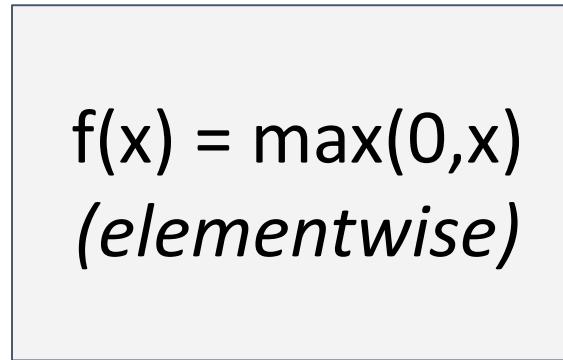
$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \longleftarrow$$

Upstream
gradient

Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \longrightarrow$$



4D output y:

$$\longrightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} dy/dx \\ dL/dy \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 4 & -1 & 5 & 9 \end{bmatrix}$$

4D dL/dy :

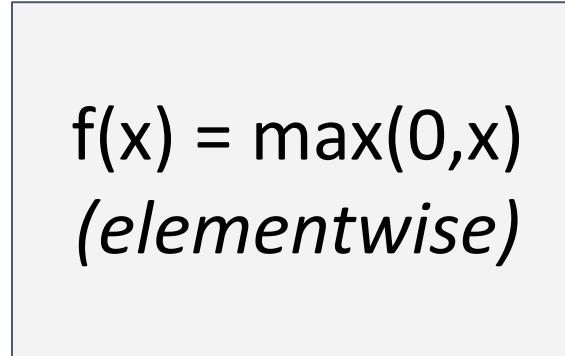
$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \longleftarrow$$

Upstream
gradient

Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \longrightarrow$$



4D output y:

$$\longrightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D dL/dx :

$$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix} \longleftarrow$$

$[dy/dx]$ $[dL/dy]$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

4D dL/dy :

$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \longleftarrow$$

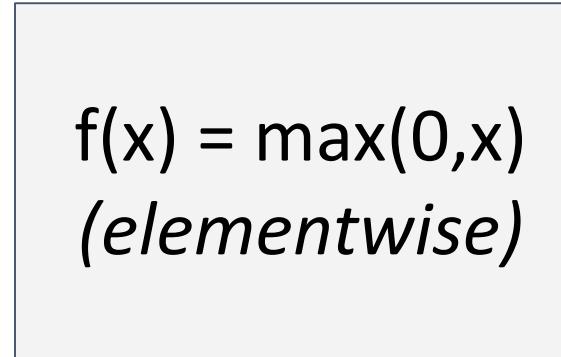
Upstream
gradient

Backprop with Vectors

Jacobian is **sparse**: off-diagonal entries all zero! Never **explicitly** form Jacobian; instead use **implicit** multiplication

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \longrightarrow$$



4D output y :

$$\longrightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D dL/dx :

$$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix} \longleftarrow$$

$[dy/dx] [dL/dy]$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

4D dL/dy :

$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \longleftarrow$$

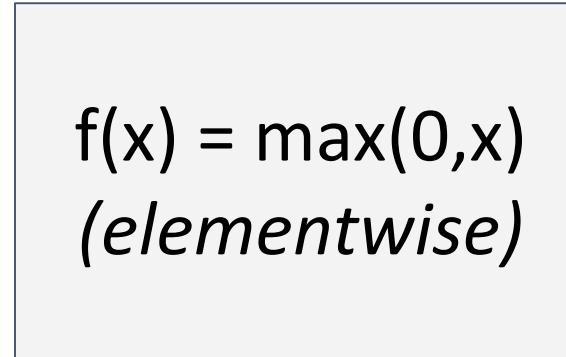
Upstream
gradient

Backprop with Vectors

Jacobian is **sparse**: off-diagonal entries all zero! Never **explicitly** form Jacobian; instead use **implicit** multiplication

4D input x :

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \longrightarrow$$



4D output y :

$$\longrightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D dL/dx :

$$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix} \leftarrow$$

$$\left(\frac{\partial L}{\partial x} \right)_i = \begin{cases} \left(\frac{\partial L}{\partial y} \right)_i, & \text{if } x_i > 0 \\ 0, & \text{otherwise} \end{cases}$$

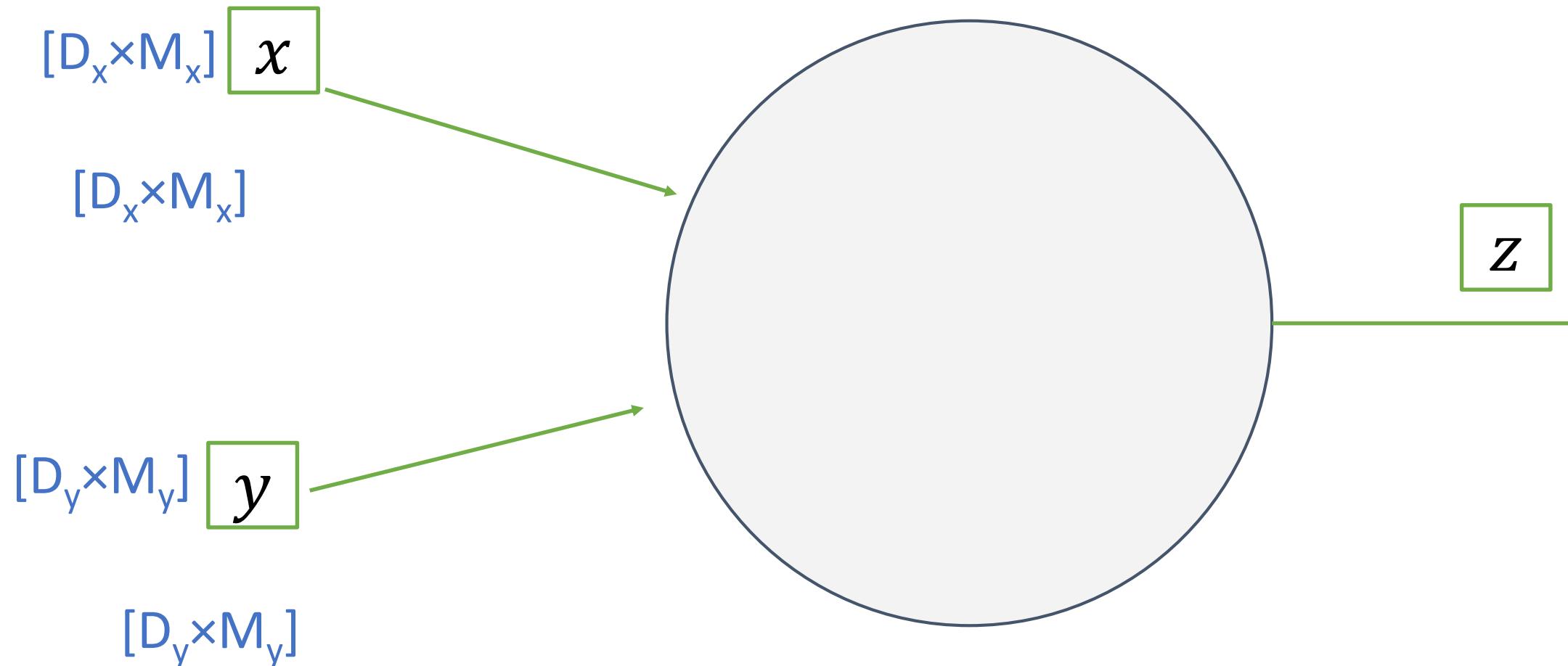
$[dy/dx]$ $[dL/dy]$

4D dL/dy :

$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow$$

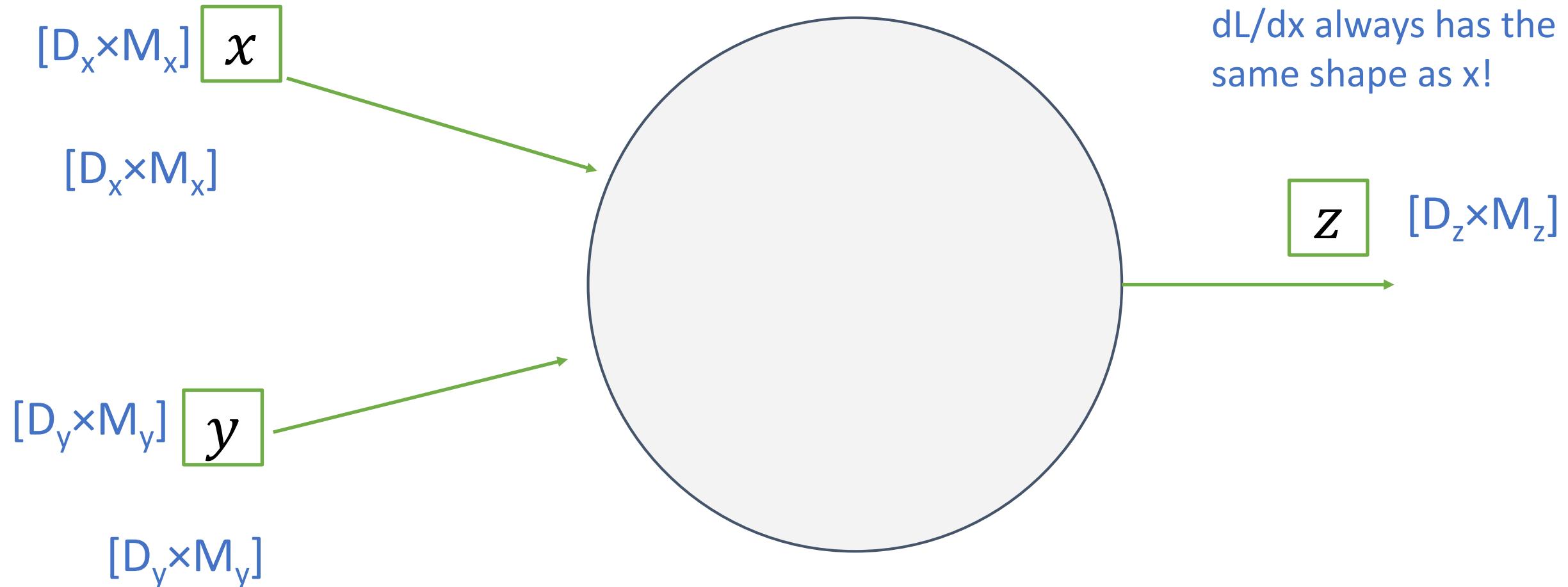
Upstream
gradient

Backprop with Matrices (or Tensors):

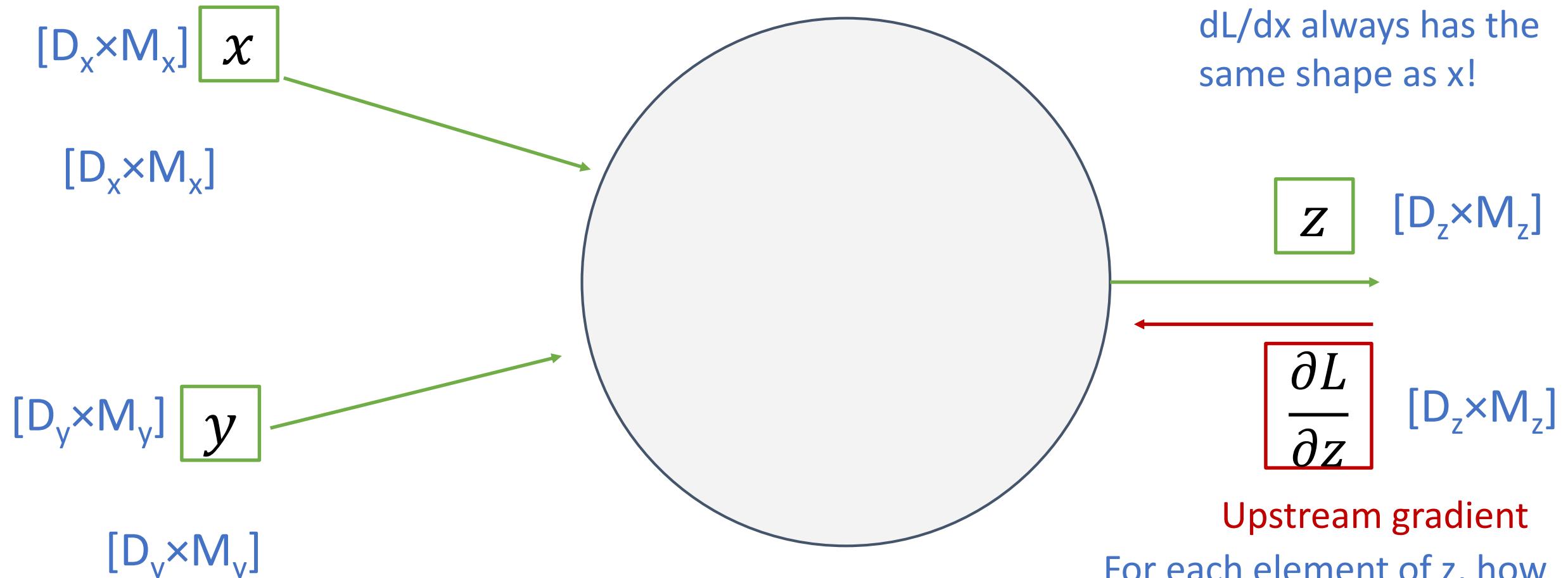


Backprop with Matrices (or Tensors):

Loss L still a scalar!



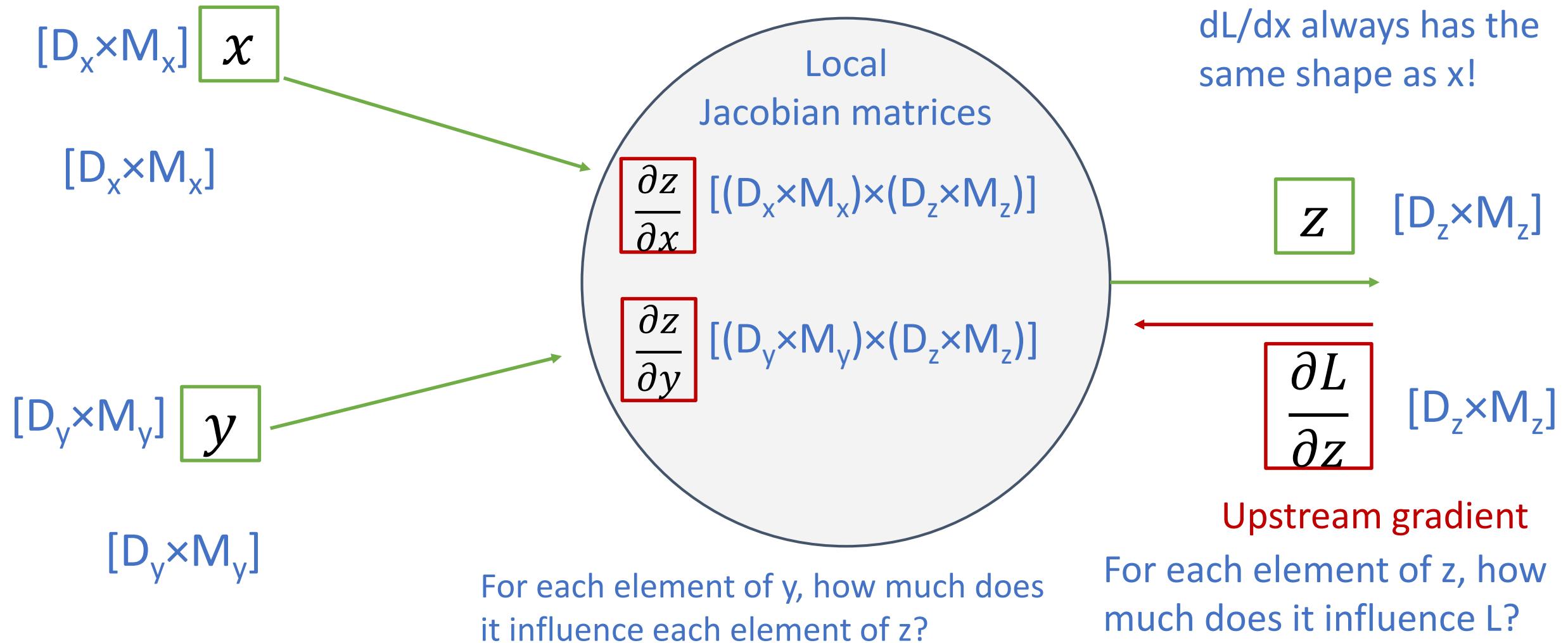
Backprop with Matrices (or Tensors):



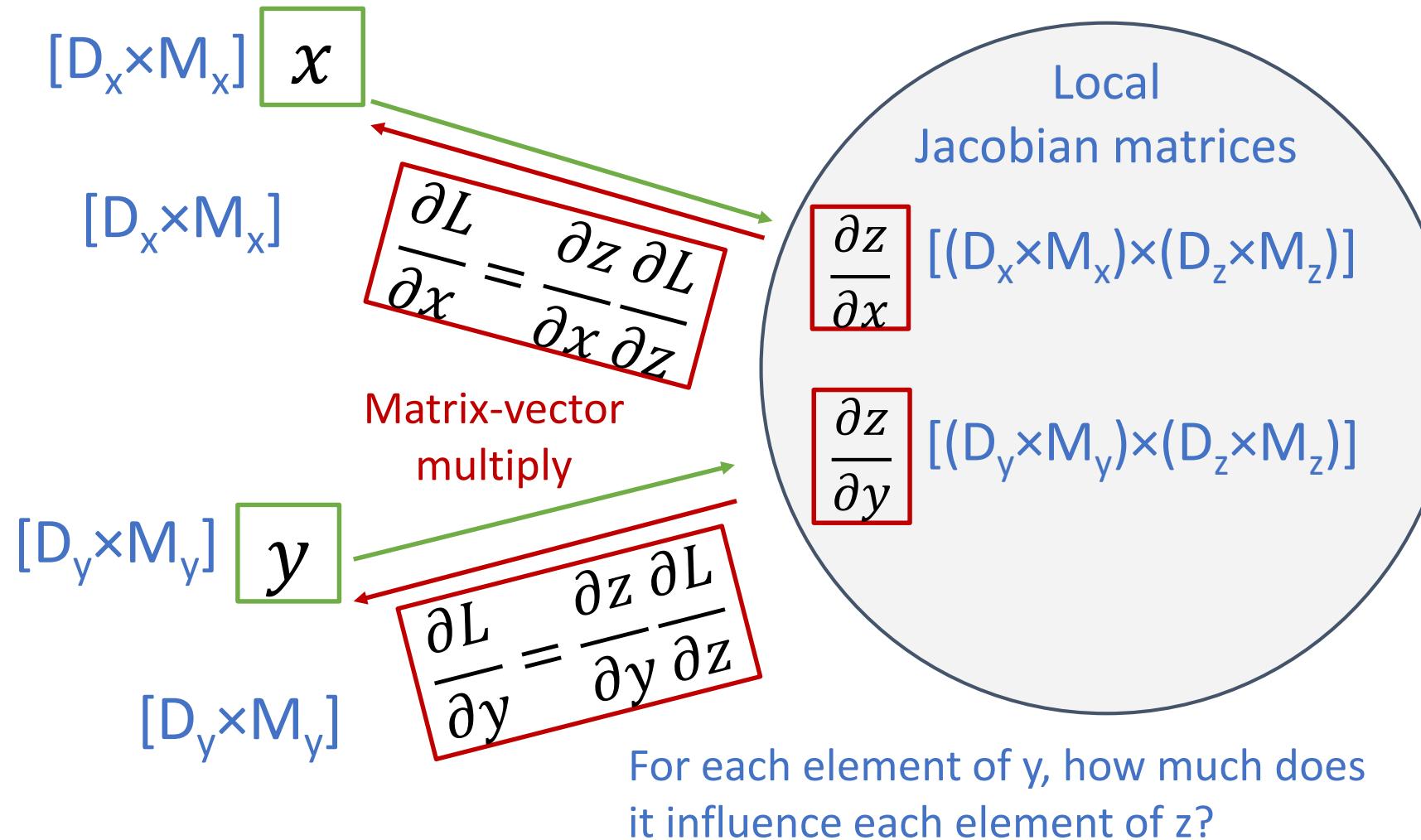
Loss L still a scalar!

dL/dx always has the same shape as x !

Backprop with Matrices (or Tensors):

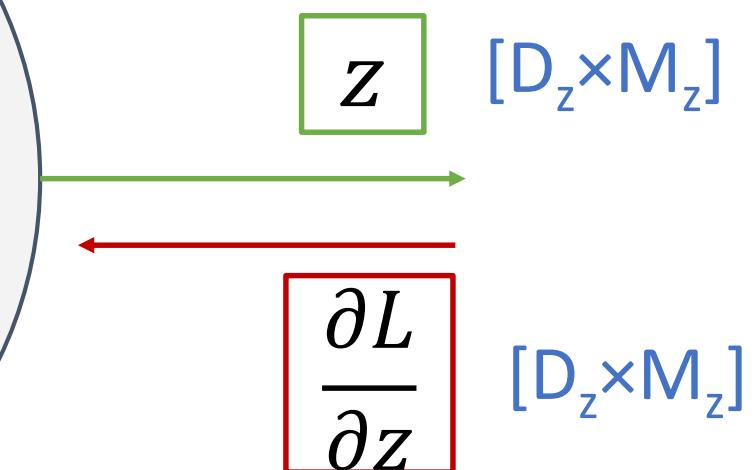


Backprop with Matrices (or Tensors):



Loss L still a scalar!

dL/dx always has the same shape as x !



Upstream gradient

For each element of z , how much does it influence L ?

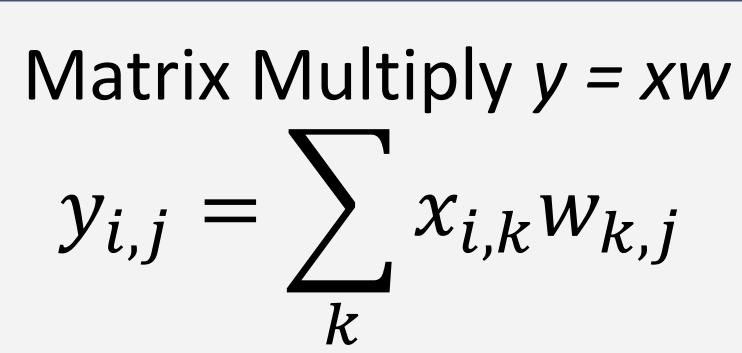
Example: Matrix Multiplication

$x: [N \times D]$

$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

$w: [D \times M]$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$



$y: [N \times M]$

$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

Example: Matrix Multiplication

$x: [N \times D]$

$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$w: [D \times M]$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$y: [N \times M]$

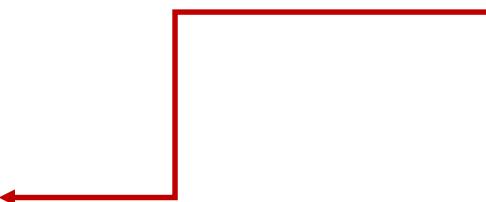
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$dL/dy: [N \times M]$

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

$dL/dx: [N \times D]$

$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$



Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Jacobians:

$$dy/dx: [(N \times D) \times (N \times M)]$$
$$dy/dw: [(D \times M) \times (N \times M)]$$

For a neural net we may have

$$N=64, D=M=4096$$

Each Jacobian takes 256 GB of memory! Must work with them implicitly!

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$$dL/dx_{1,1} = (dy/dx_{1,1}) \cdot (dL/dy)$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Local Gradient Slice:

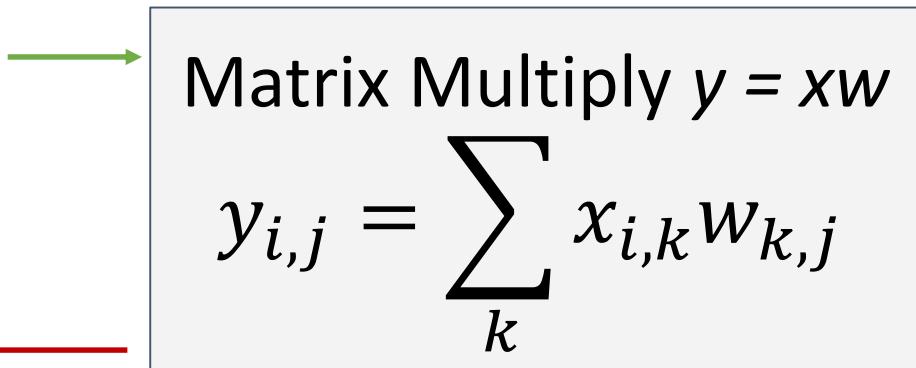
$$dy/dx_{1,1}$$
$$\begin{bmatrix} ? & ? & ? & ? \\ ? & ? & ? & ? \end{bmatrix}$$

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$$dL/dx_{1,1} = (dy/dx_{1,1}) \cdot (dL/dy)$$



$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Local Gradient Slice:

$$dy_{1,1}/dx_{1,1} \quad \begin{bmatrix} dy/dx_{1,1} \\ \begin{bmatrix} ? & ? & ? & ? \\ ? & ? & ? & ? \end{bmatrix} \end{bmatrix}$$

Example: Matrix Multiplication

$x: [N \times D]$

$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

$w: [D \times M]$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$dL/dx: [N \times D]$

$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$dL/dx_{1,1}$

$$= (dy/dx_{1,1}) \cdot (dL/dy)$$

$y: [N \times M]$

$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$dL/dy: [N \times M]$

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Local Gradient Slice:

$$dy_{1,1}/dx_{1,1} \quad \begin{bmatrix} ? & ? & ? & ? \\ ? & ? & ? & ? \end{bmatrix}$$

$$y_{1,1} = x_{1,1}w_{1,1} + x_{1,2}w_{2,1} + x_{1,3}w_{3,1}$$

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$

$[2 \quad 1 \quad -3]$	$[3 \quad 2 \quad 1 \quad -1]$
$[-3 \quad 4 \quad 2]$	$[2 \quad 1 \quad 3 \quad 2]$

$$dL/dx: [N \times D]$$

$[\boxed{?} \quad ? \quad ?]$
$[? \quad ? \quad ?]$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$$y: [N \times M]$$

$[-1 \quad -1 \quad 2 \quad 6]$
$[5 \quad 2 \quad 11 \quad 7]$

$$dL/dy: [N \times M]$$

$[2 \quad 3 \quad -3 \quad 9]$
$[-8 \quad 1 \quad 4 \quad 6]$

Local Gradient Slice:

$$dy/dx_{1,1}$$

$$dy_{1,1}/dx_{1,1} \quad \boxed{3} \quad ? \quad ? \quad ?$$

$$[? \quad ? \quad ? \quad ?]$$

$$y_{1,1} = x_{1,1} \boxed{w_{1,1}} + x_{1,2} w_{2,1} + x_{1,3} w_{3,1}$$

$$\Rightarrow dy_{1,1}/dx_{1,1} = \boxed{w_{1,1}}$$

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$$dL/dx_{1,1} = (dy/dx_{1,1}) \cdot (dL/dy)$$

Matrix Multiply $y = xw$

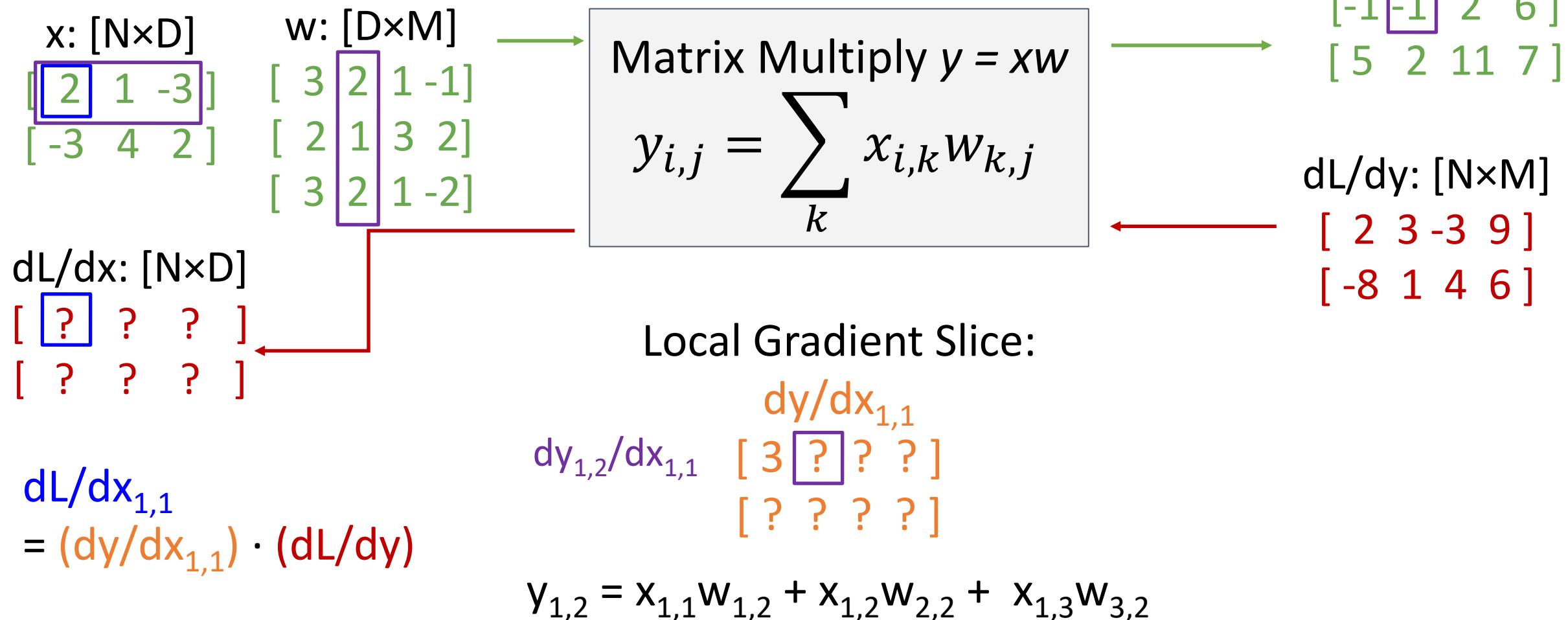
$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$
$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

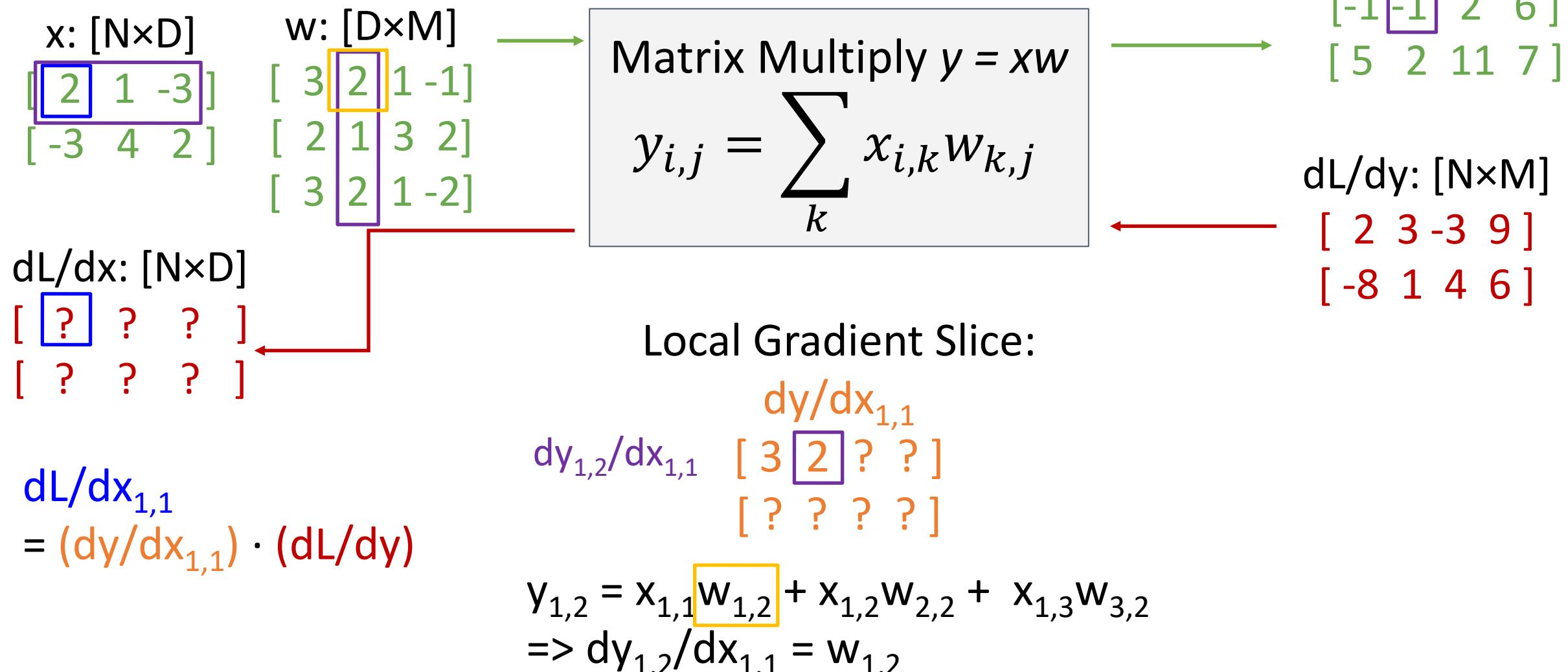
Local Gradient Slice:

$$dy/dx_{1,1}$$
$$dy_{1,2}/dx_{1,1} \quad \begin{bmatrix} 3 & ? & ? & ? \\ ? & ? & ? & ? \end{bmatrix}$$

Example: Matrix Multiplication



Example: Matrix Multiplication



Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$$dL/dx_{1,1} = (dy/dx_{1,1}) \cdot (dL/dy)$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

Local Gradient Slice:

$$dy/dx_{1,1}$$
$$dy_{1,2}/dx_{1,1} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ ? & ? & ? & ? \end{bmatrix}$$

$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$
$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Example: Matrix Multiplication

$$x: [N \times D]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$
$$w: [D \times M]$$
$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$dL/dx: [N \times D]$$

$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$$dL/dx_{1,1} = (dy/dx_{1,1}) \cdot (dL/dy)$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$$y: [N \times M]$$

$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$$dL/dy: [N \times M]$$

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Local Gradient Slice:

$$dy/dx_{1,1}$$
$$dy_{1,2}/dx_{1,1} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ ? & ? & ? & ? \end{bmatrix}$$

$$y_{2,1} = x_{2,1}w_{1,1} + x_{2,2}w_{2,1} + x_{2,3}w_{3,1}$$

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$$dL/dx_{1,1} = (dy/dx_{1,1}) \cdot (dL/dy)$$

Local Gradient Slice:

$$dy/dx_{1,1}$$
$$dy_{1,2}/dx_{1,1} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 0 & ? & ? & ? \end{bmatrix}$$

$$y_{2,1} = x_{2,1}w_{1,1} + x_{2,2}w_{2,1} + x_{2,3}w_{3,1}$$
$$\Rightarrow dy_{2,1}/dx_{1,1} = 0$$

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$$dL/dx_{1,1} = (dy/dx_{1,1}) \cdot (dL/dy)$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

Local Gradient Slice:

$$dy/dx_{1,1}$$
$$dy_{1,2}/dx_{1,1} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

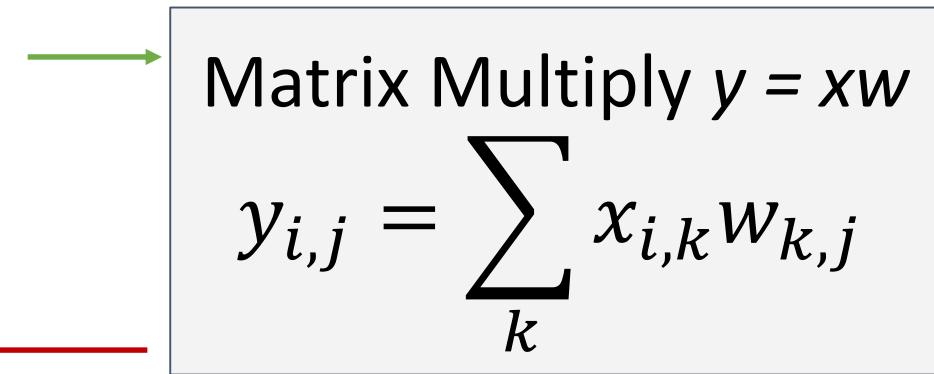
$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} ? & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$$dL/dx_{1,1} = (dy/dx_{1,1}) \cdot (dL/dy)$$



$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Local Gradient Slice:

$$dy/dx_{1,1}$$
$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} 0 & ? & ? \\ ? & ? & ? \end{bmatrix}$$

$$dL/dx_{1,1}$$
$$= (dy/dx_{1,1}) \cdot (dL/dy)$$
$$= (w_{1,:}) \cdot (dL/dy_{1,:})$$
$$= 3*2 + 2*3 + 1*(-3) + (-1)*9 = 0$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

Local Gradient Slice:

$$dy/dx_{1,1}$$
$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} 0 & ? & ? \\ ? & ? & -30 \end{bmatrix}$$

$$dL/dx_{2,3} = (dy/dx_{2,3}) \cdot (dL/dy)$$

Local Gradient Slice:

$$dy/dx_{2,3}$$
$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Example: Matrix Multiplication

$$x: [N \times D] \quad w: [D \times M]$$
$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix} \quad \begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

$$y: [N \times M]$$
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$$dL/dy: [N \times M]$$
$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

$$dL/dx: [N \times D]$$
$$\begin{bmatrix} 0 & ? & ? \\ ? & ? & -30 \end{bmatrix}$$

$$dL/dx_{2,3}$$
$$= (dy/dx_{2,3}) \cdot (dL/dy)$$
$$= (w_{3,:}) \cdot (dL/dy_{2,:})$$
$$= 3*(-8) + 2*1 + 1*4 + (-2)*6 = -30$$

Local Gradient Slice:

$$dy/dx_{2,3}$$
$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Example: Matrix Multiplication

$x: [N \times D]$

$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

$w: [D \times M]$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$



Matrix Multiply $y = xw$

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$y: [N \times M]$

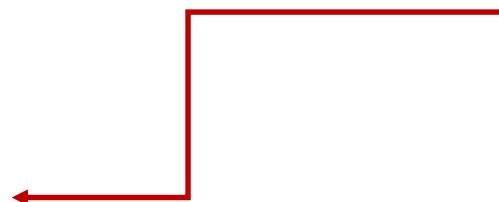
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$dL/dy: [N \times M]$

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

$dL/dx: [N \times D]$

$$\begin{bmatrix} 0 & 16 & -9 \\ -24 & 9 & -30 \end{bmatrix}$$



$dL/dx_{i,j}$

$$= (dy/dx_{i,j}) \cdot (dL/dy)$$

$$= (w_{j,:}) \cdot (dL/dy_{i,:})$$

Example: Matrix Multiplication

$x: [N \times D]$

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$w: [D \times M]$

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$dL/dx_{i,j}$

$$= (\frac{dy}{dx_{i,j}}) \cdot (\frac{dL}{dy})$$

$$= (w_{j,:}) \cdot (\frac{dL}{dy}_{i,:})$$

$$dL/dx = (dL/dy) w^T$$

$[N \times D] \quad [N \times M] \quad [M \times D]$

Easy way to remember:
It's the only way the
shapes work out!

Example: Matrix Multiplication

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$w: [D \times M]$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \end{bmatrix}$$



Matrix Multiply $y = xw$

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$y: [N \times M]$

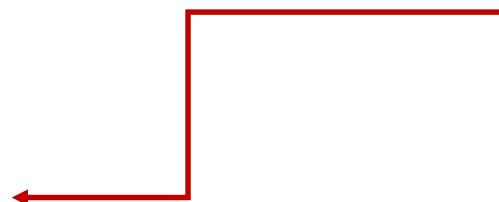
$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

$dL/dy: [N \times M]$

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$$dL/dx = (dL/dy) w^T$$

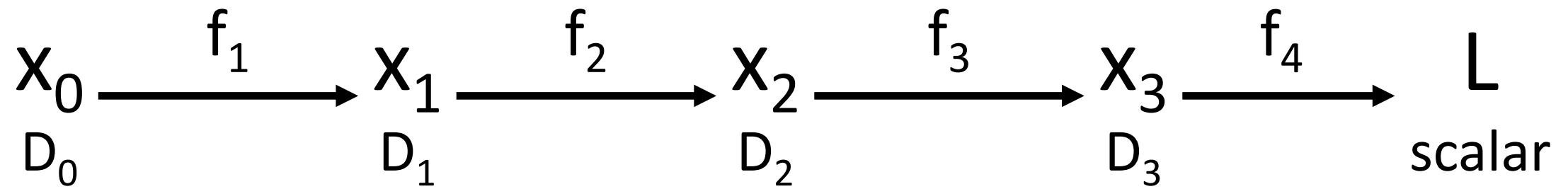
$[N \times D] \quad [N \times M] \quad [M \times D]$

$$dL/dw = x^T (dL/dy)$$

$[D \times M] \quad [D \times N] \quad [N \times M]$

Easy way to remember:
It's the only way the
shapes work out!

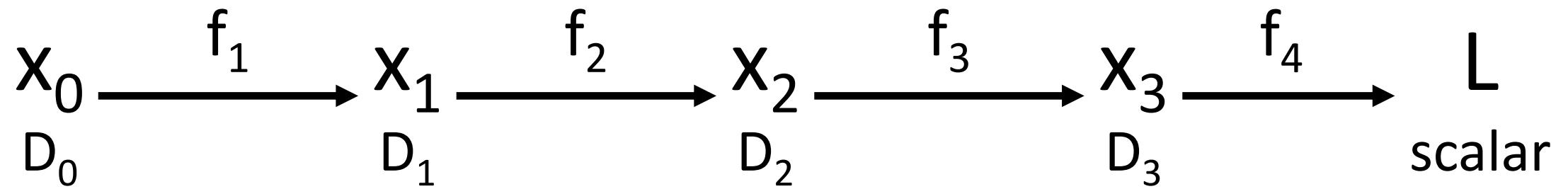
Backpropagation: Another View



Chain
rule

$$\frac{\partial L}{\partial x_0} = \left(\frac{\partial x_1}{\partial x_0} \right) \left(\frac{\partial x_2}{\partial x_1} \right) \left(\frac{\partial x_3}{\partial x_2} \right) \left(\frac{\partial L}{\partial x_3} \right)$$

Backpropagation: Another View



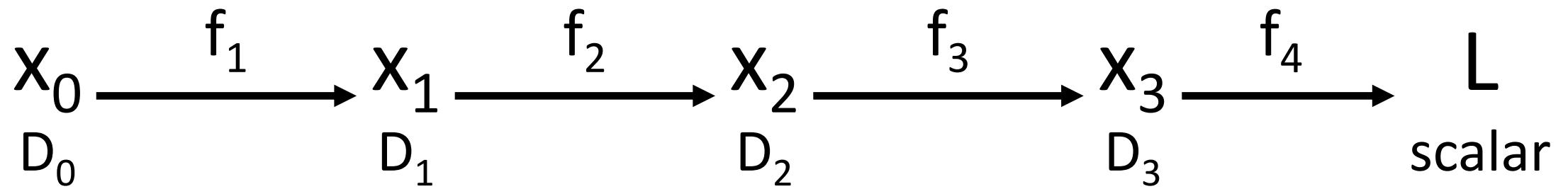
Matrix multiplication is **associative**: we can compute products in any order

Chain
rule

$$\frac{\partial L}{\partial x_0} = \left(\frac{\partial x_1}{\partial x_0} \right) \left(\frac{\partial x_2}{\partial x_1} \right) \left(\frac{\partial x_3}{\partial x_2} \right) \left(\frac{\partial L}{\partial x_3} \right)$$

$[D_0 \times D_1] \quad [D_1 \times D_2] \quad [D_2 \times D_3] \quad [D_3]$

Reverse-Mode Automatic Differentiation

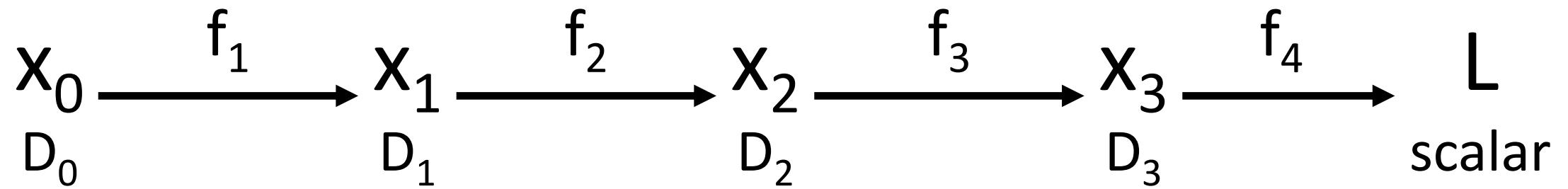


Matrix multiplication is **associative**: we can compute products in any order
Computing products right-to-left avoids matrix-matrix products; only needs matrix-vector

Chain rule

$$\frac{\partial L}{\partial x_0} = \overbrace{\left(\frac{\partial x_1}{\partial x_0} \right) \left(\frac{\partial x_2}{\partial x_1} \right) \left(\frac{\partial x_3}{\partial x_2} \right) \left(\frac{\partial L}{\partial x_3} \right)}^{[D_0 \times D_1] [D_1 \times D_2] [D_2 \times D_3] [D_3]}$$

Reverse-Mode Automatic Differentiation



Matrix multiplication is **associative**: we can compute products in any order

Computing products right-to-left avoids matrix-matrix products; only needs matrix-vector

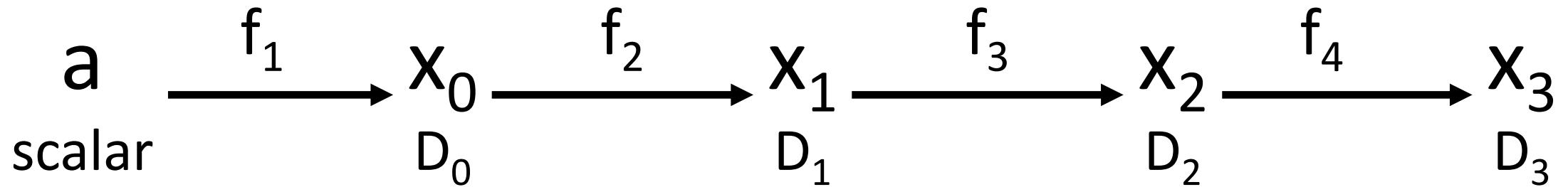
Chain rule

$$\frac{\partial L}{\partial x_0} = \overbrace{\left(\frac{\partial x_1}{\partial x_0} \right) \left(\frac{\partial x_2}{\partial x_1} \right) \left(\frac{\partial x_3}{\partial x_2} \right) \left(\frac{\partial L}{\partial x_3} \right)}^{\text{What if we want grads of scalar input w/ respect to vector outputs?}}$$

Compute grad of scalar output w/ respect to all vector inputs

$[D_0 \times D_1]$ $[D_1 \times D_2]$ $[D_2 \times D_3]$ $[D_3]$

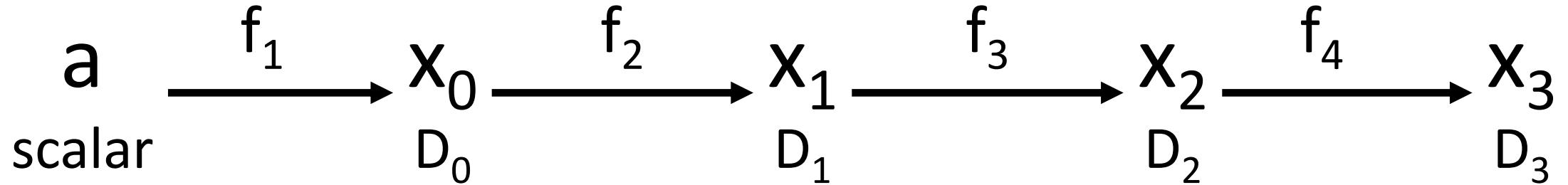
Forward-Mode Automatic Differentiation



Chain
rule

$$\frac{\partial x_3}{\partial a} = \left(\frac{\partial x_0}{\partial a} \right)_{[D_0]} \left(\frac{\partial x_1}{\partial x_0} \right)_{[D_0 \times D_1]} \left(\frac{\partial x_2}{\partial x_1} \right)_{[D_1 \times D_2]} \left(\frac{\partial x_3}{\partial x_2} \right)_{[D_2 \times D_3]}$$

Forward-Mode Automatic Differentiation

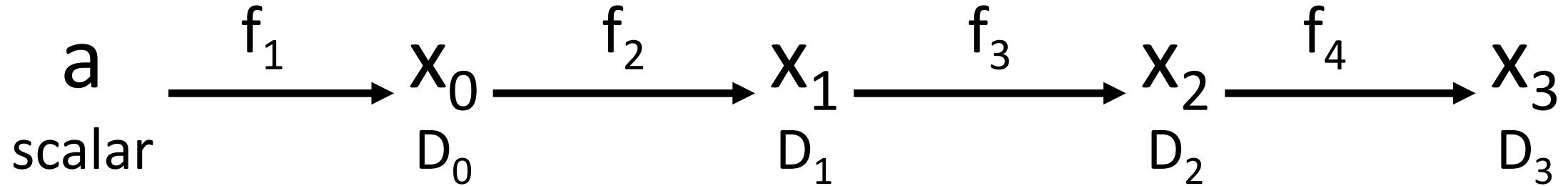


Computing products left-to-right avoids matrix-matrix products; only needs matrix-vector

Chain rule

$$\frac{\partial x_3}{\partial a} = \overbrace{\left(\frac{\partial x_0}{\partial a} \right) \left(\frac{\partial x_1}{\partial x_0} \right) \left(\frac{\partial x_2}{\partial x_1} \right) \left(\frac{\partial x_3}{\partial x_2} \right)}^{[D_0] \times [D_0 \times D_1] \times [D_1 \times D_2] \times [D_2 \times D_3]}$$

Forward-Mode Automatic Differentiation



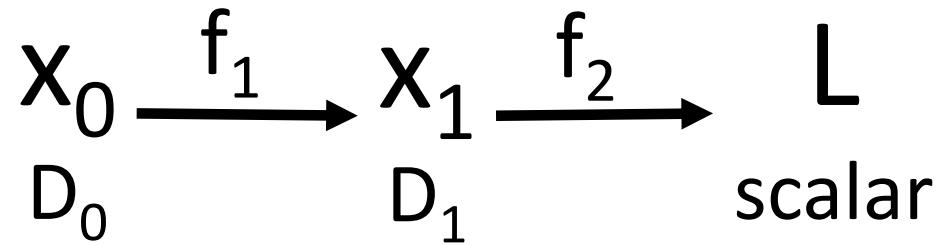
Computing products left-to-right avoids matrix-matrix products; only needs matrix-vector
Not implemented in PyTorch / TensorFlow =(

Chain rule

$$\frac{\partial x_3}{\partial a} = \overbrace{\left(\frac{\partial x_0}{\partial a} \right) \left(\frac{\partial x_1}{\partial x_0} \right) \left(\frac{\partial x_2}{\partial x_1} \right) \left(\frac{\partial x_3}{\partial x_2} \right)}^{[D_0] \times [D_0 \times D_1] \times [D_1 \times D_2] \times [D_2 \times D_3]}$$

But you can implement forward-mode AD using [two calls to reverse-mode AD!](#)
(Inefficient but elegant)

Backprop: Higher-Order Derivatives

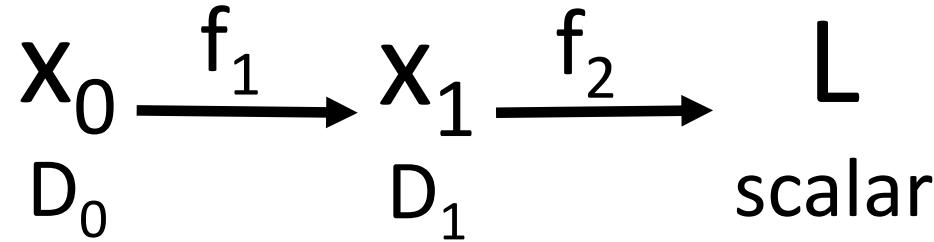


$\frac{\partial^2 L}{\partial x_0^2}$ **Hessian matrix**

$\frac{\partial^2 L}{\partial x_0^2}$ H of second
derivatives.

$[D_0 \times D_0]$

Backprop: Higher-Order Derivatives



$$\frac{\partial^2 L}{\partial x_0^2}$$

$[D_0 \times D_0]$

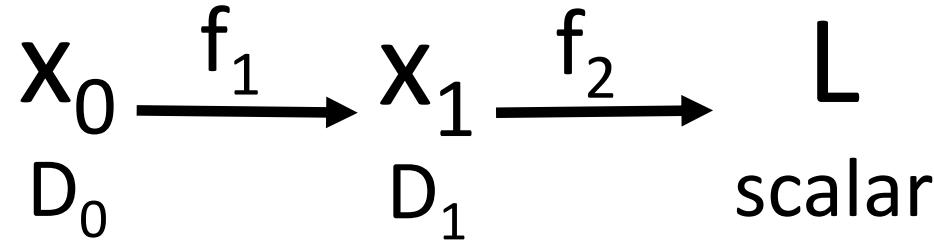
Hessian matrix
H of second
derivatives.

$$\frac{\partial^2 L}{\partial x_0^2} v$$

$[D_0 \times D_0] [D_0]$

Hessian / vector multiply

Backprop: Higher-Order Derivatives



$$\frac{\partial^2 L}{\partial x_0^2}$$

Hessian matrix
H of second
derivatives.

$$[D_0 \times D_0]$$

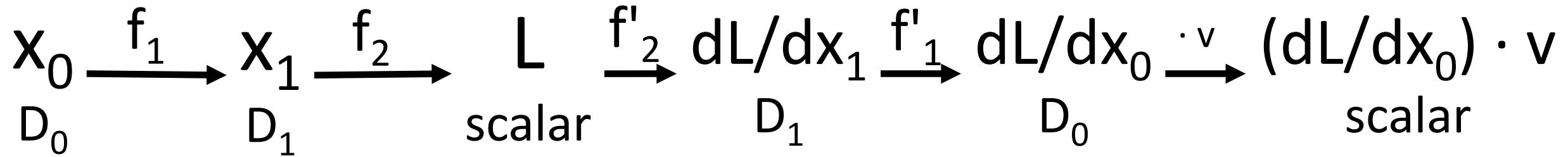
Hessian / vector multiply

$$\frac{\partial^2 L}{\partial x_0^2} v = \frac{\partial}{\partial x_0} \left[\frac{\partial L}{\partial x_0} \cdot v \right]$$

(if v doesn't
depend on x_0)

$$[D_0 \times D_0] [D_0]$$

Backprop: Higher-Order Derivatives



$$\frac{\partial^2 L}{\partial x_0^2}$$

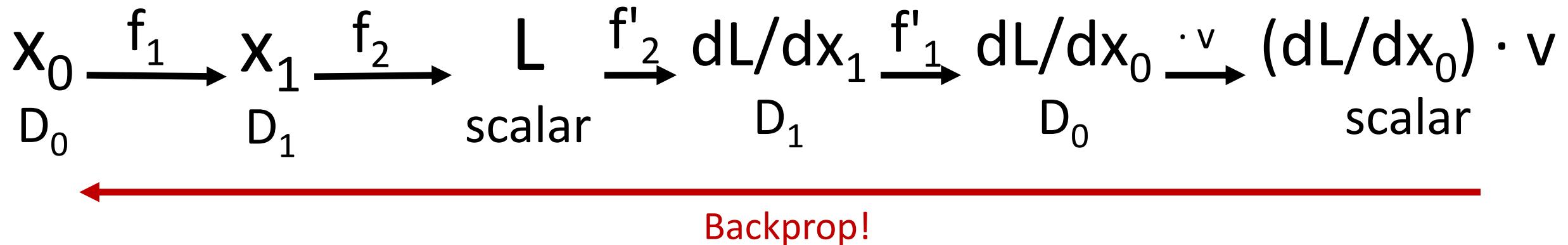
Hessian matrix
H of second derivatives.
[$D_0 \times D_0$]

Hessian / vector multiply

$$\frac{\partial^2 L}{\partial x_0^2} v = \frac{\partial}{\partial x_0} \left[\frac{\partial L}{\partial x_0} \cdot v \right]$$

(if v doesn't depend on x_0)
[$D_0 \times D_0$] [D_0]

Backprop: Higher-Order Derivatives



$$\frac{\partial^2 L}{\partial x_0^2} \quad \begin{array}{l} \text{Hessian matrix} \\ \text{H of second} \\ \text{derivatives.} \end{array}$$

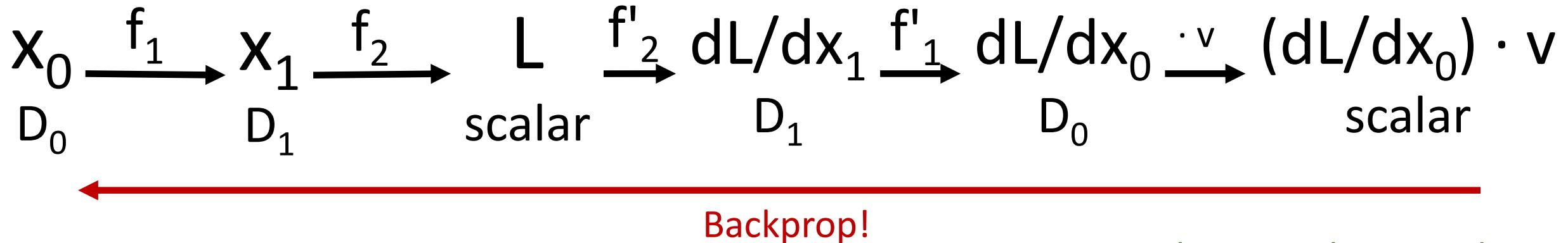
$[D_0 \times D_0]$

Hessian / vector multiply

$$\frac{\partial^2 L}{\partial x_0^2} v = \frac{\partial}{\partial x_0} \left[\frac{\partial L}{\partial x_0} \cdot v \right] \quad (\text{if } v \text{ doesn't depend on } x_0)$$

$[D_0 \times D_0] [D_0]$

Backprop: Higher-Order Derivatives



$$\frac{\partial^2 L}{\partial x_0^2}$$

Hessian matrix
H of second
derivatives.

$$[D_0 \times D_0]$$

Hessian / vector multiply

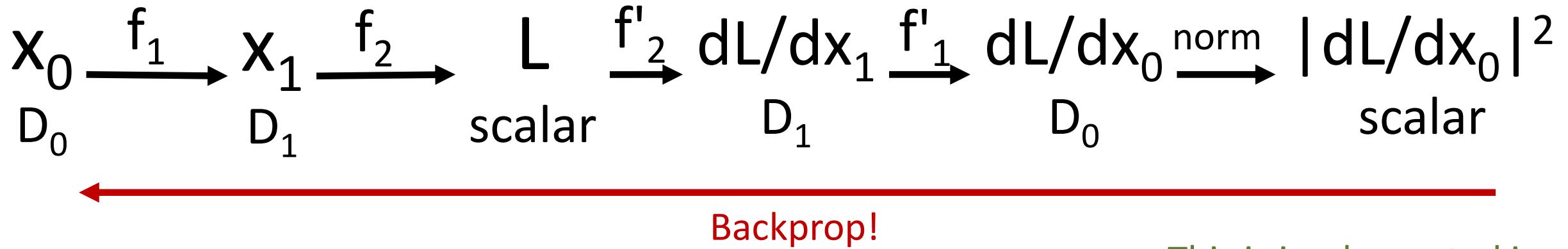
$$\frac{\partial^2 L}{\partial x_0^2} v = \frac{\partial}{\partial x_0} \left[\frac{\partial L}{\partial x_0} \cdot v \right]$$

$$[D_0 \times D_0] [D_0]$$

This is implemented in
PyTorch / Tensorflow!

(if v doesn't
depend on x_0)

Backprop: Higher-Order Derivatives



This is implemented in
PyTorch / Tensorflow!

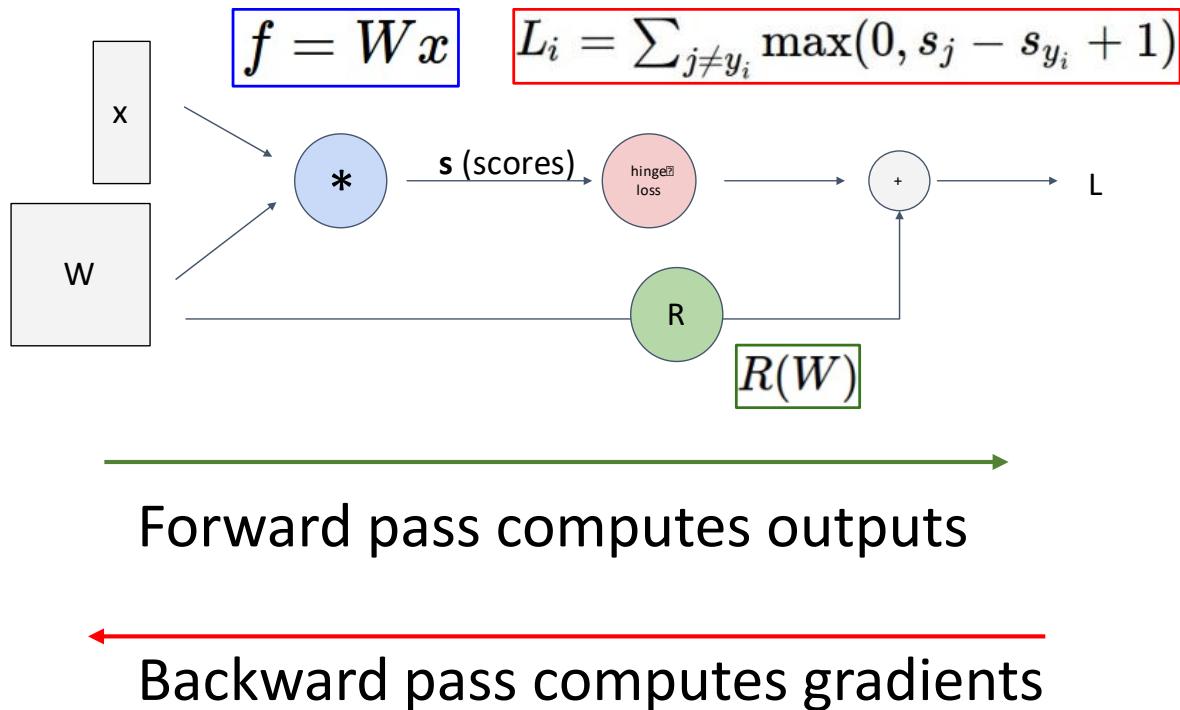
Example: Regularization to penalize the norm of the gradient

$$R(W) = \left\| \frac{\partial L}{\partial W} \right\|_2^2 = \left(\frac{\partial L}{\partial W} \right) \cdot \left(\frac{\partial L}{\partial W} \right) \frac{\partial}{\partial x_0} [R(W)] = 2 \left(\frac{\partial^2 L}{\partial x_0^2} \right) \left(\frac{\partial L}{\partial x_0} \right)$$

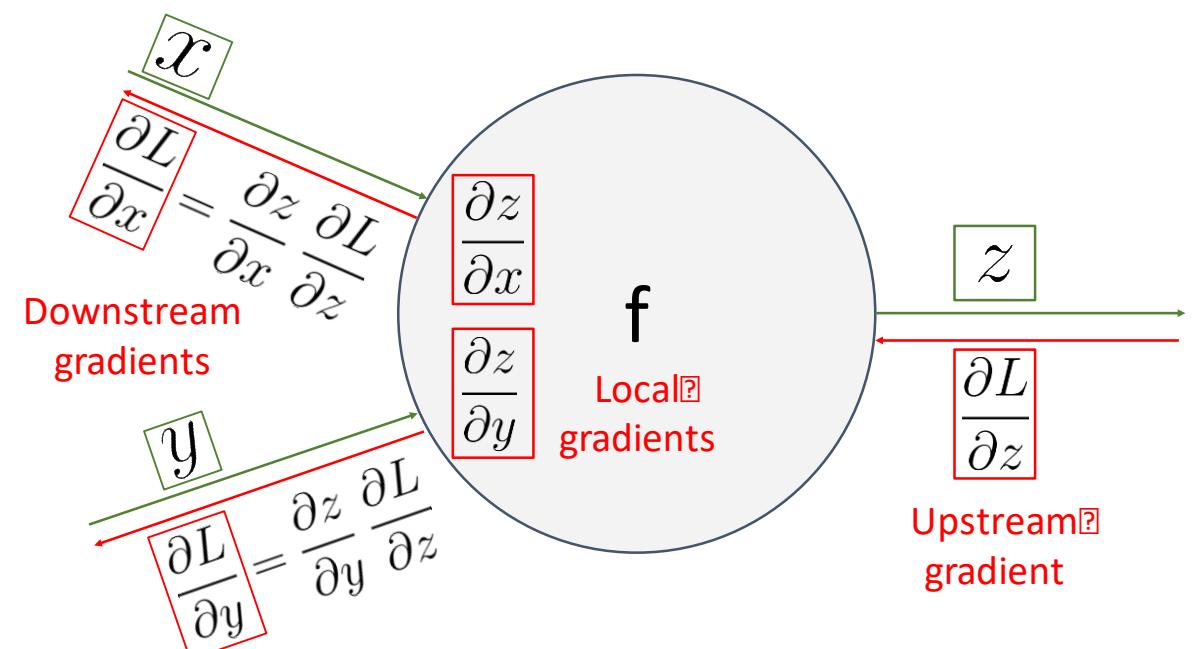
Gulrajani et al, "Improved Training of Wasserstein GANs", NeurIPS 2017

Summary

Represent complex expressions
as **computational graphs**



During the backward pass, each node in the graph receives **upstream gradients** and multiplies them by **local gradients** to compute **downstream gradients**



Summary

Backprop can be implemented with “flat” code where the backward pass looks like forward pass reversed (Use this for A2!)

```
def f(w0, x0, w1, x1, w2):
    s0 = w0 * x0
    s1 = w1 * x1
    s2 = s0 + s1
    s3 = s2 + w2
    L = sigmoid(s3)

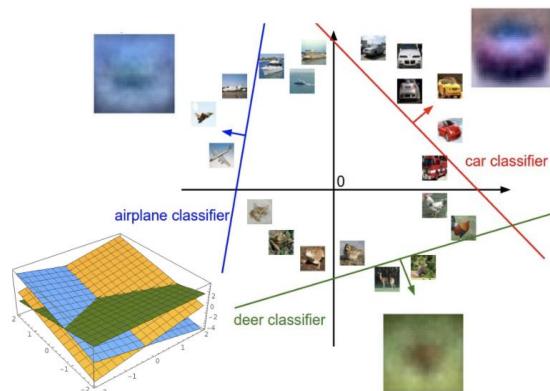
    grad_L = 1.0
    grad_s3 = grad_L * (1 - L) * L
    grad_w2 = grad_s3
    grad_s2 = grad_s3
    grad_s0 = grad_s2
    grad_s1 = grad_s2
    grad_w1 = grad_s1 * x1
    grad_x1 = grad_s1 * w1
    grad_w0 = grad_s0 * x0
    grad_x0 = grad_s0 * w0
```

Backprop can be implemented with a modular API, as a set of paired forward/backward functions (We will do this on A3!)

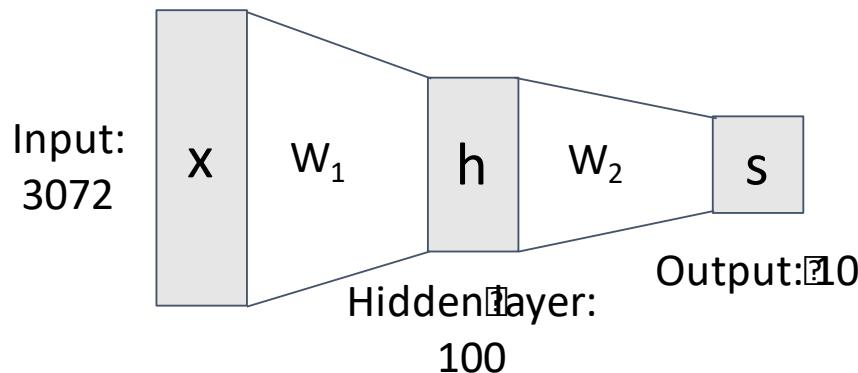
```
class Multiply(torch.autograd.Function):
    @staticmethod
    def forward(ctx, x, y):
        ctx.save_for_backward(x, y)
        z = x * y
        return z

    @staticmethod
    def backward(ctx, grad_z):
        x, y = ctx.saved_tensors
        grad_x = y * grad_z    # dz/dx * dL/dz
        grad_y = x * grad_z    # dz/dy * dL/dz
        return grad_x, grad_y
```

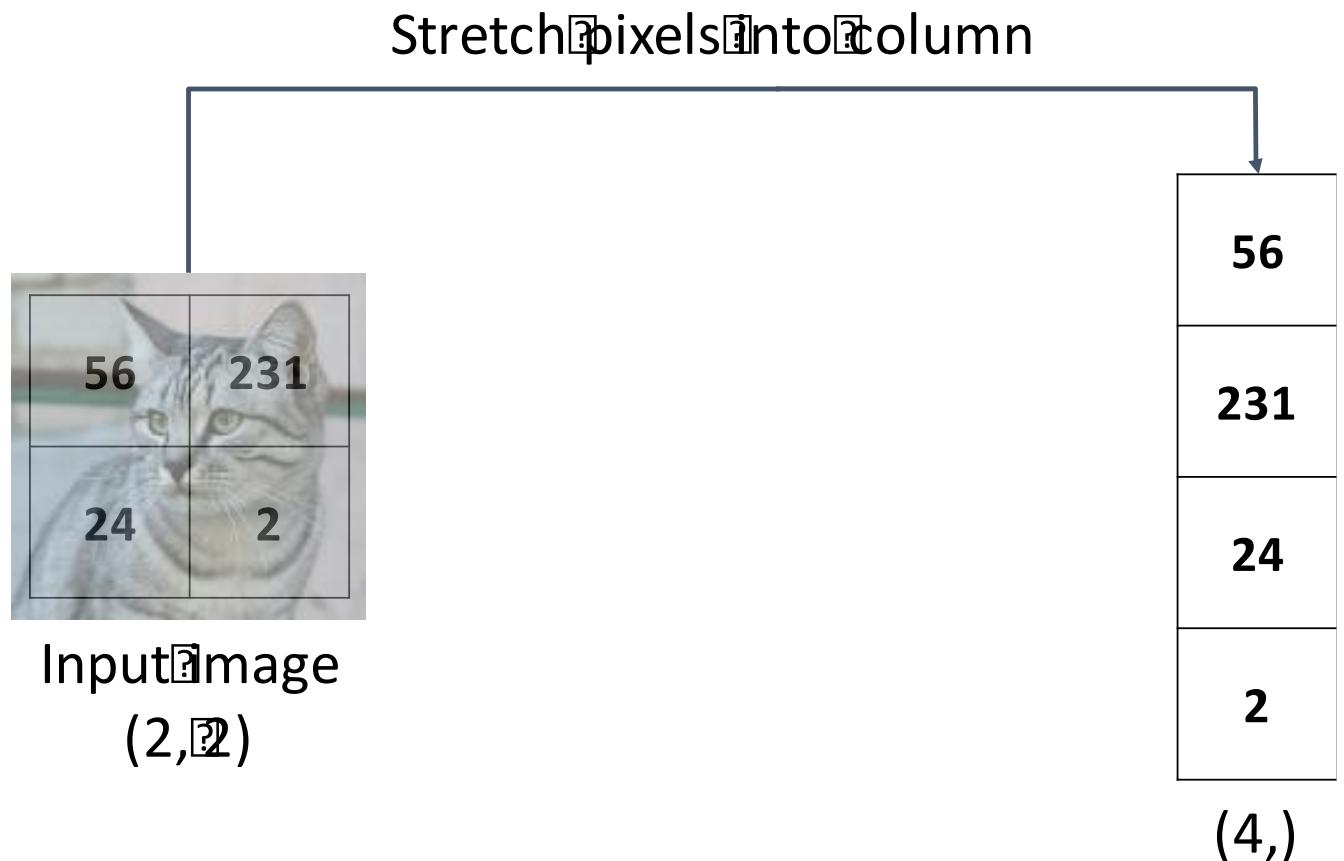
$$f(x, W) = Wx$$



$$f = W_2 \max(0, W_1 x)$$



Problem: So far our classifiers don't respect the spatial structure of images!



Next time:
Convolutional Neural Networks