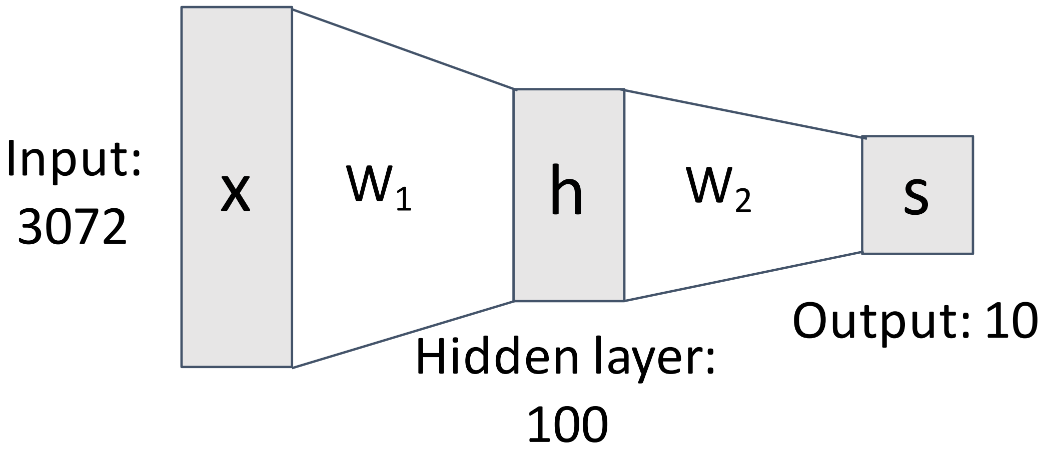
Lecture 6: Backpropagation

Justin Johnson
2022

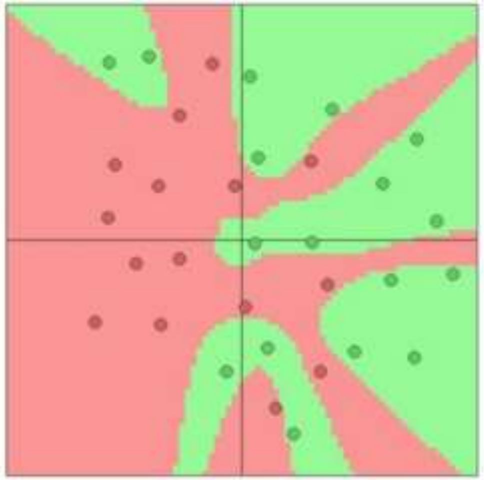
Last time: Neural Networks

From linear classifiers to
fully-connected networks

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



Space Warping



Problem: How to compute gradients?

$$s = f(x; W_1, W_2) = W_2 \max(0, W_1 x)$$ Nonlinear score function

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

$$R(W) = \sum_k W_k^2$$ Regularization

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \lambda R(W_1) + \lambda R(W_2)$$ Total loss: data loss + regularization

If we can compute $\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial W_2}$ n we can learn W_1 and W_2

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

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

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

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

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

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

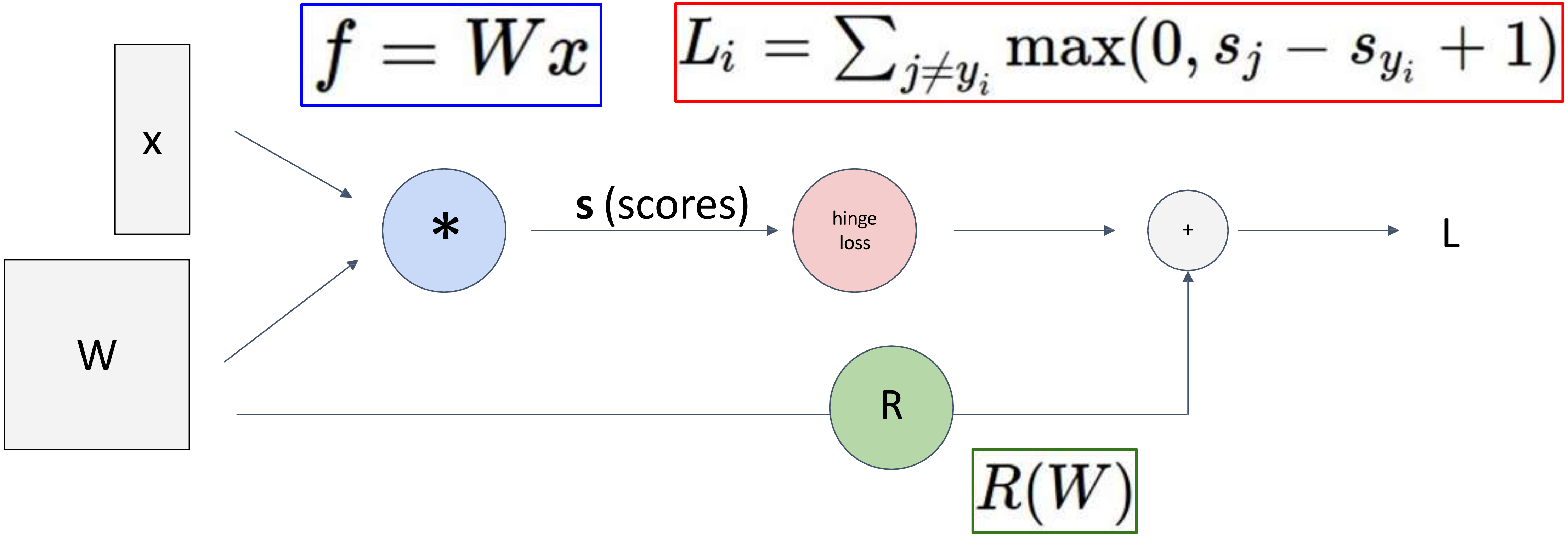
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

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

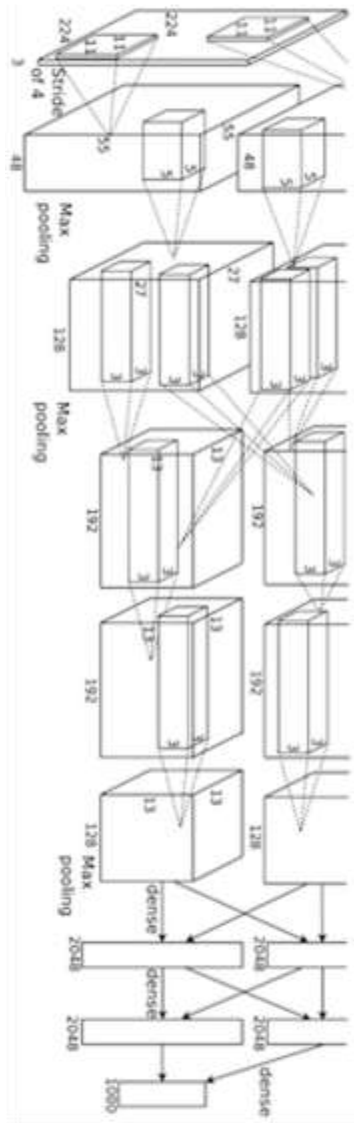


Deep Network (AlexNet)

input image

weights

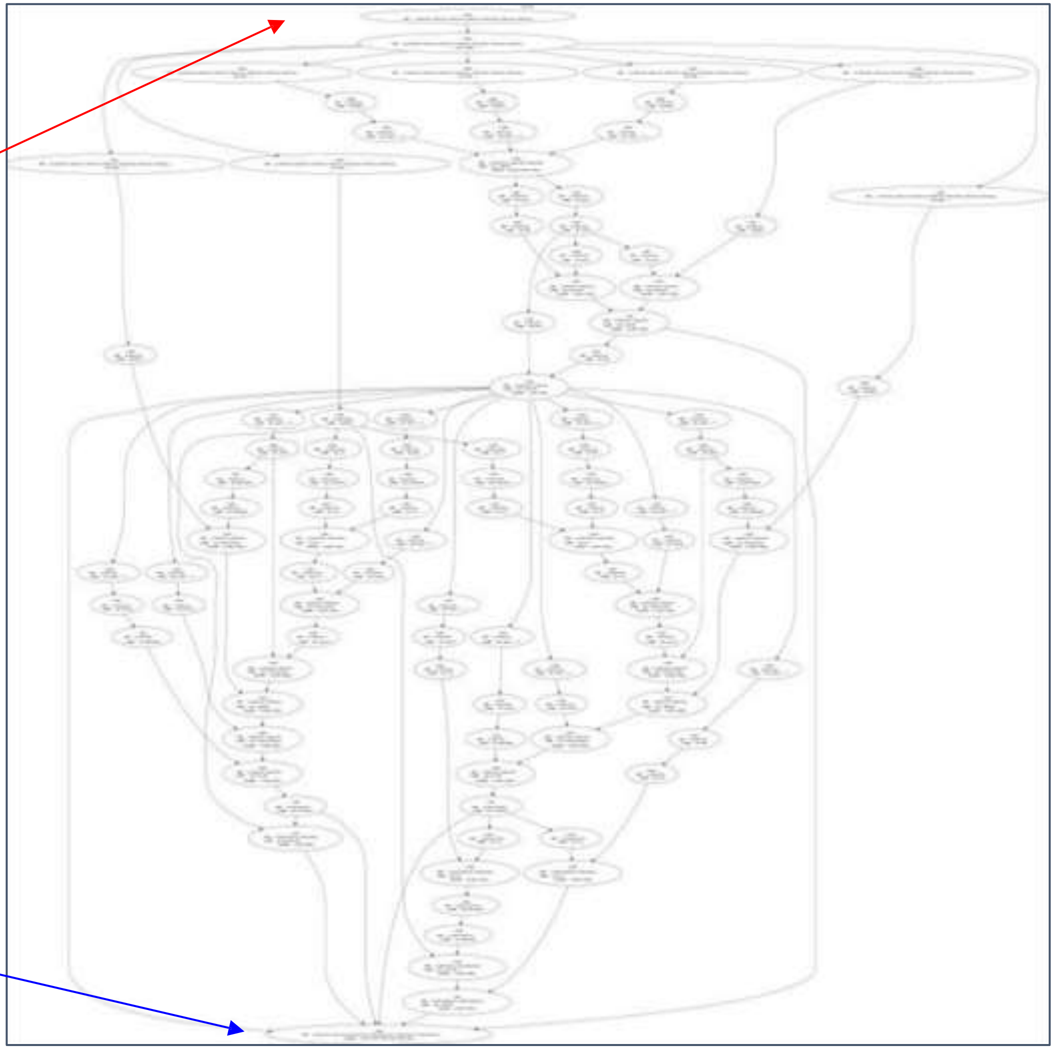
loss



Neural Turing Machine

input image

loss



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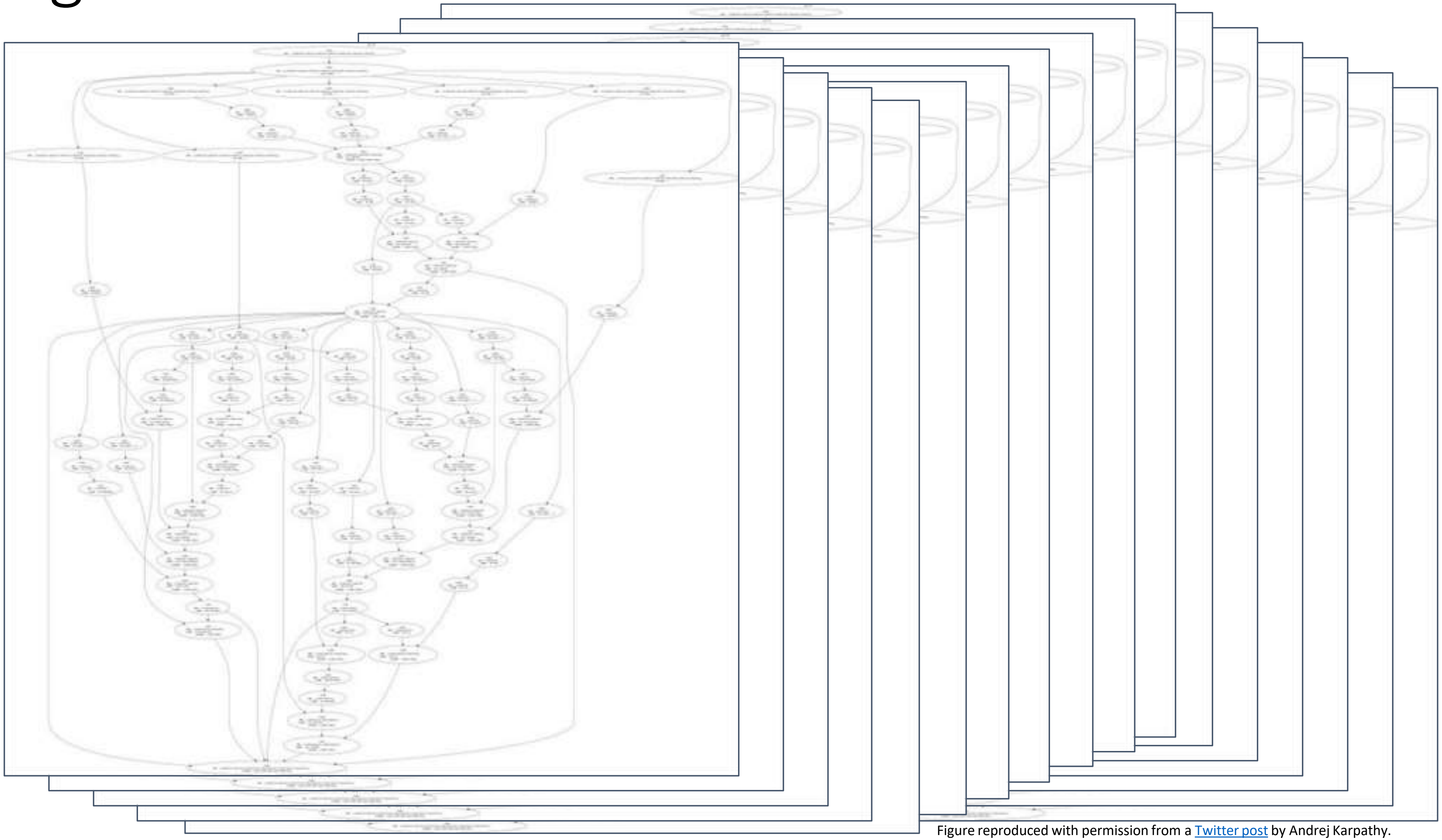
Graves et al, arXiv 2014

Neural Turing Machine



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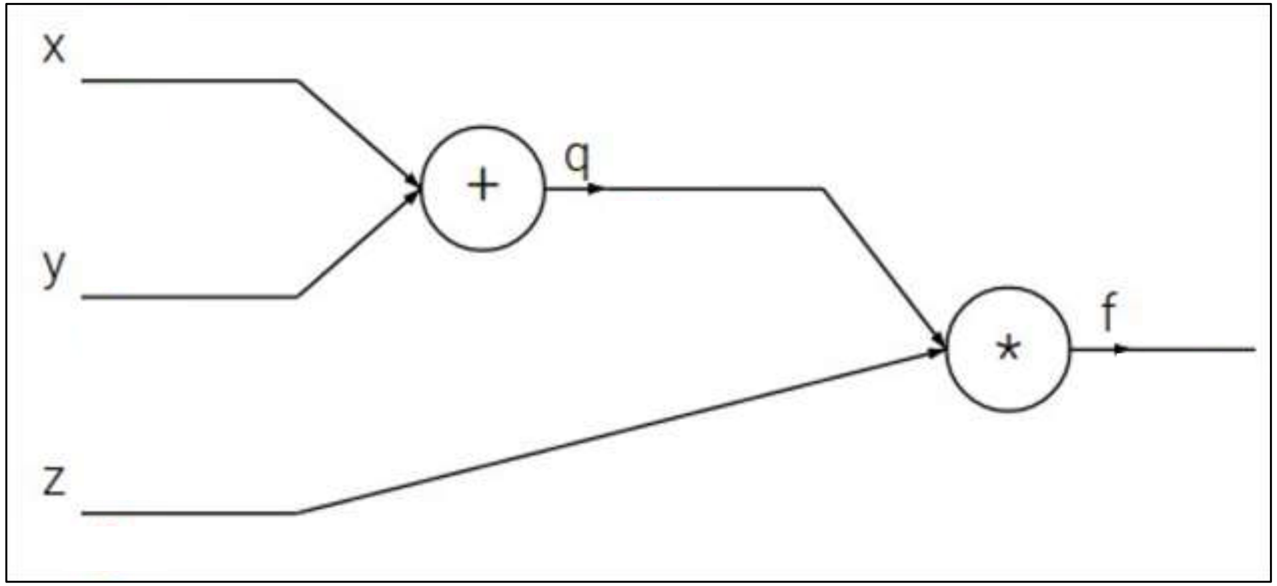
Backpropagation: Simple Example

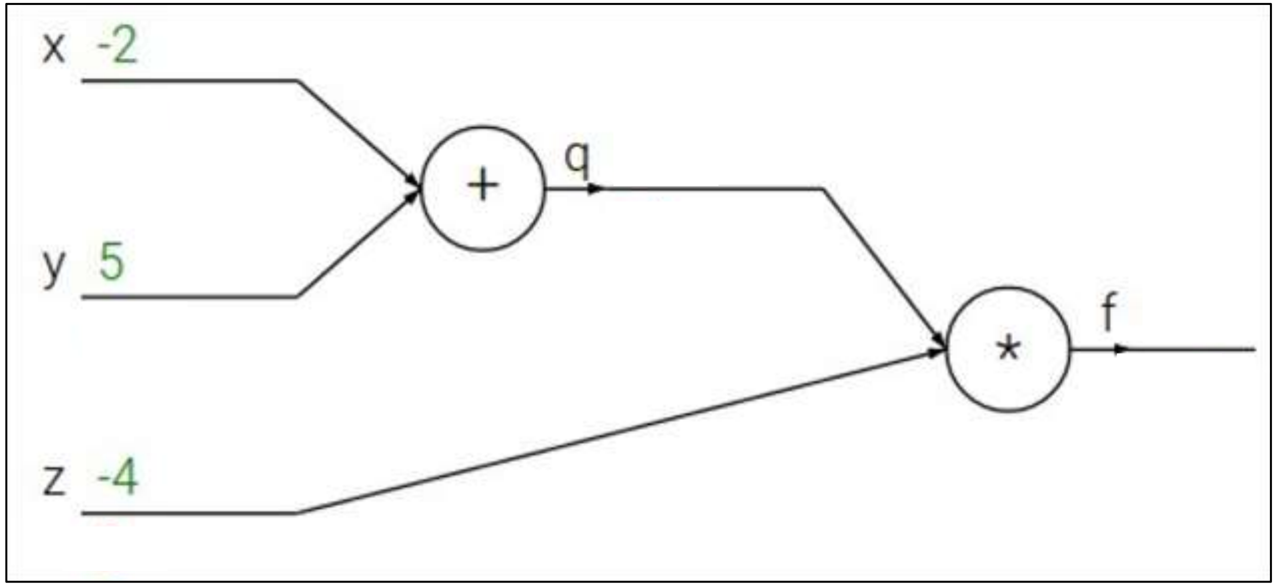
$$f(x, y, z) = (x + y)z$$



Backpropagation: Simple Example

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

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



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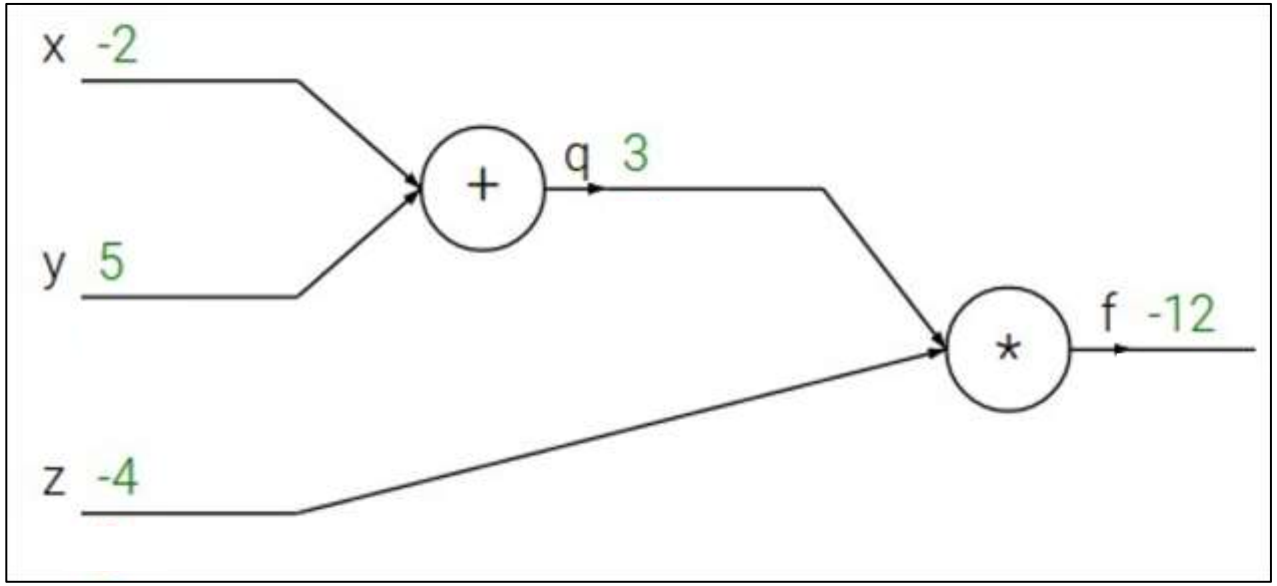
1. Forward pass: Compute outputs

$$q = x + y \qquad f = qz$$



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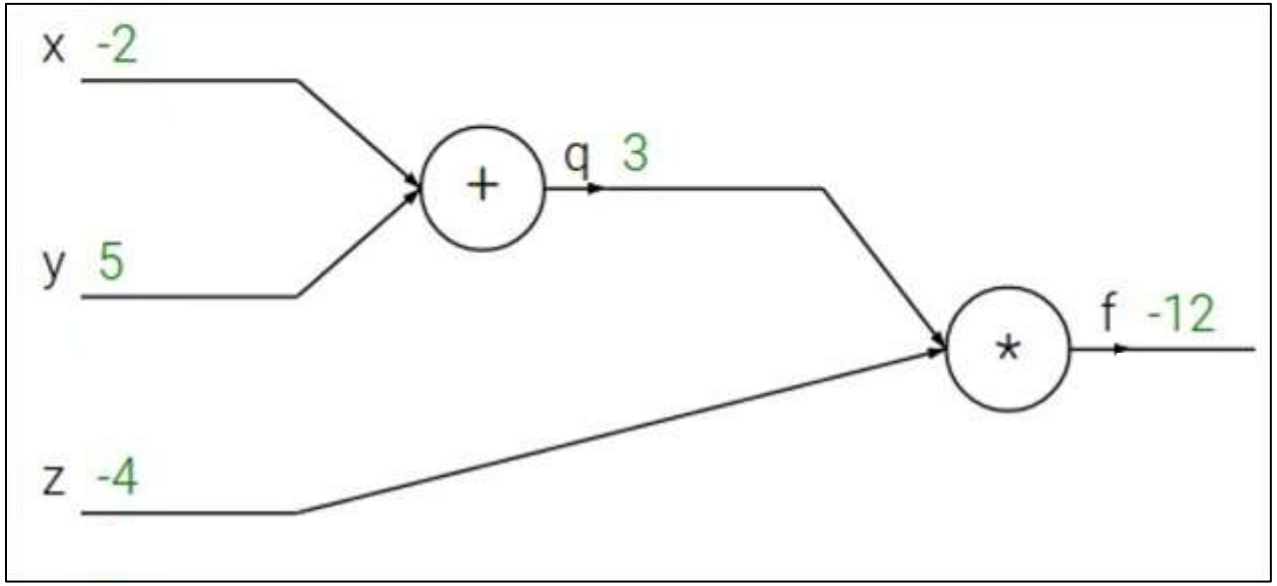

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2. Backward pass: Compute derivatives

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

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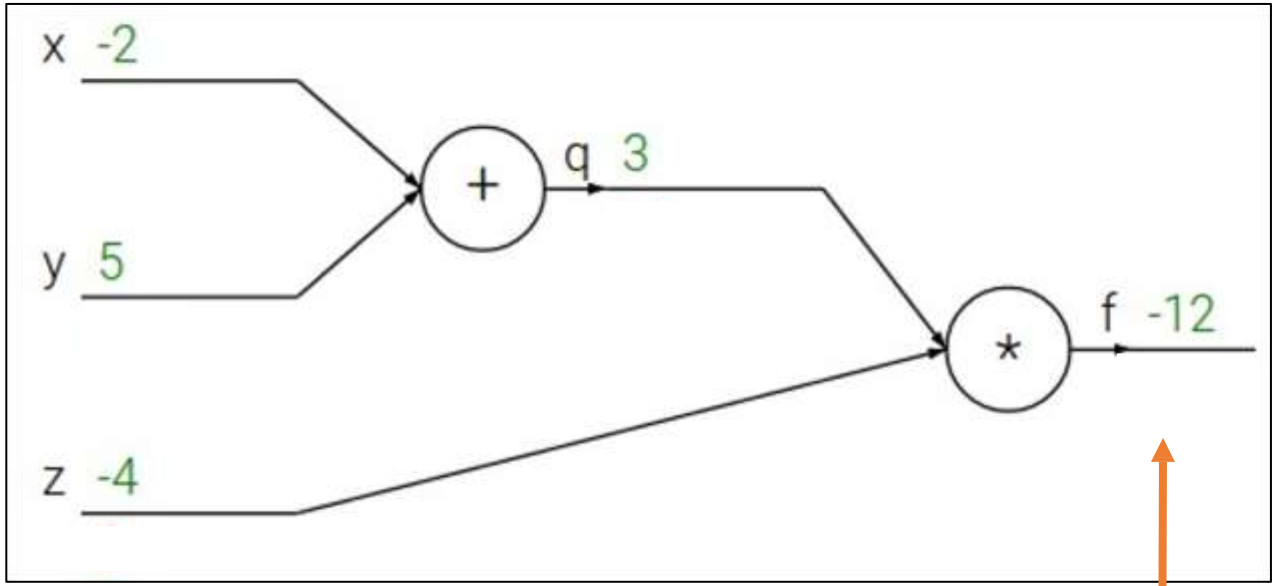

$$\frac{\partial f}{\partial f}$$

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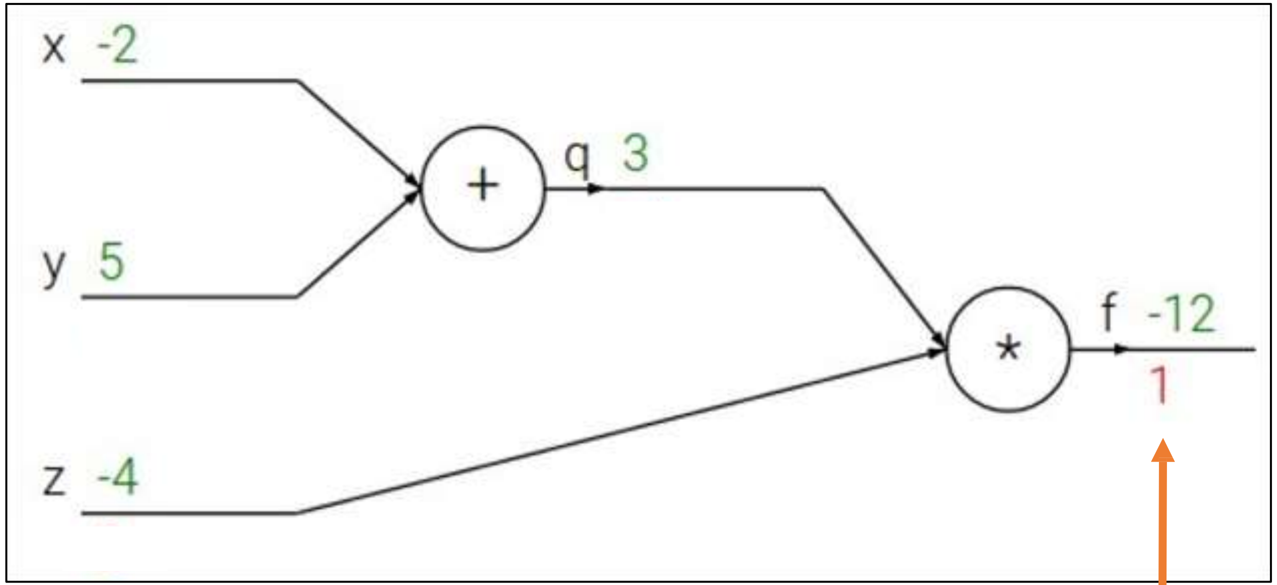

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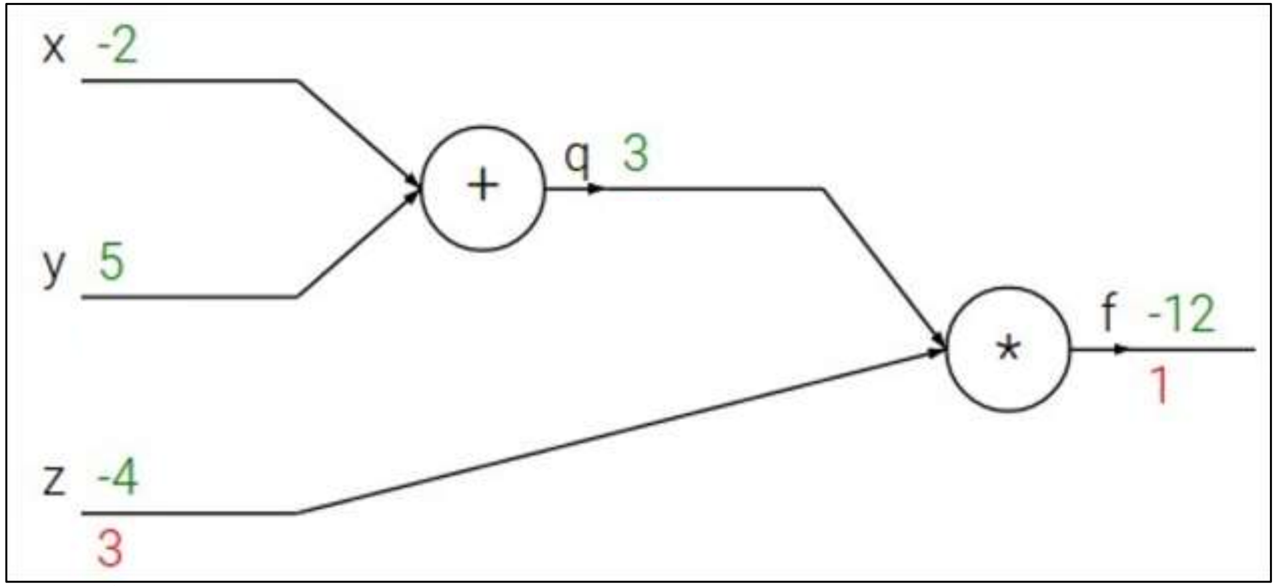

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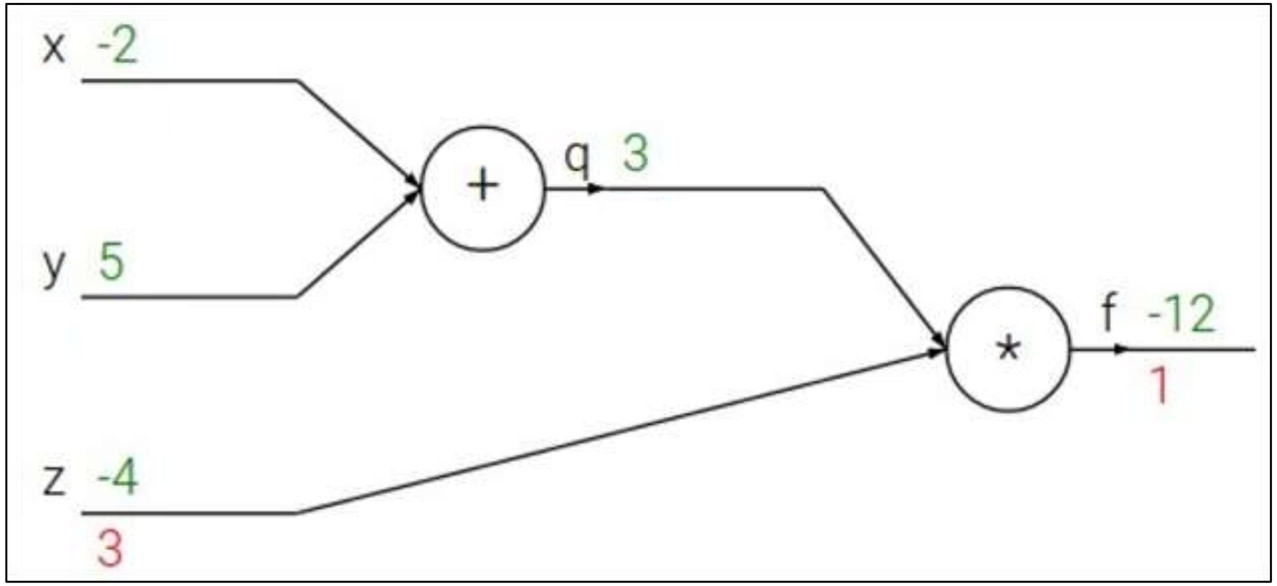

1. Forward pass: Compute outputs

$$q = x + y \qquad \boxed{f = qz}$$

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

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

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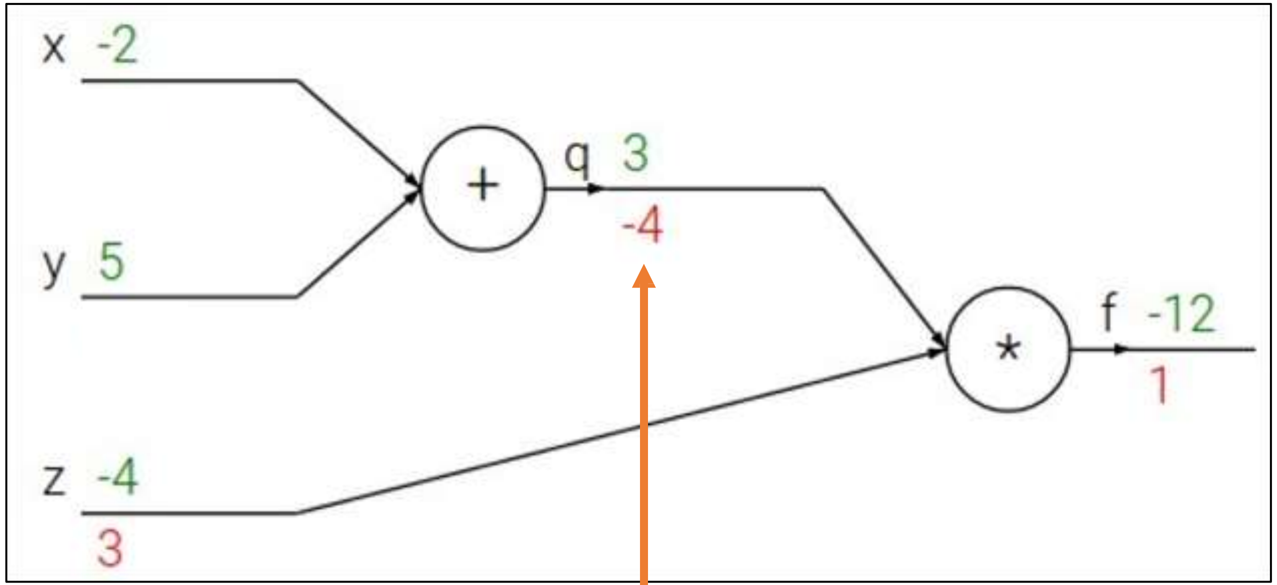

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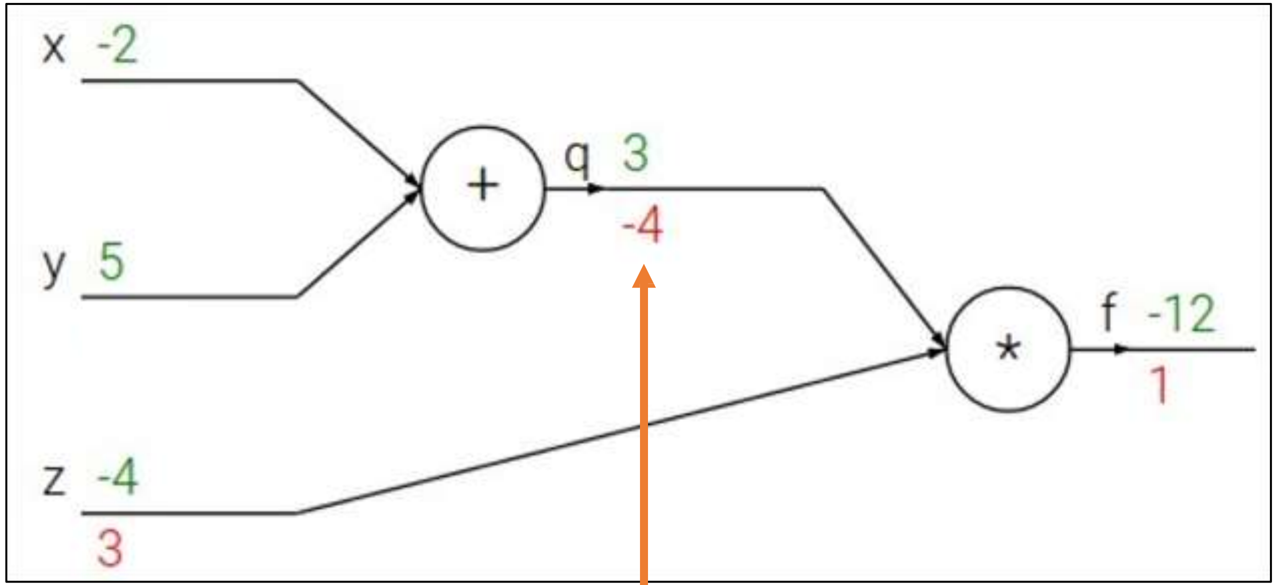

$$\boxed{\frac{\partial f}{\partial q} = z}$$

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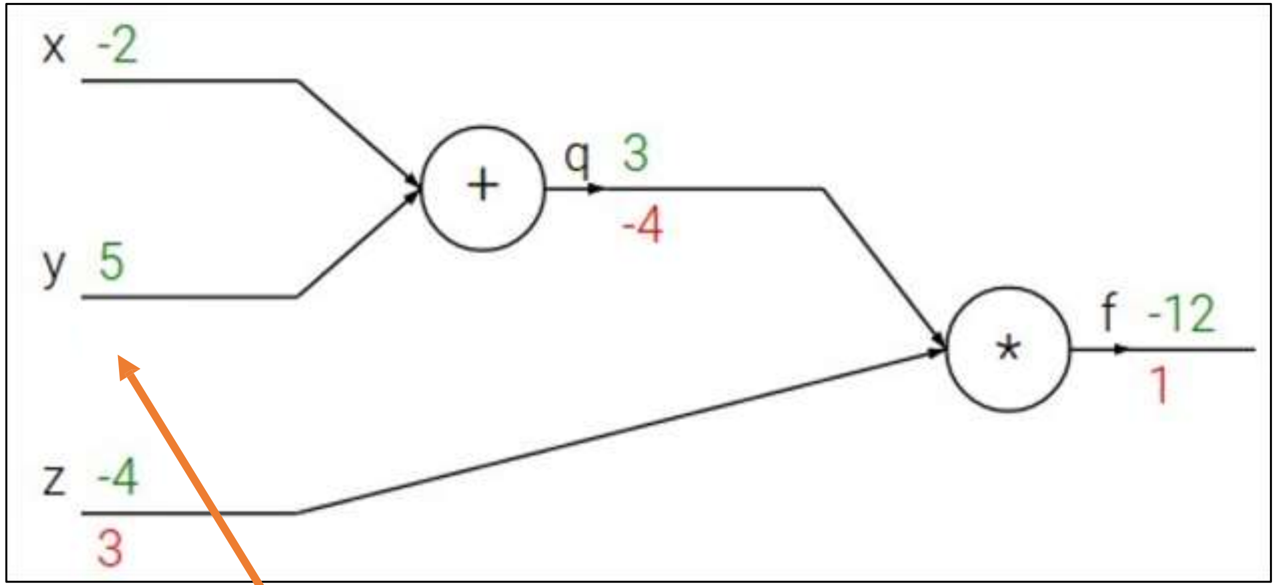

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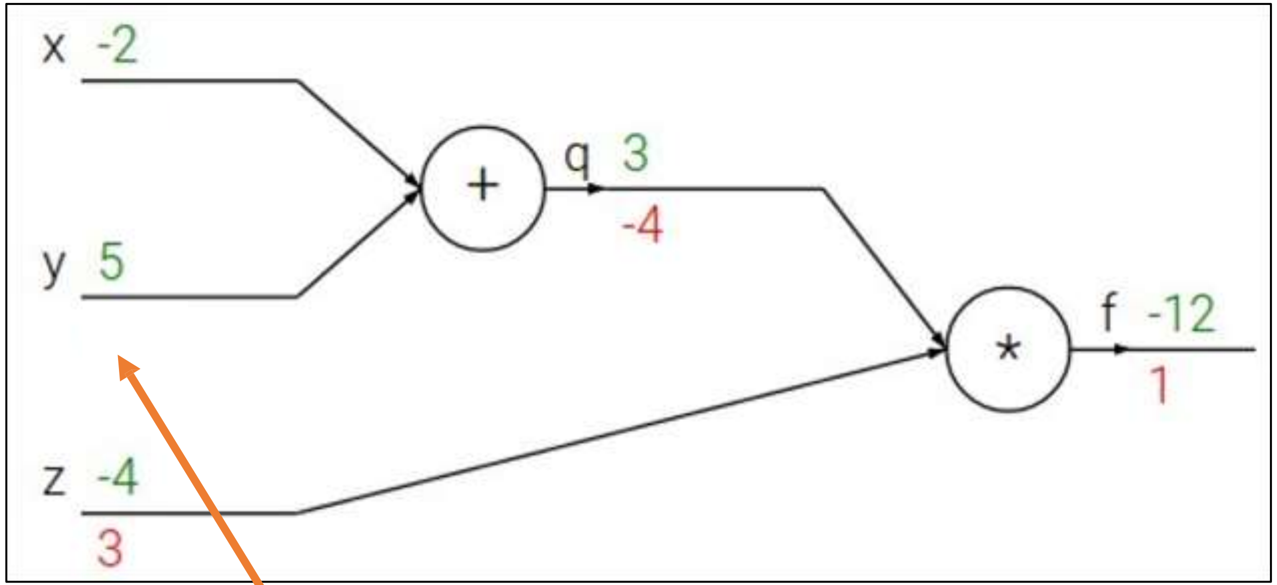

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Chain Rule

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

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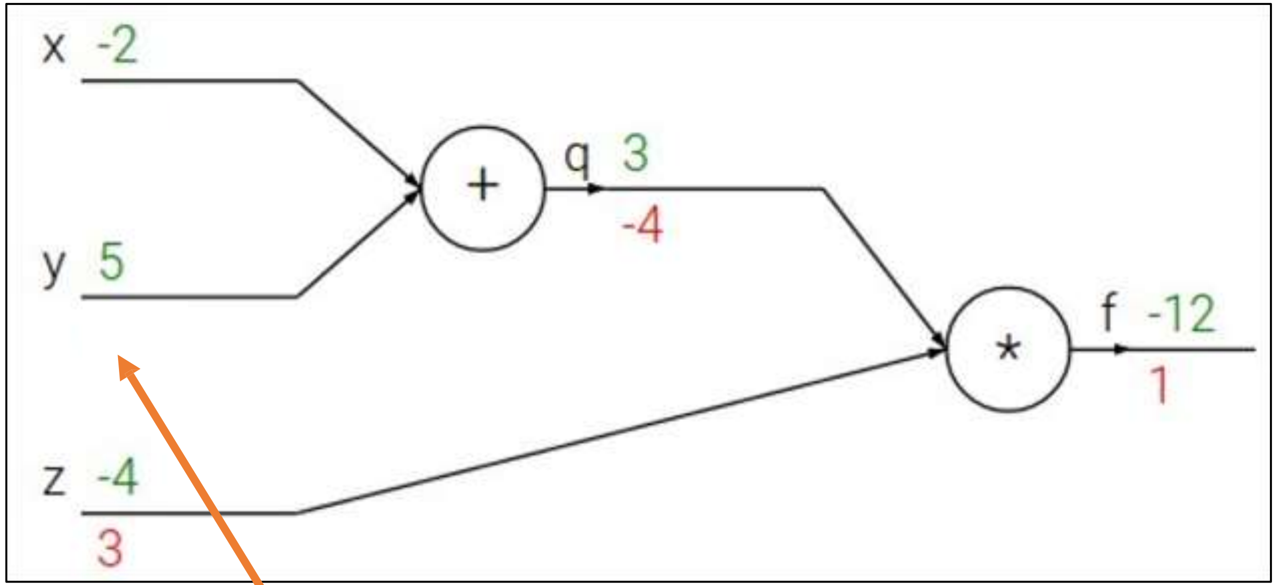

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Downstream Gradient **Local Gradient** **Upstream Gradient**

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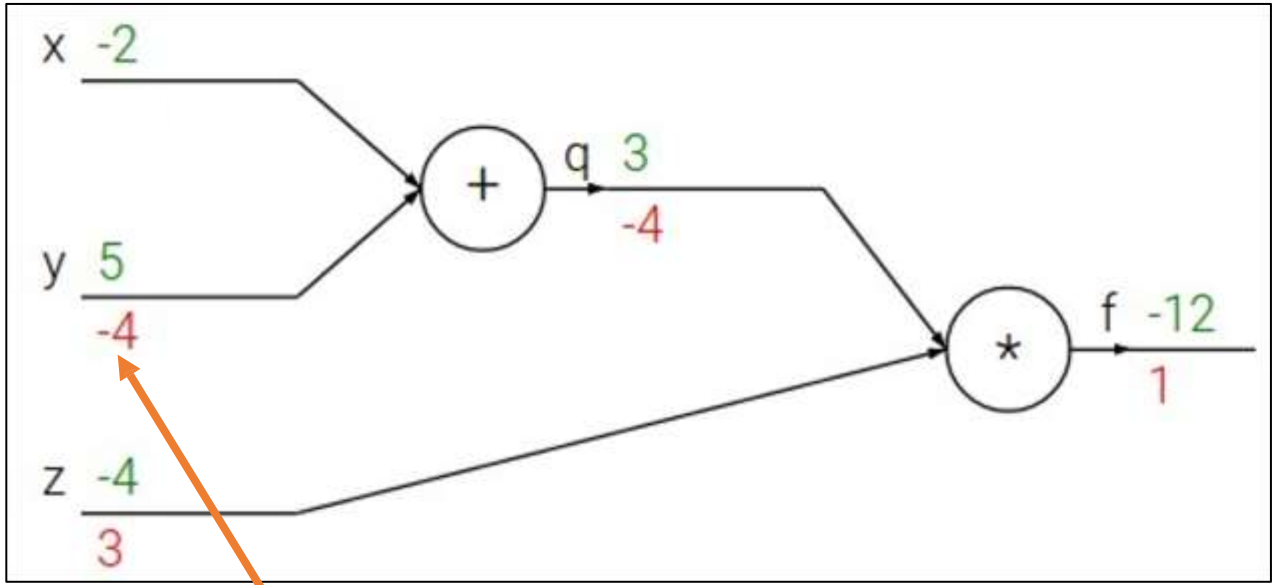

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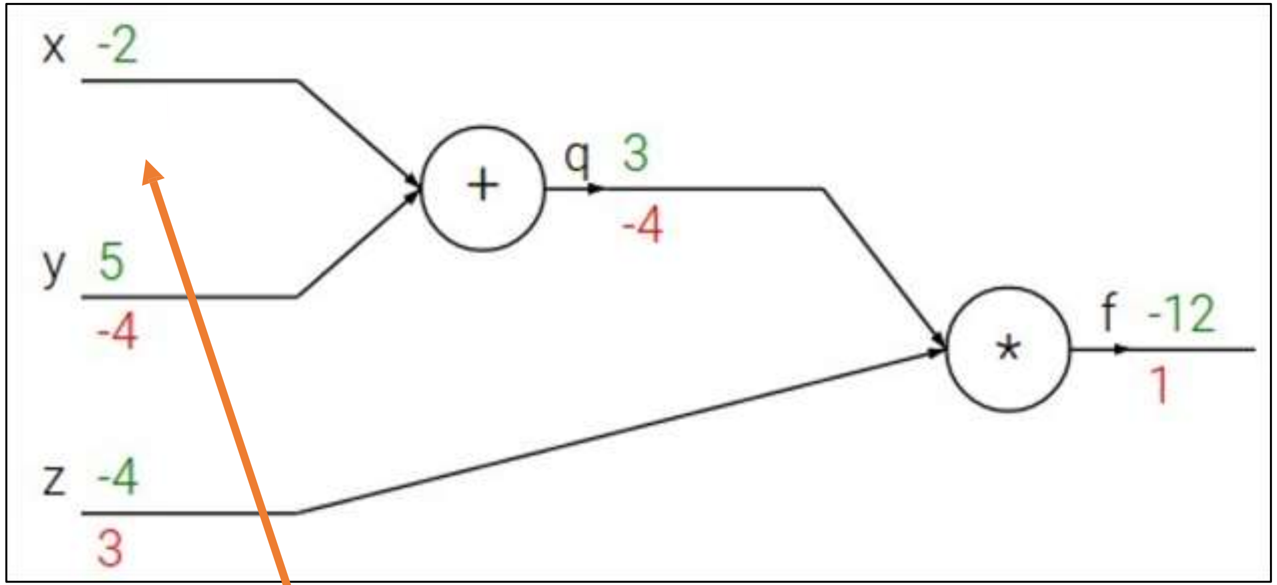

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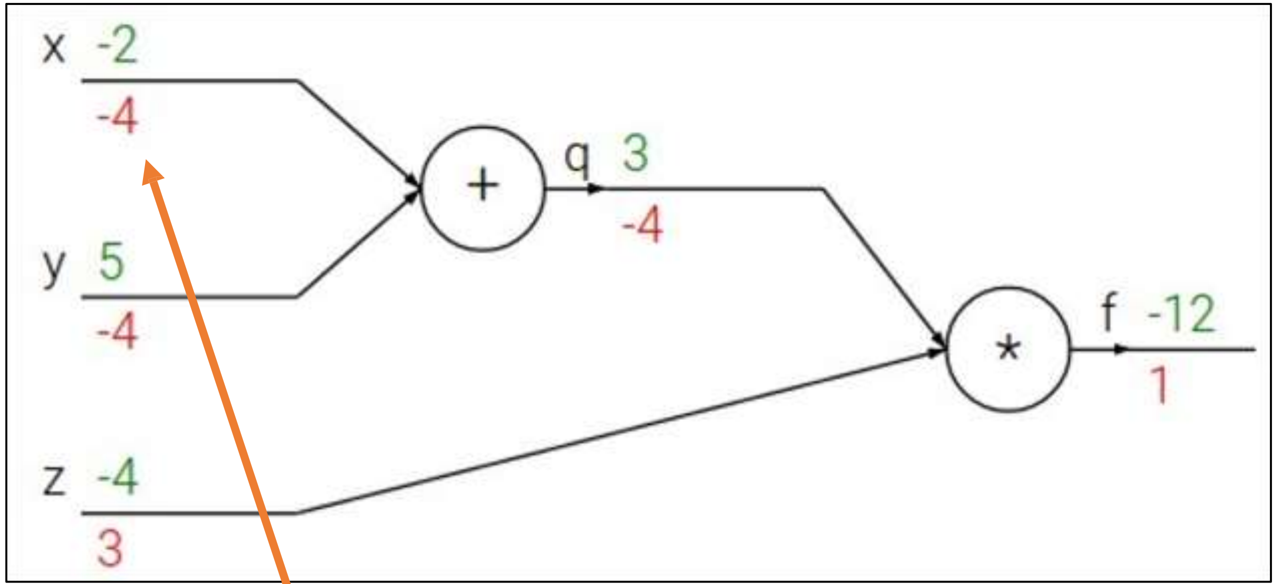

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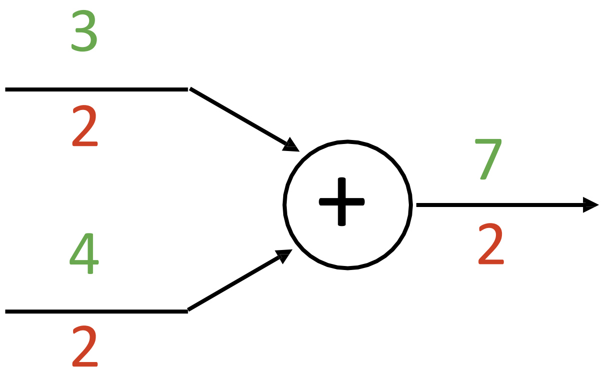
Patterns in Gradient Flow

add gate: gradient distributor



Patterns in Gradient Flow

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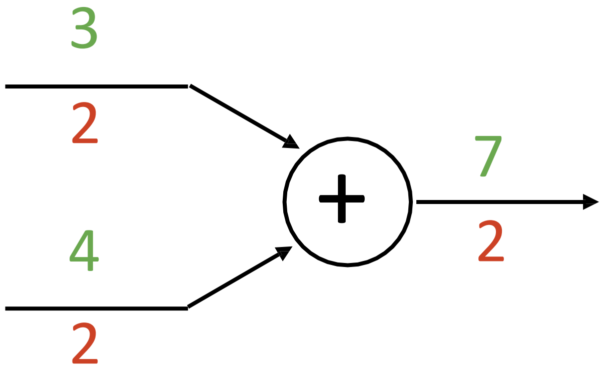
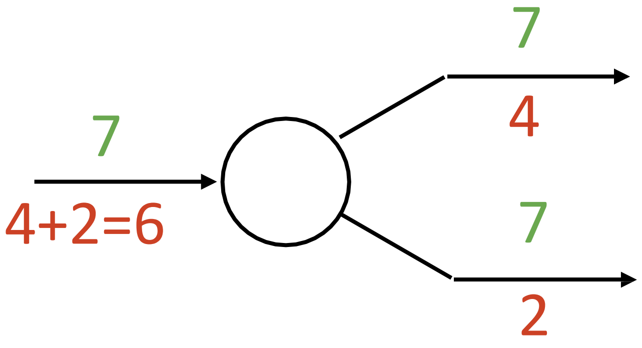


copy gate: gradient adder



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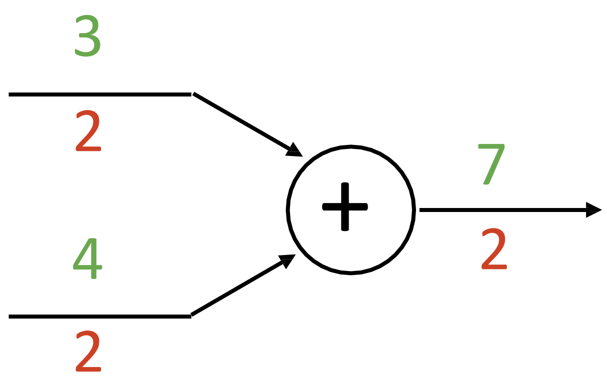
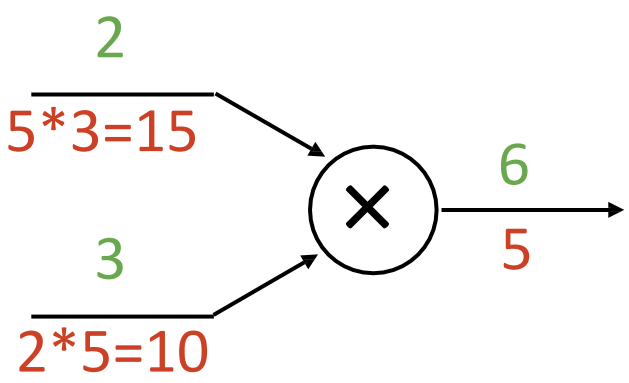


mul gate: "swap multiplier"



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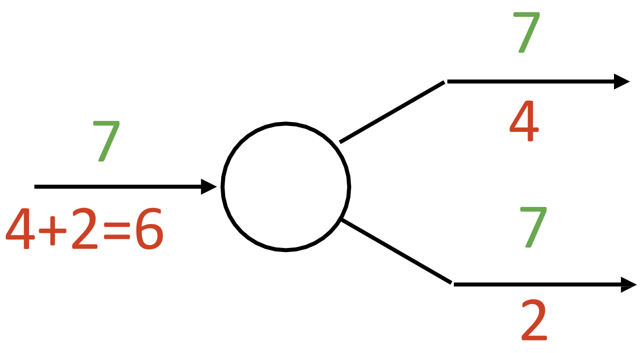

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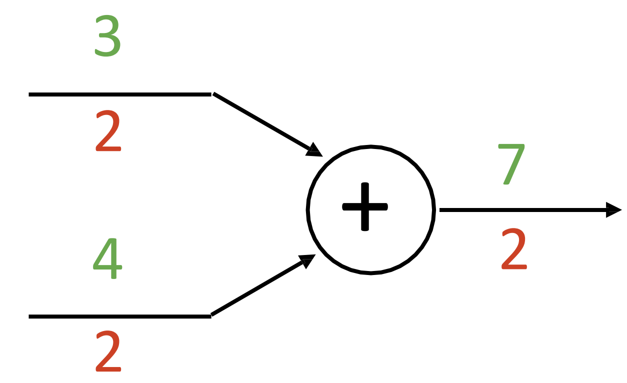

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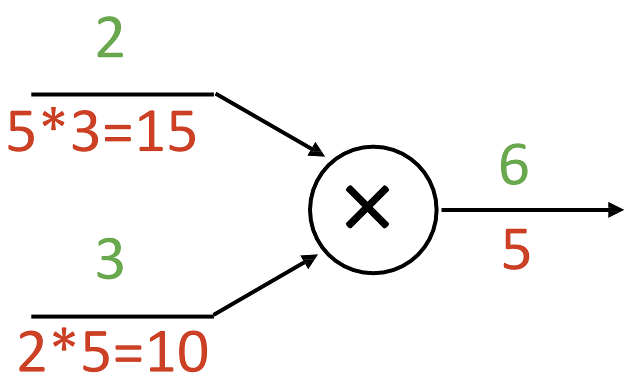

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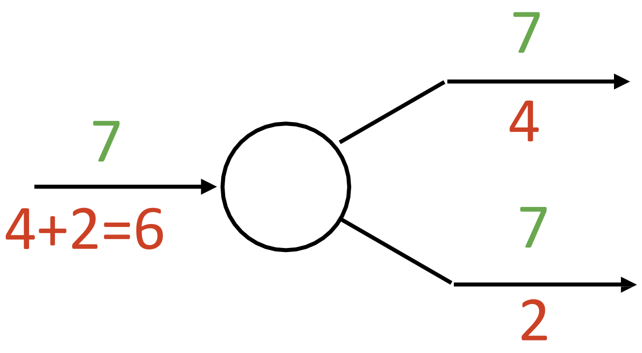
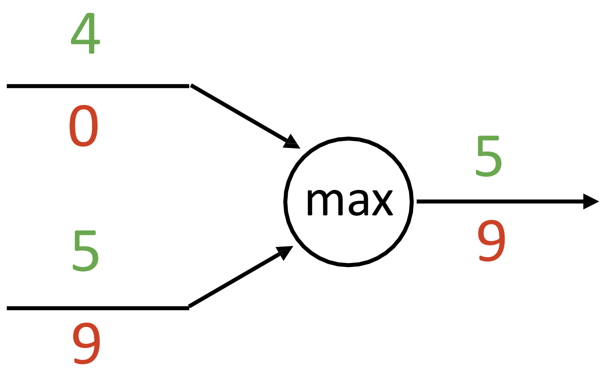
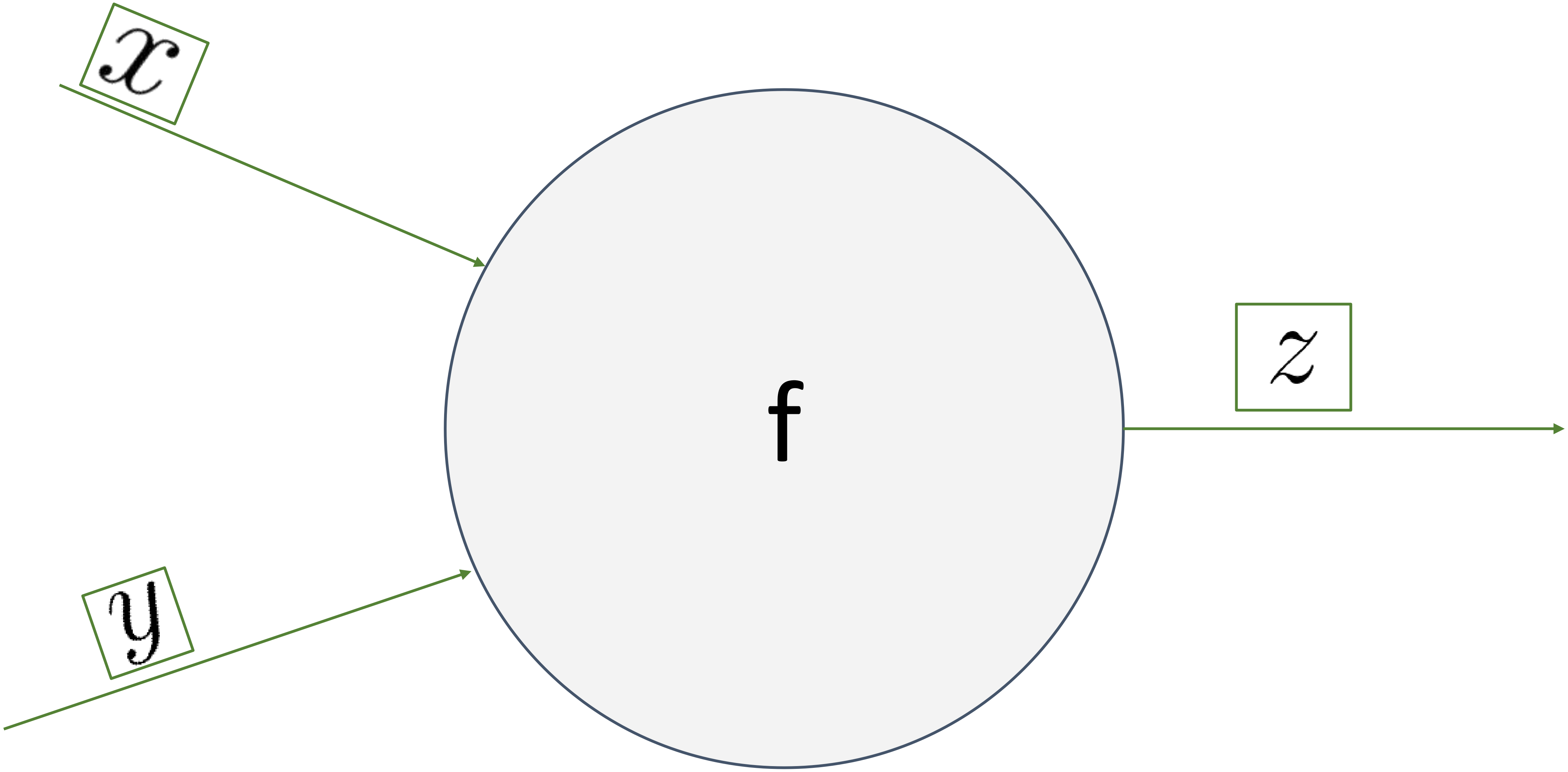
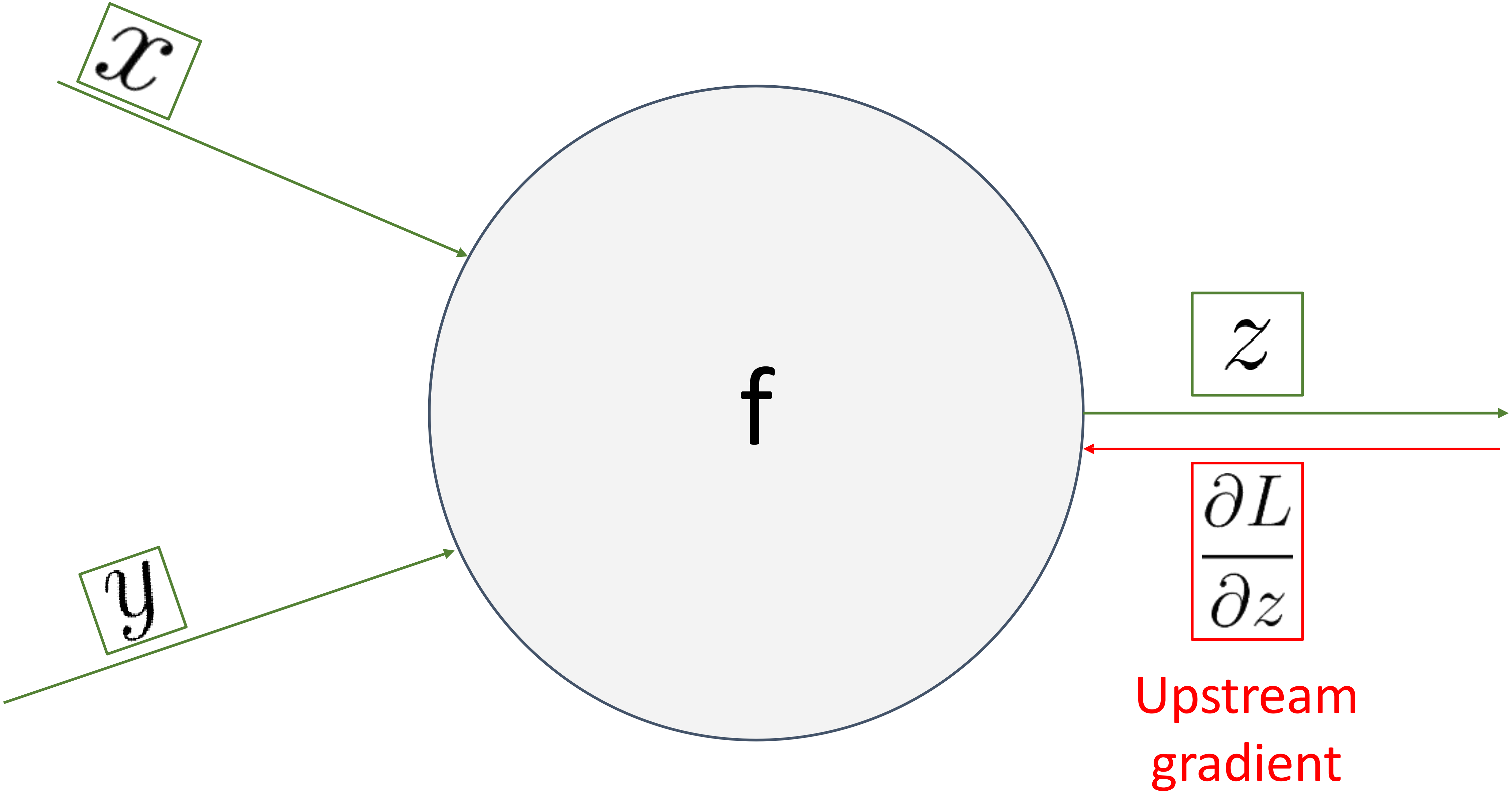


max gate: gradient router

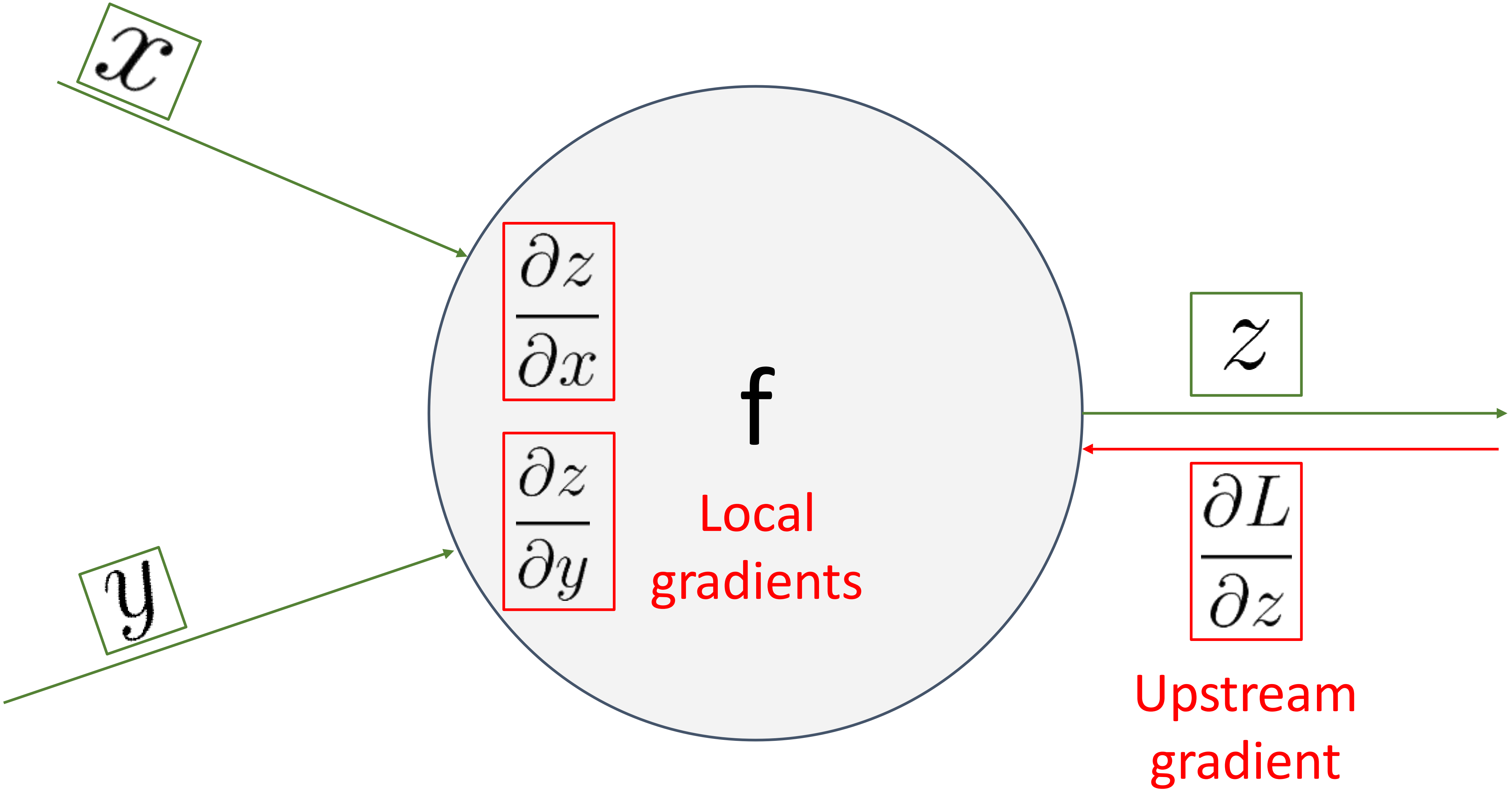


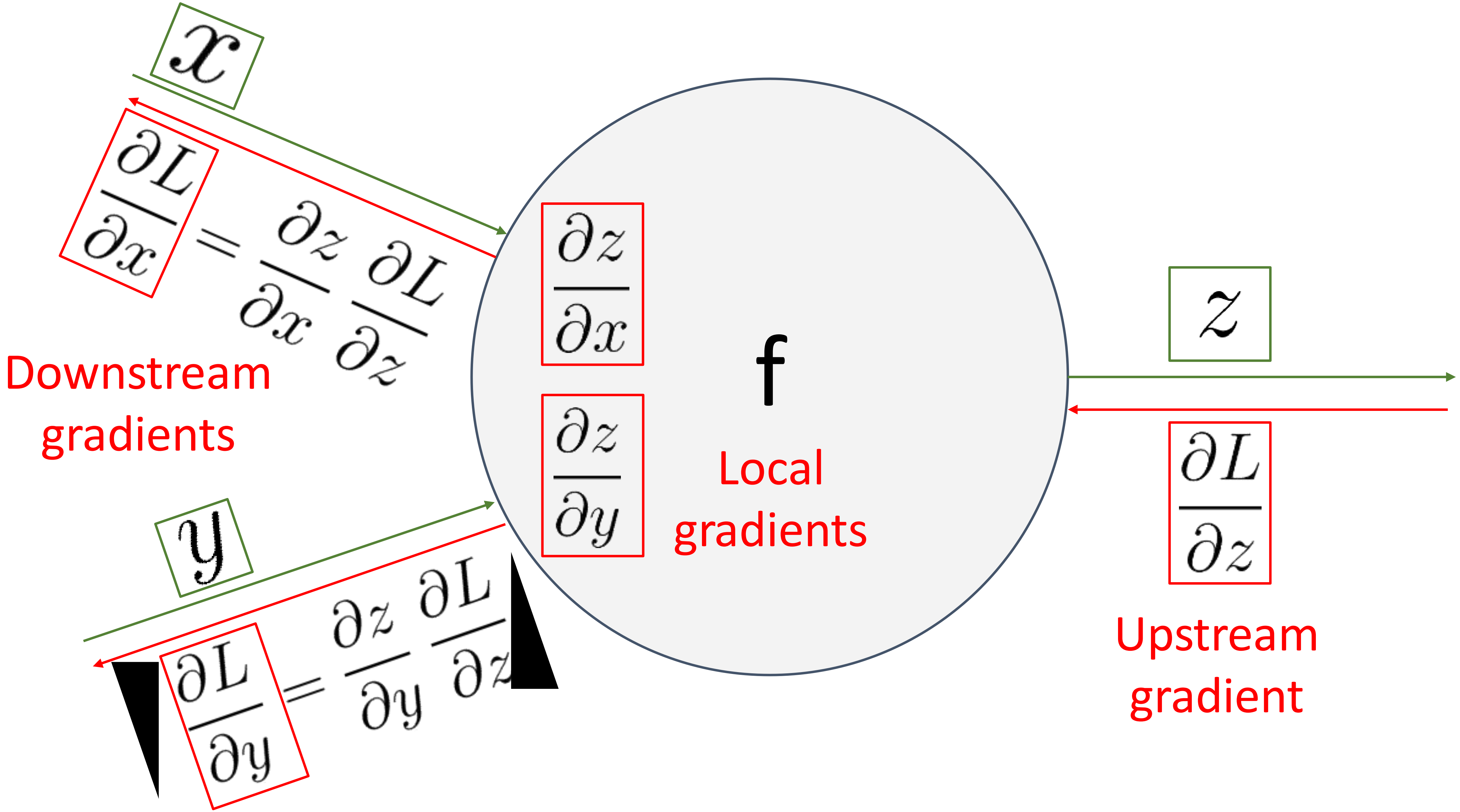


x
y
f
z



x
y
f
z
$\frac{\partial L}{\partial z}$
Upstream gradient


x
y
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
Local gradients
z
$\frac{\partial L}{\partial z}$
Upstream gradient


x
$\frac{\partial L}{\partial x} = \frac{\partial z}{\partial x}\frac{\partial L}{\partial z}$
Downstream gradients
y
$\frac{\partial L}{\partial y} = \frac{\partial z}{\partial y}\frac{\partial L}{\partial z}$
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
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z
$\frac{\partial L}{\partial z}$
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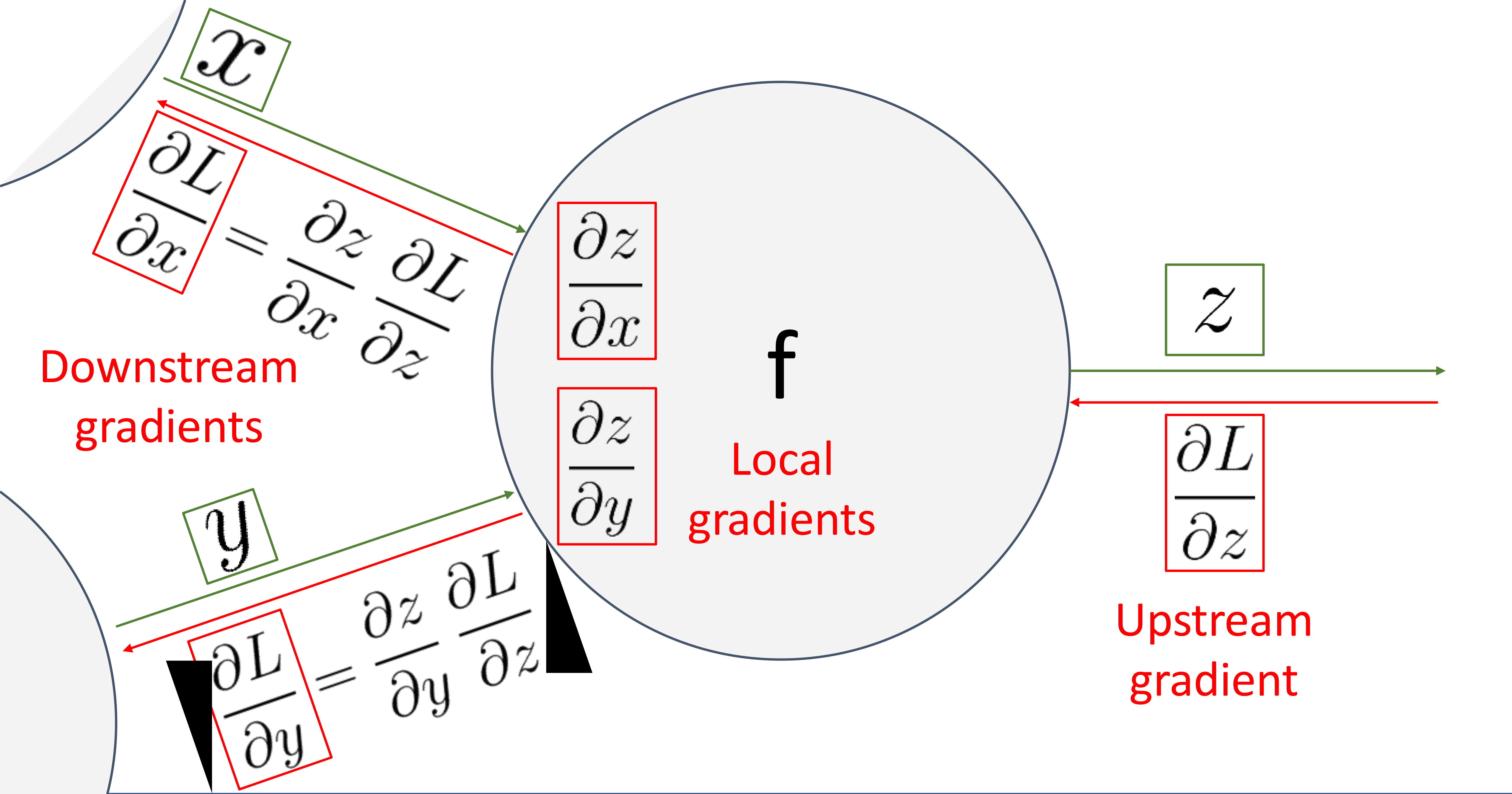

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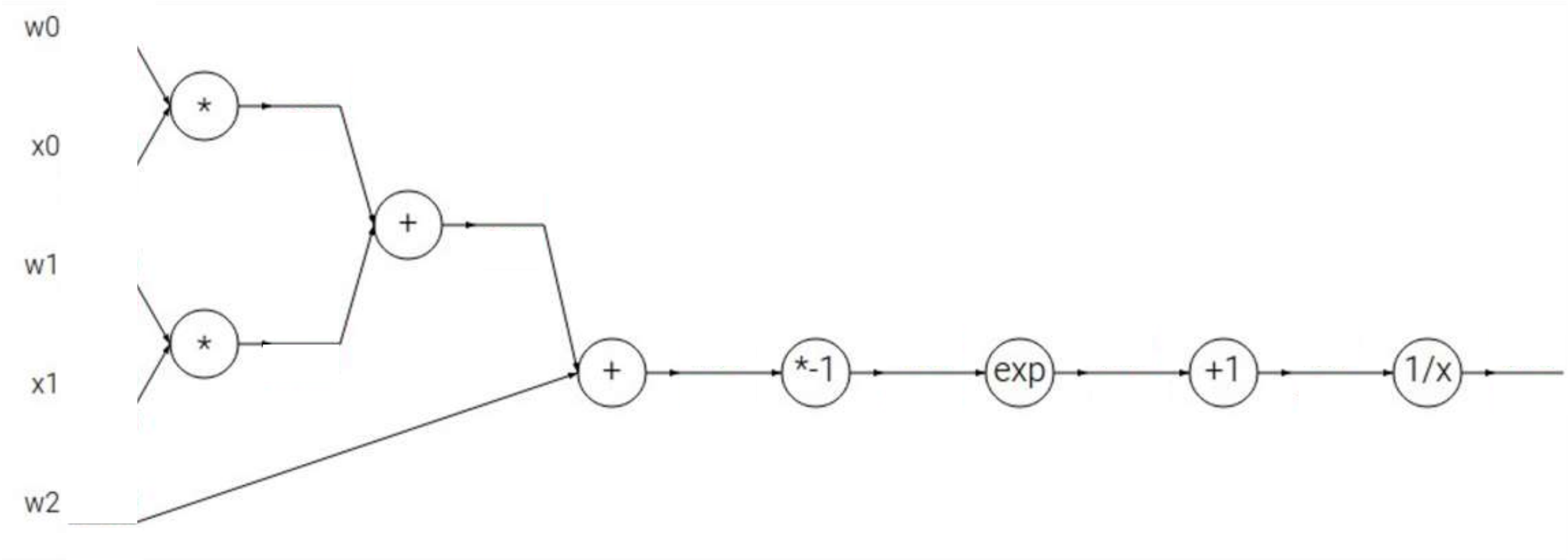
Upstream gradient

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



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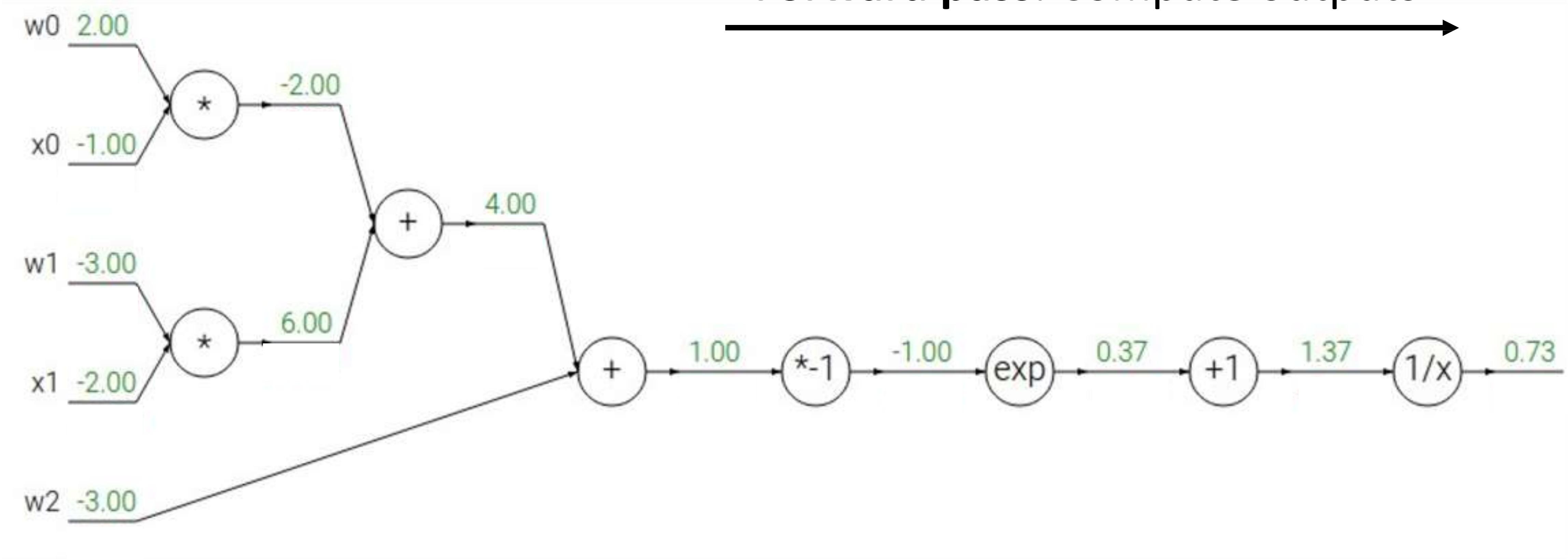

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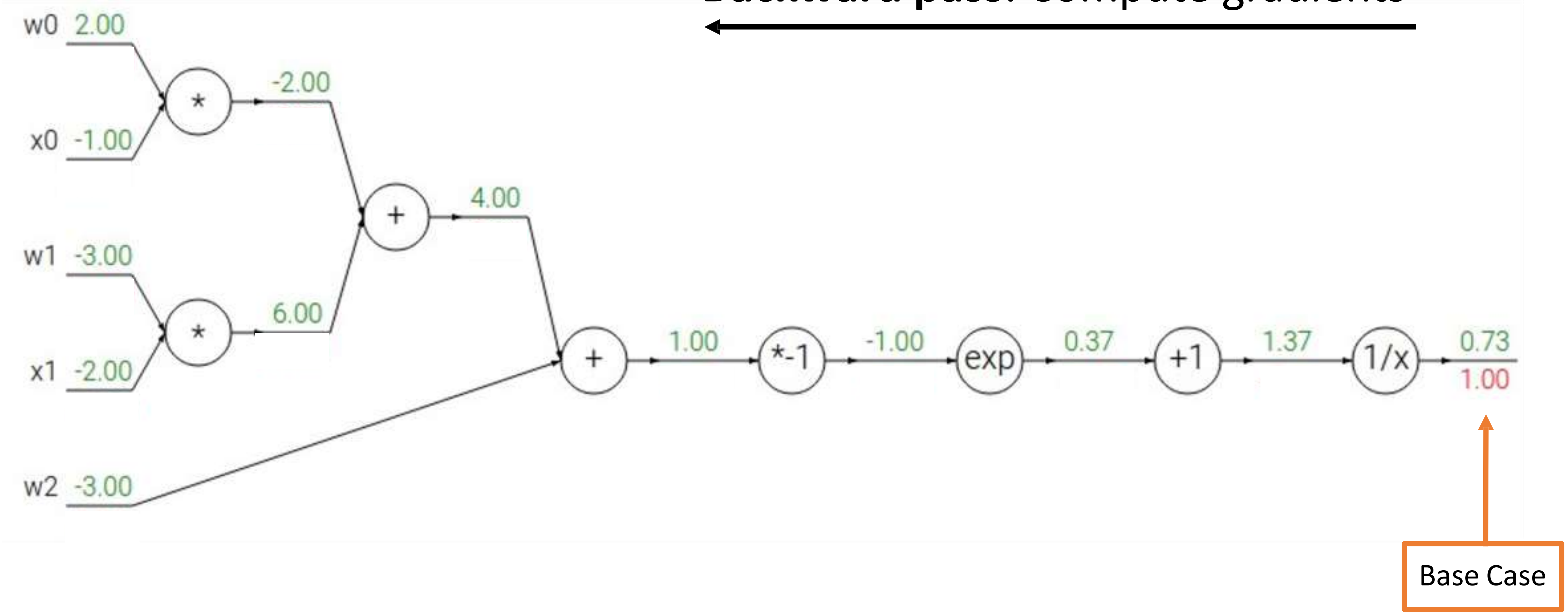
Backward pass: Compute gradients



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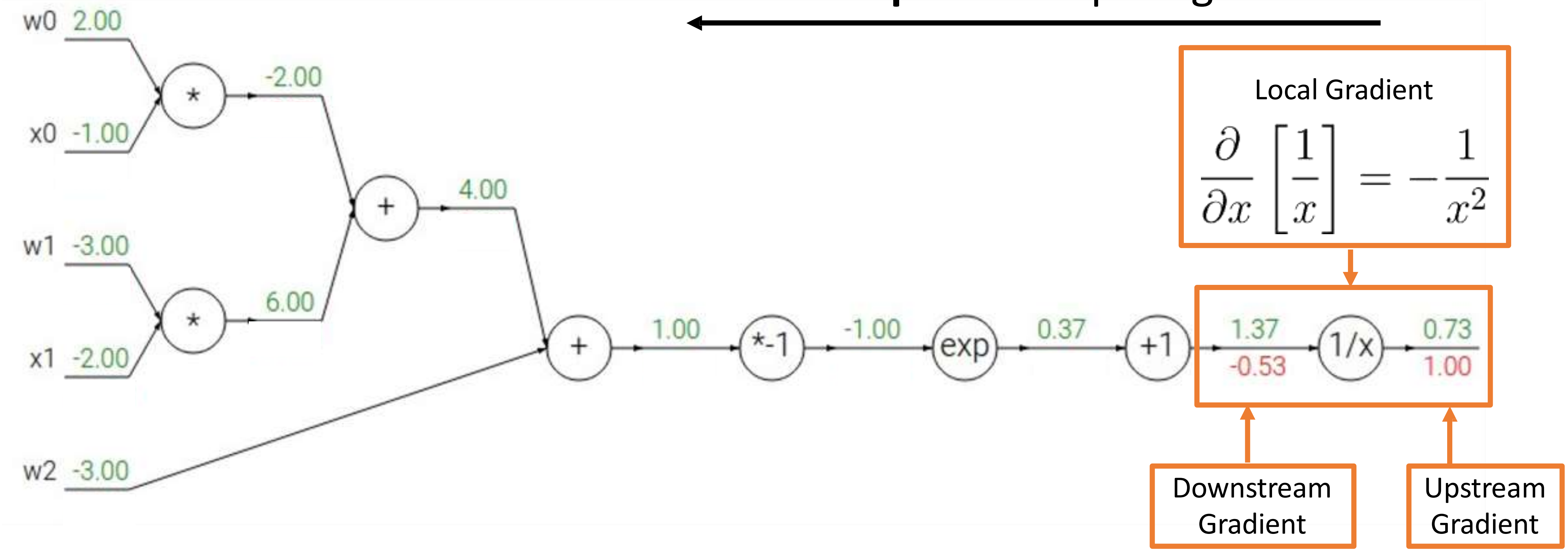

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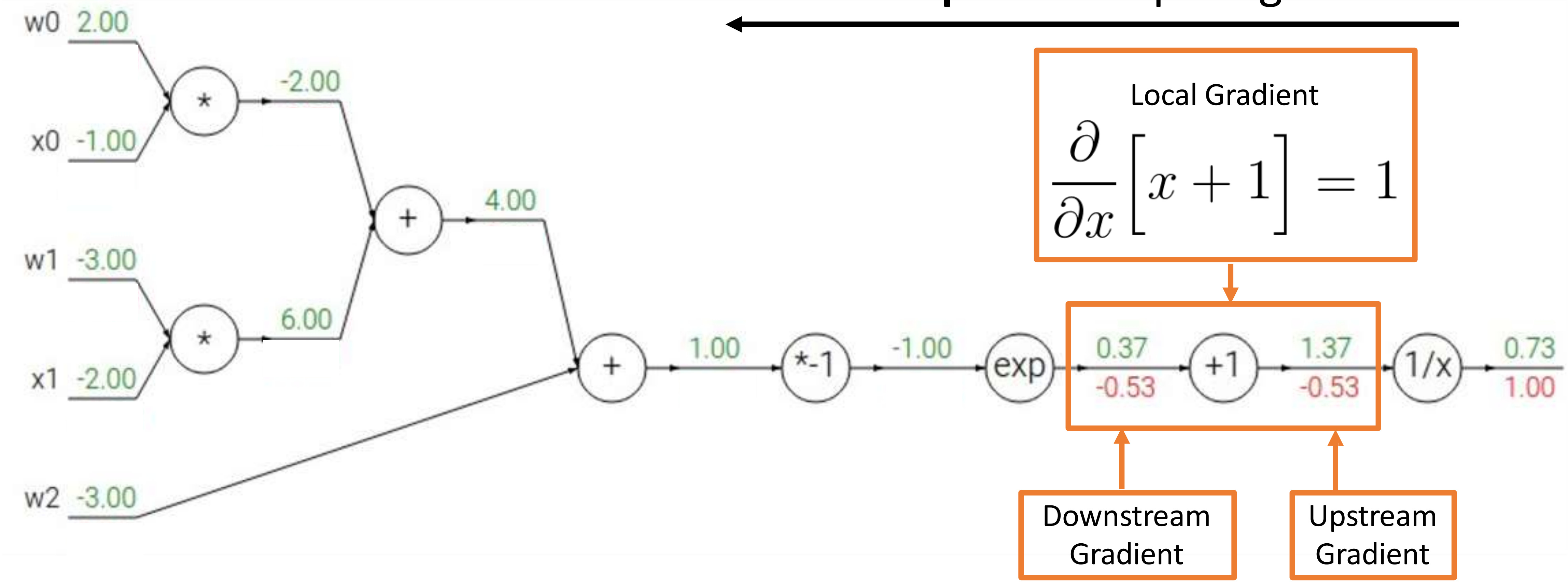

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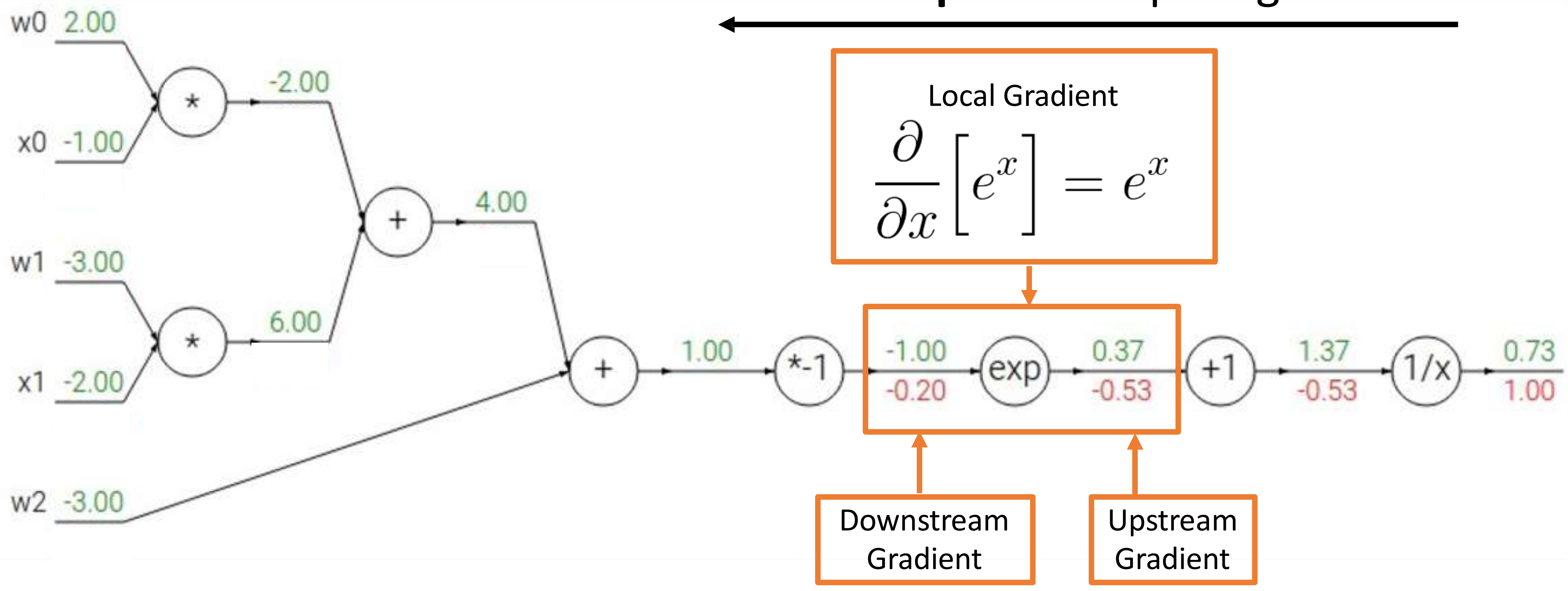

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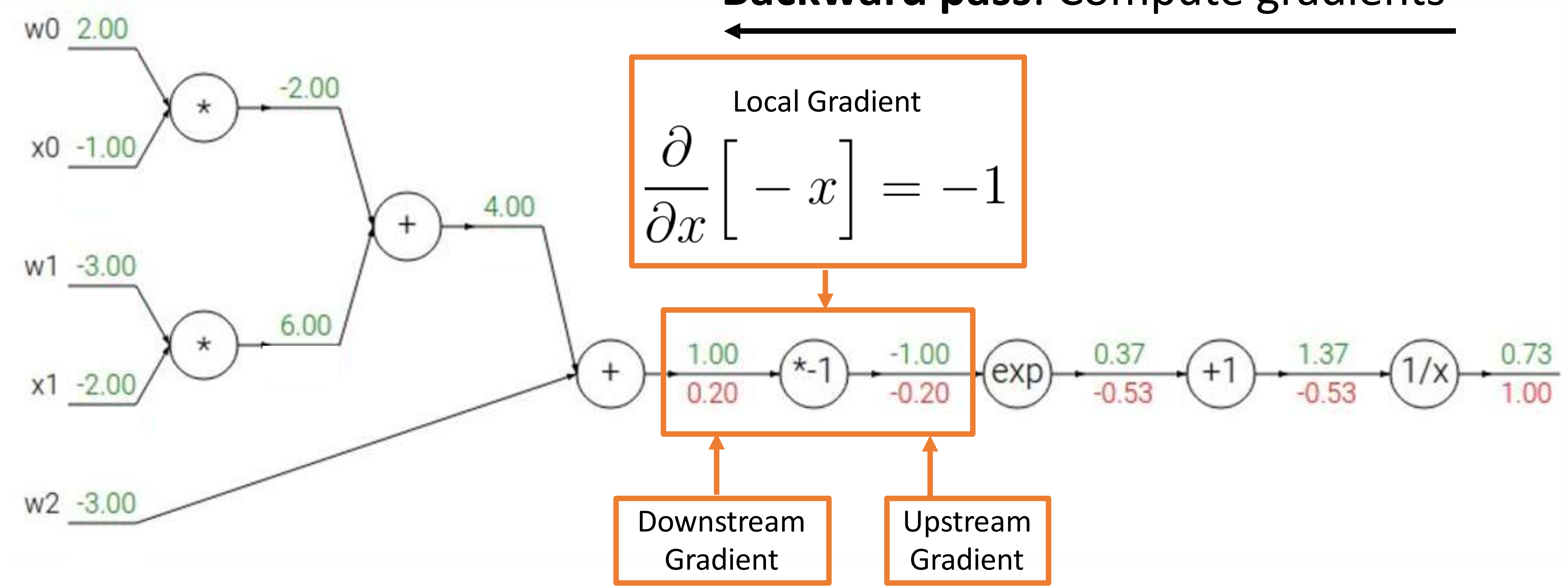

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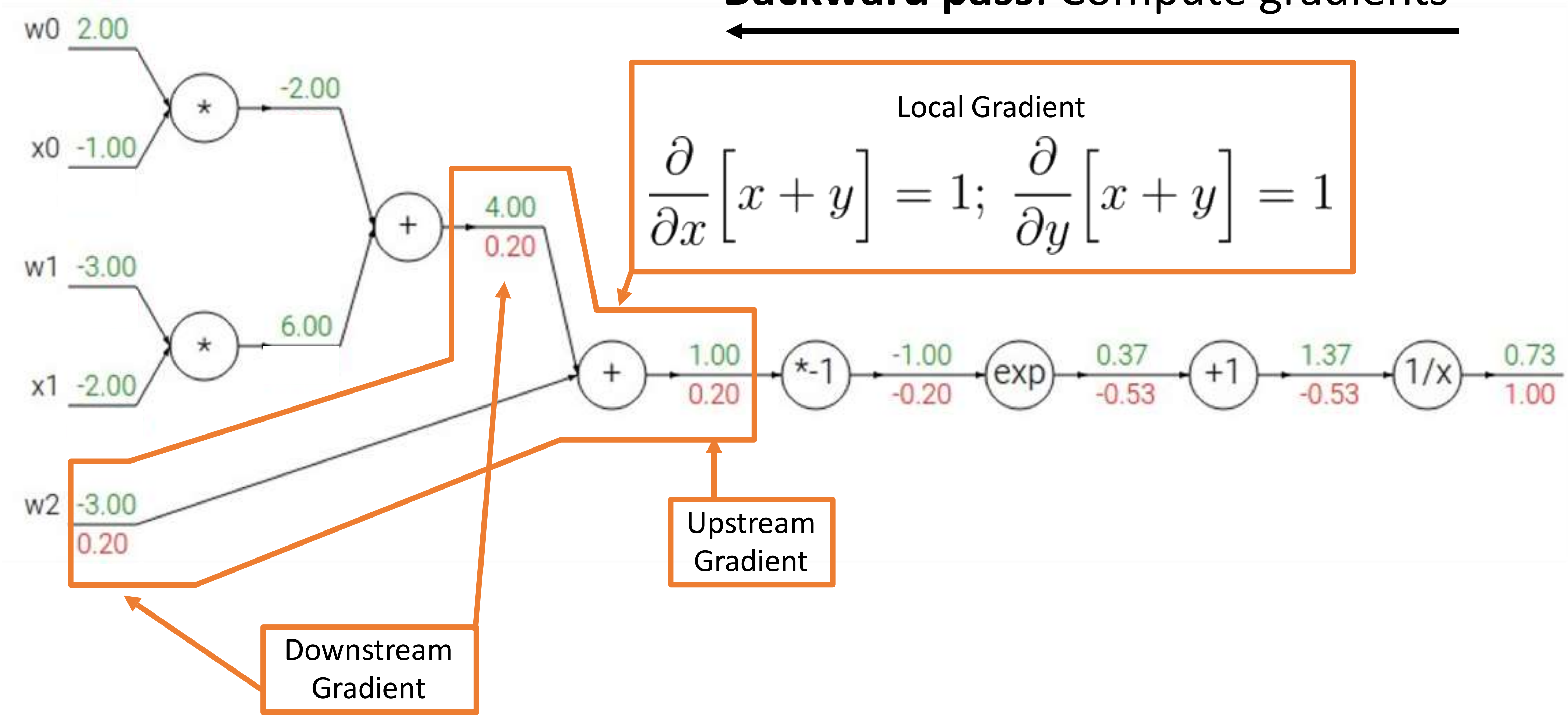
Backward pass: Compute gradients



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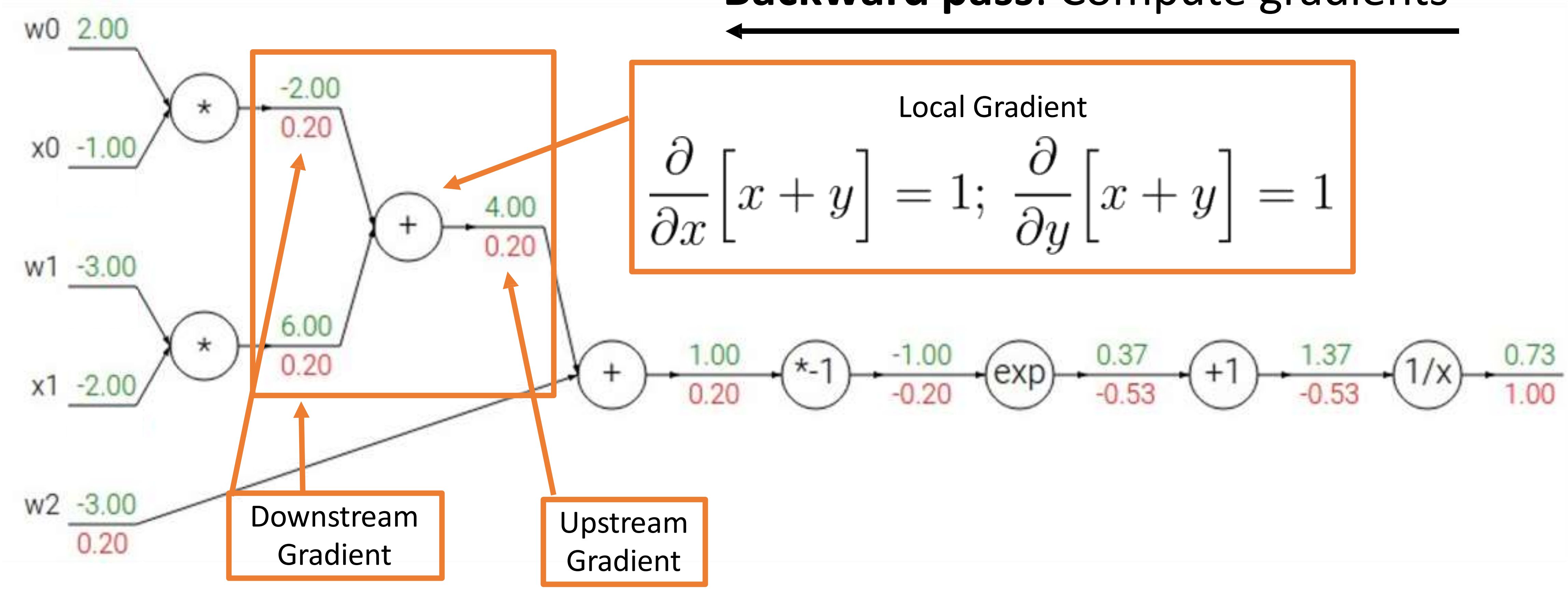
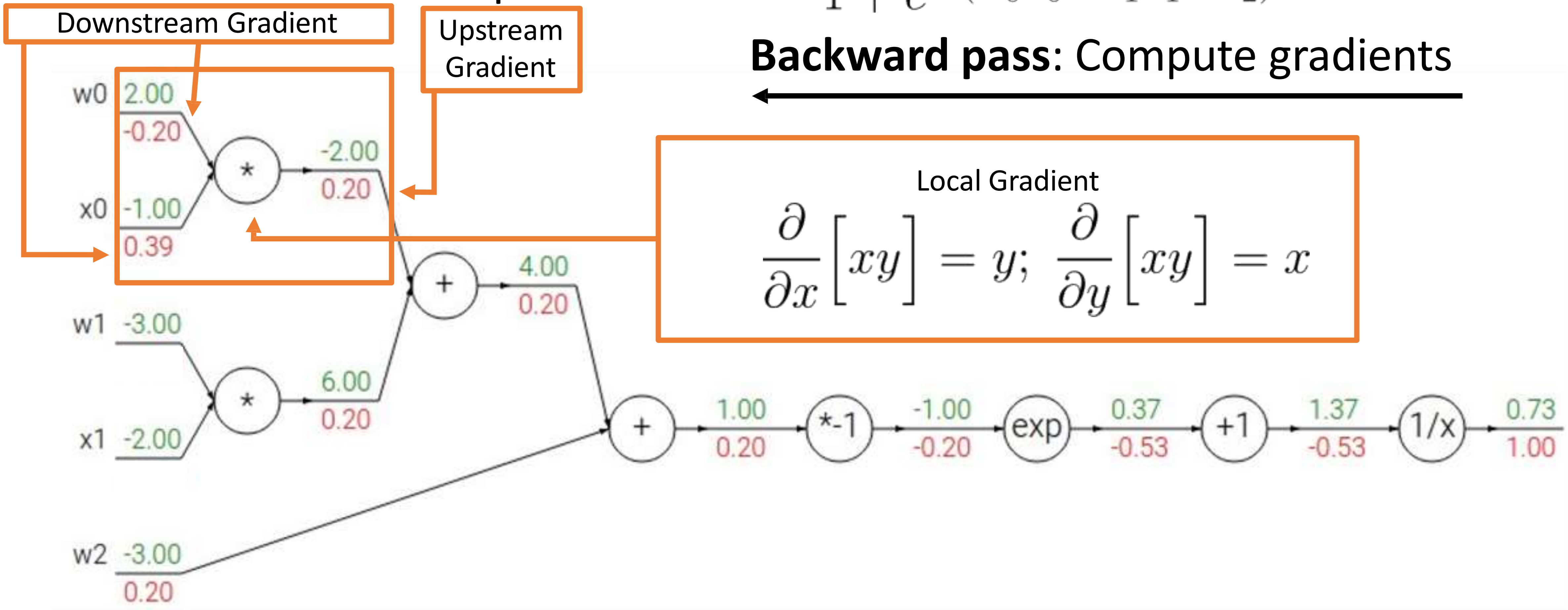
Backward pass: Compute gradients



Another Example

$$f(x, w) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$$

Backward pass: Compute gradients



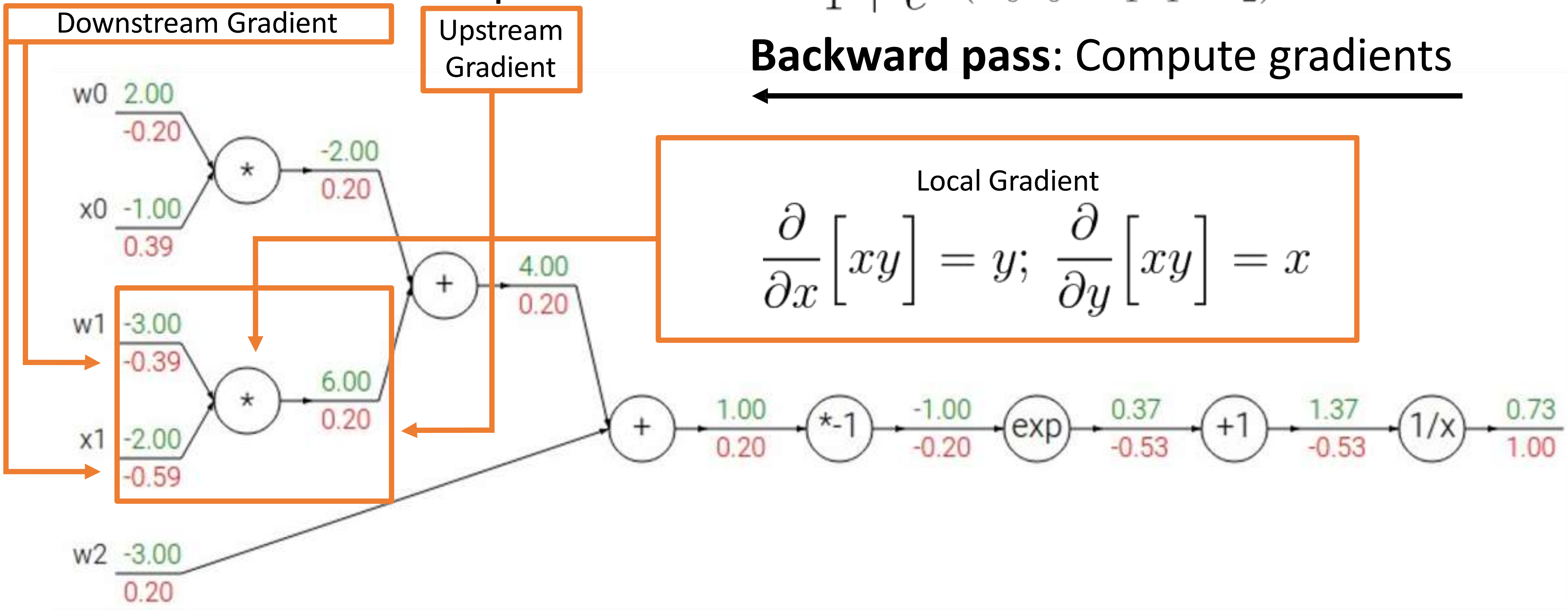
Local Gradient

$$\frac{\partial}{\partial x}\left[xy\right] = y; \quad \frac{\partial}{\partial y}\left[xy\right] = x$$

Another Example

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

Backward pass: Compute gradients



Local Gradient

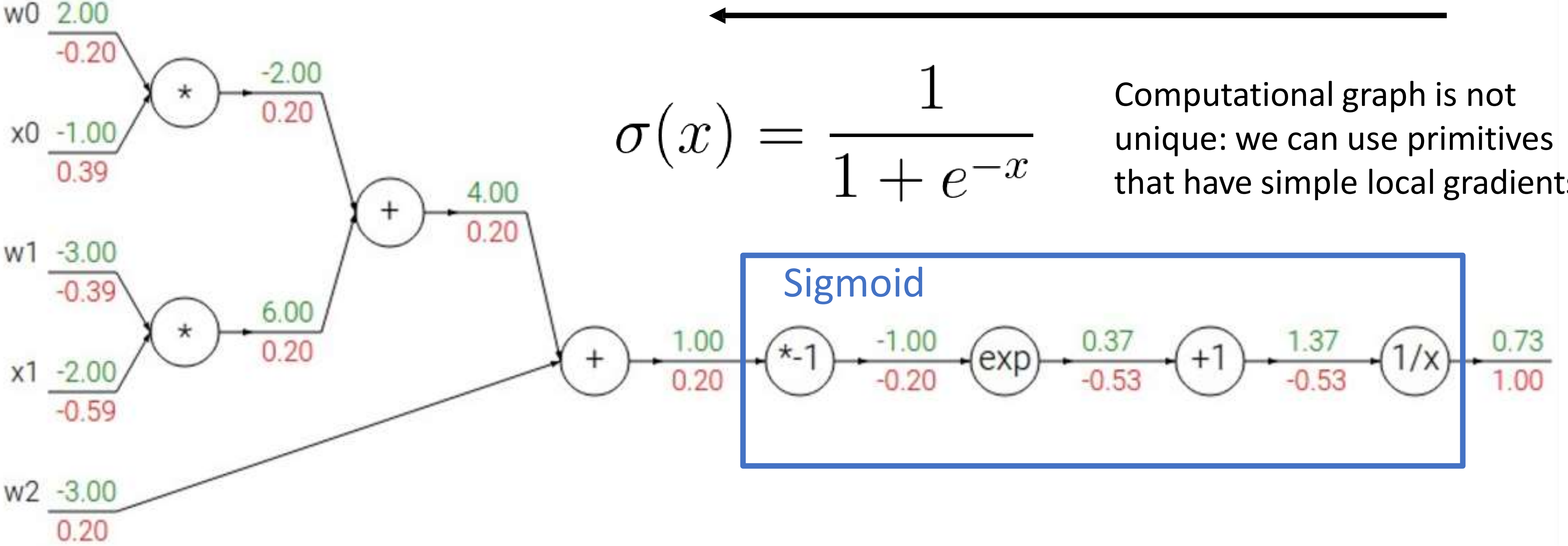
$$\frac{\partial}{\partial x}\left[xy\right] = y; \quad \frac{\partial}{\partial y}\left[xy\right] = x$$

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

Backward pass: Compute gradients

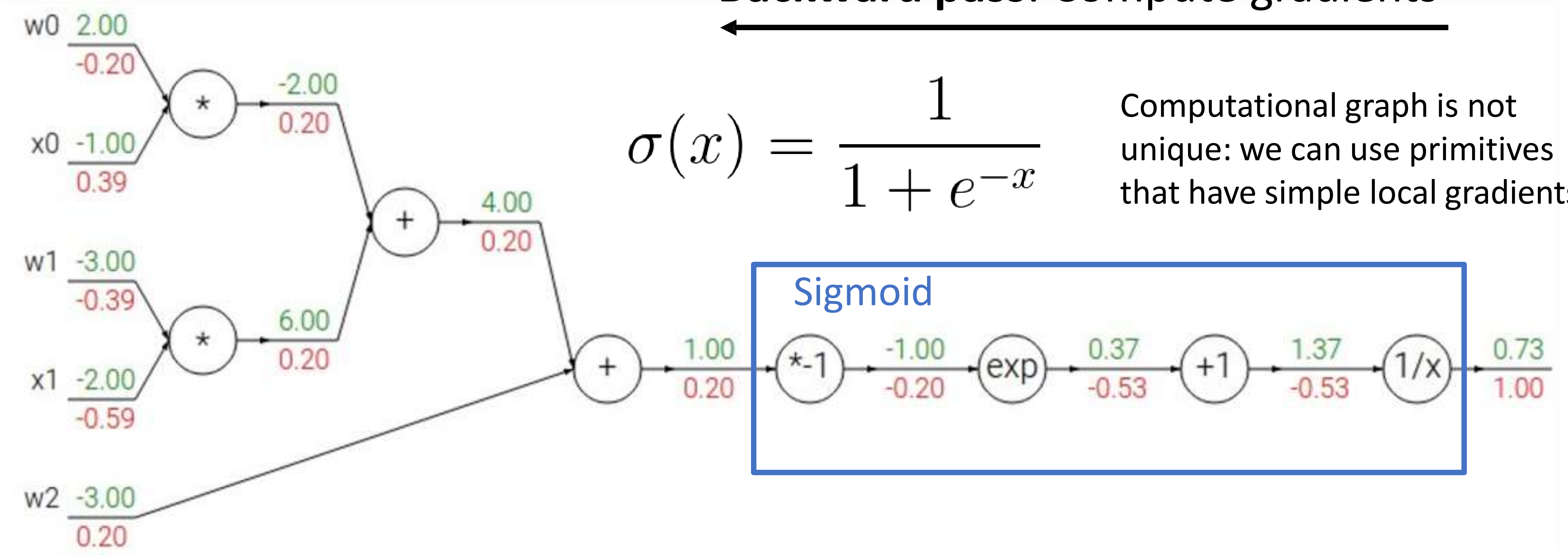
$$\sigma(x) = \frac{1}{1+e^{-x}}$$

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



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

Backward pass: Compute gradients



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

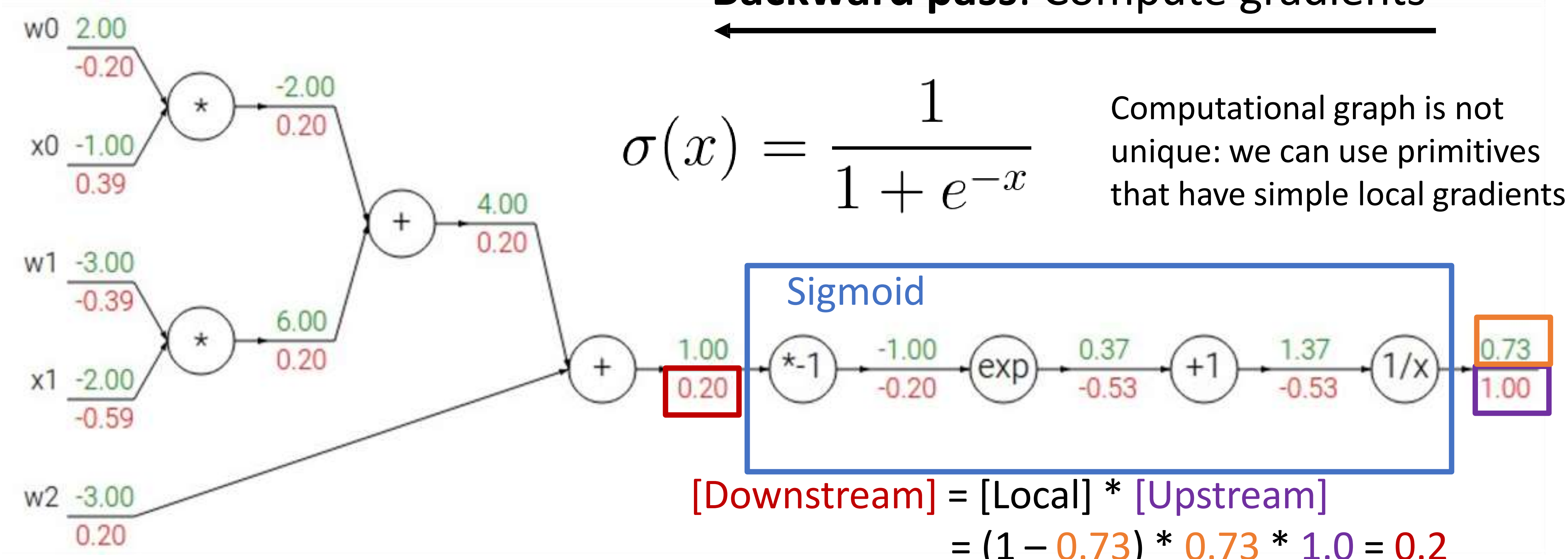
Computational graph is not unique: we can use primitives that have simple local gradients

Sigmoid local gradient:

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

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

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

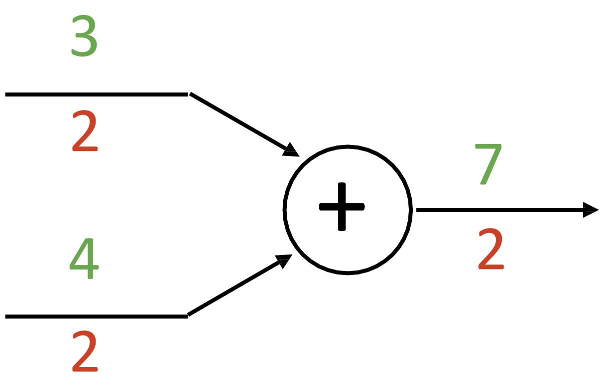
[Downstream] = [Local] * [Upstream]

= (1 – 0.73) * 0.73 * 1.0 = 0.2

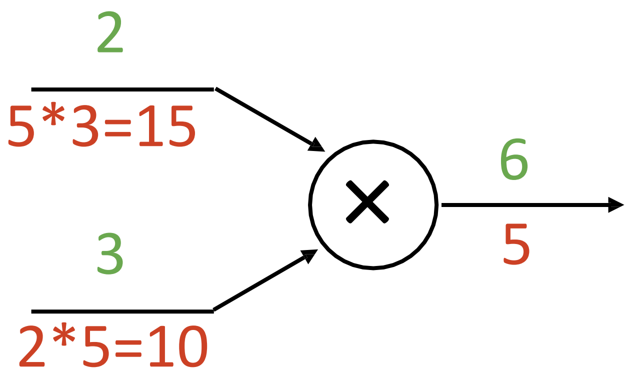
Sigmoid local gradient: $$\frac{\partial}{\partial x}\left[\sigma(x)\right] = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$

Patterns in Gradient Flow

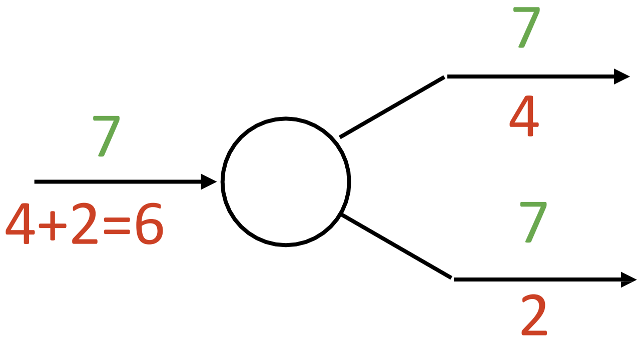
add gate: gradient distributor



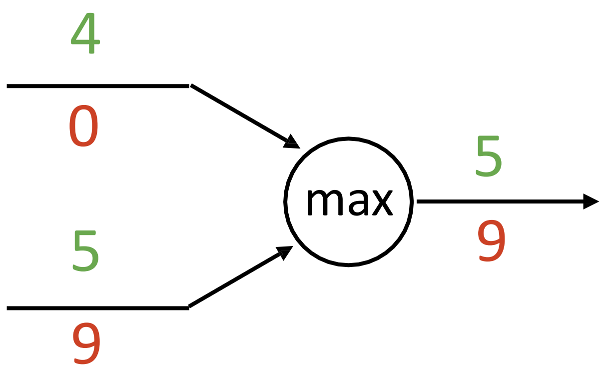
mul gate: “swap multiplier”



copy gate: gradient adder



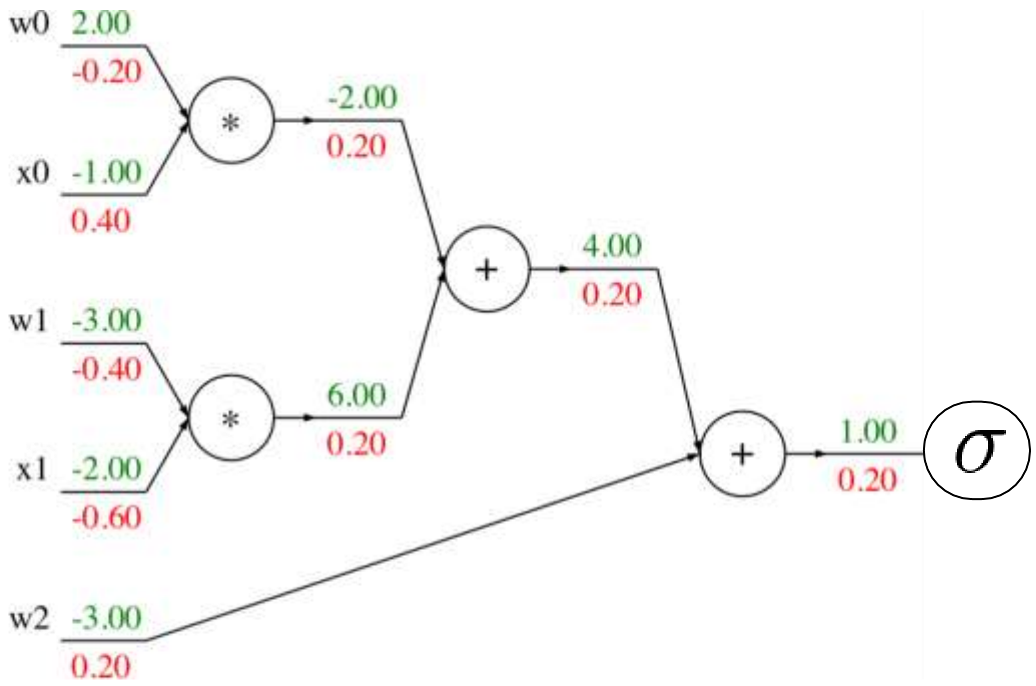
max gate: gradient router



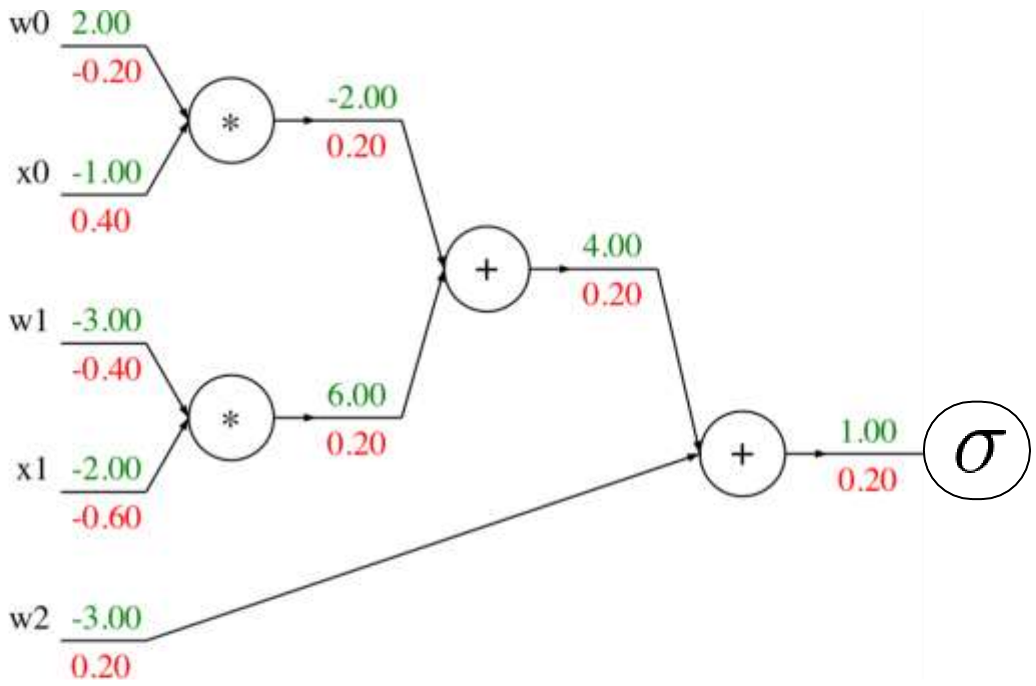
Backprop Implementation: "Flat" gradient code:

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:



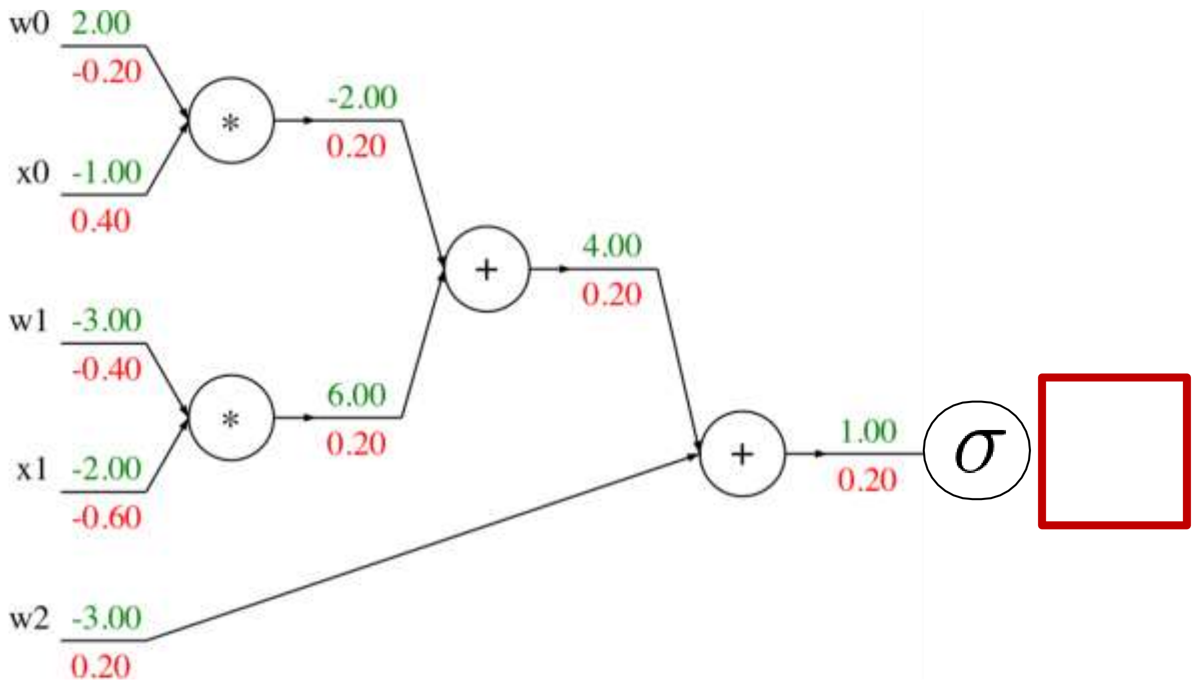
Forward pass: Compute output

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

Backward pass: Compute grads

```
    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

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

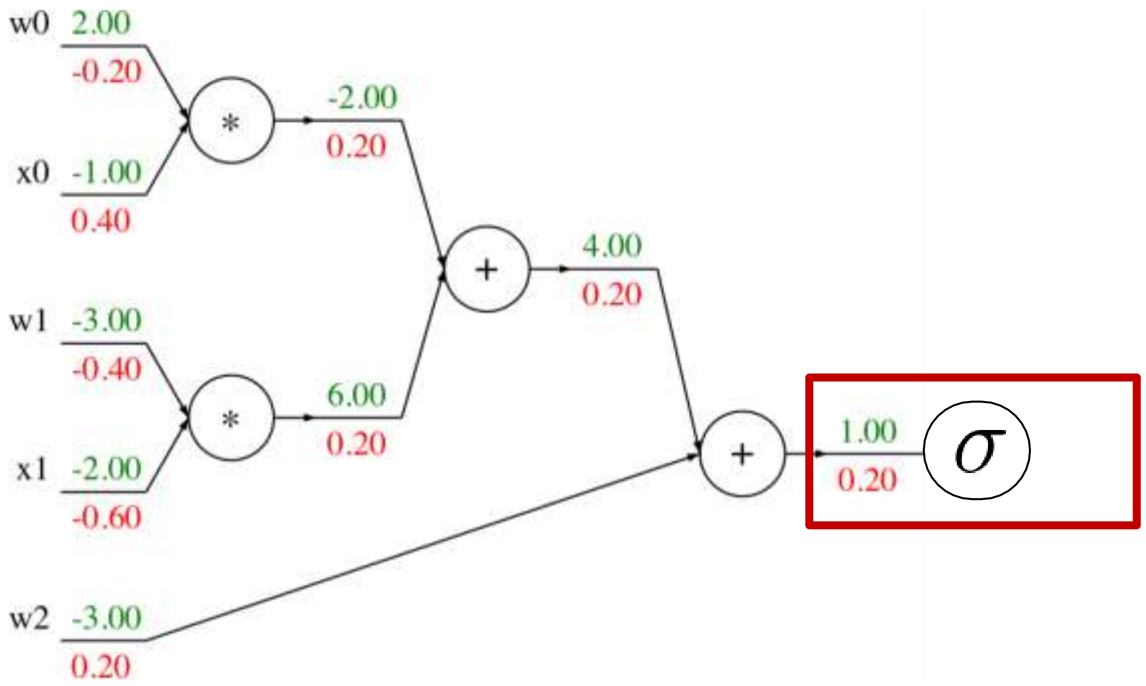
Base case

```
    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
```

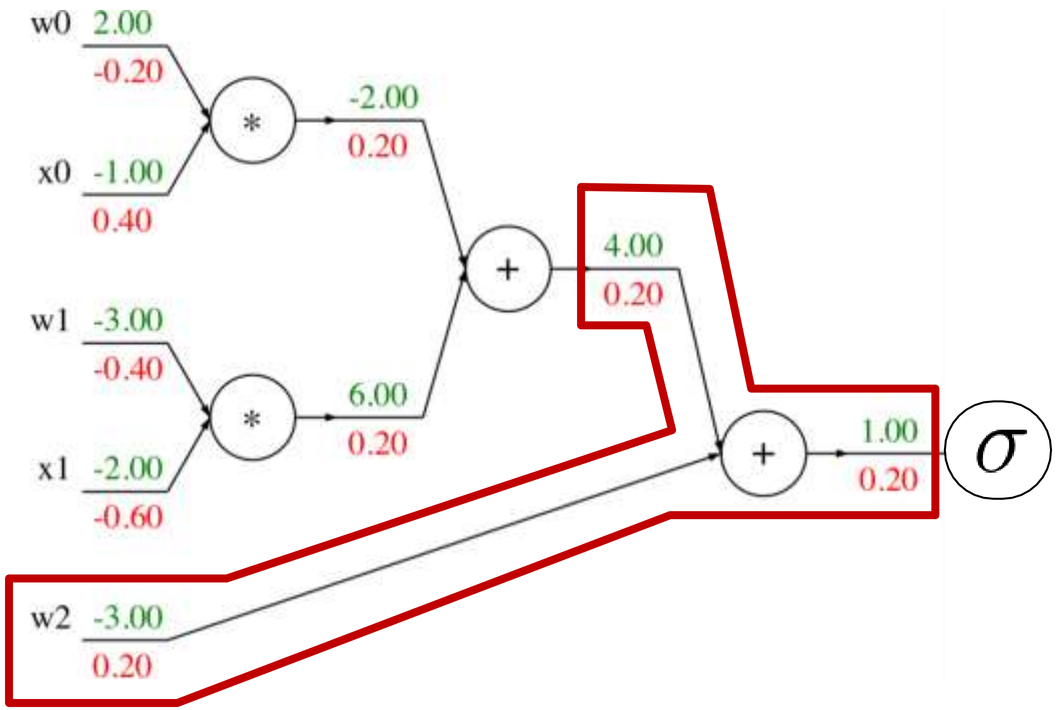
Backprop Implementation: ”Flat” gradient code:

Forward pass:
Compute output

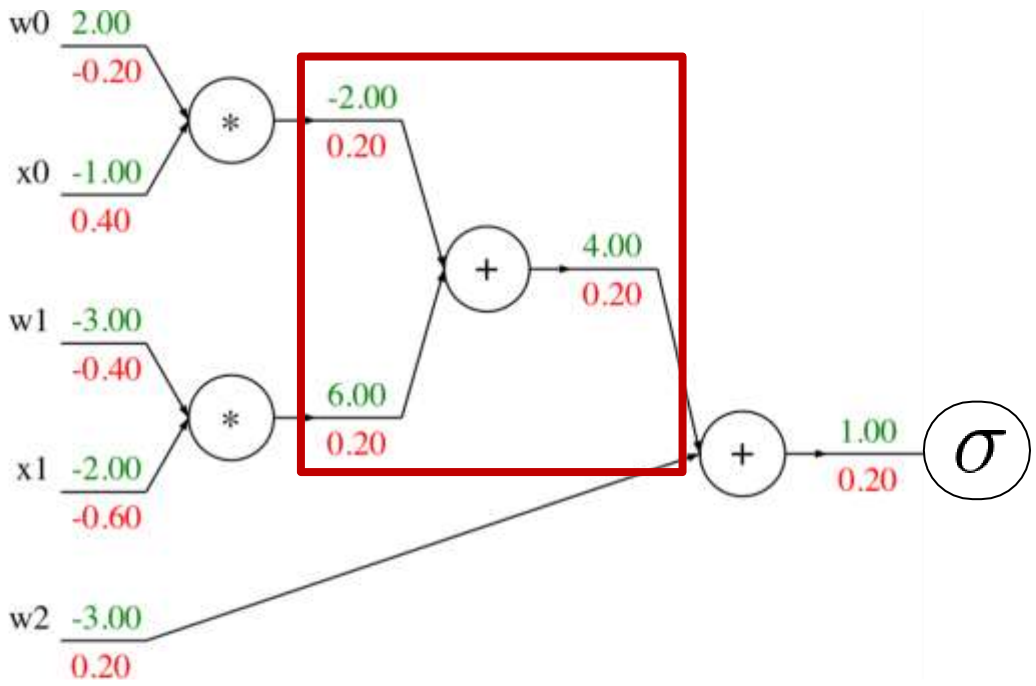
```python
def f(w0, x0, w1, x1, w2):
    s0 = w0 * x0
    s1 = w1 * x1
    s2 = s0 + s1
    s3 = s2 + w2
    L = sigmoid(s3)

    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
```

Add



Backprop Implementation: "Flat" gradient code:



Forward pass: Compute output

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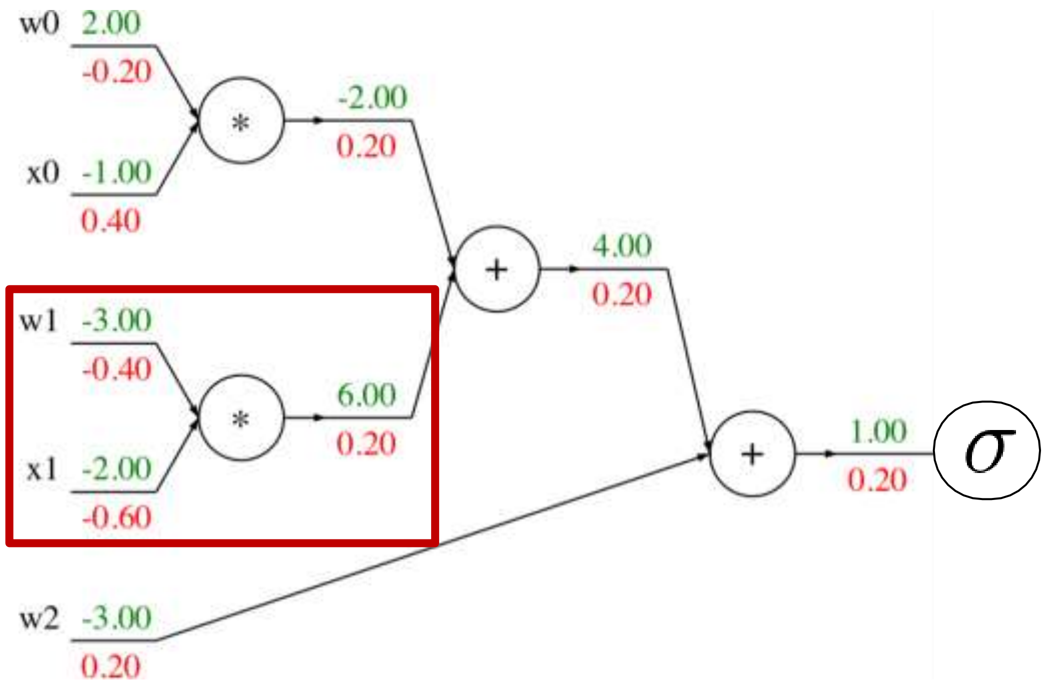

Add

Backprop Implementation: "Flat" gradient code:



Forward pass: Compute output

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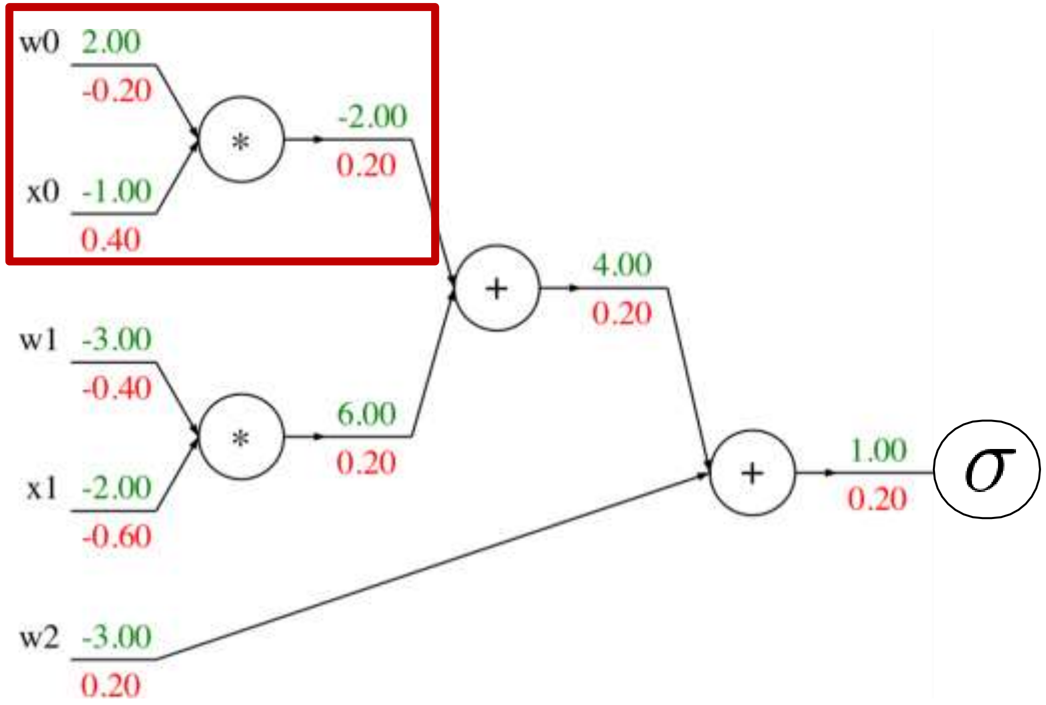

Multiply

Backprop Implementation: ”Flat” gradient code:



Forward pass:
Compute output

Multiply

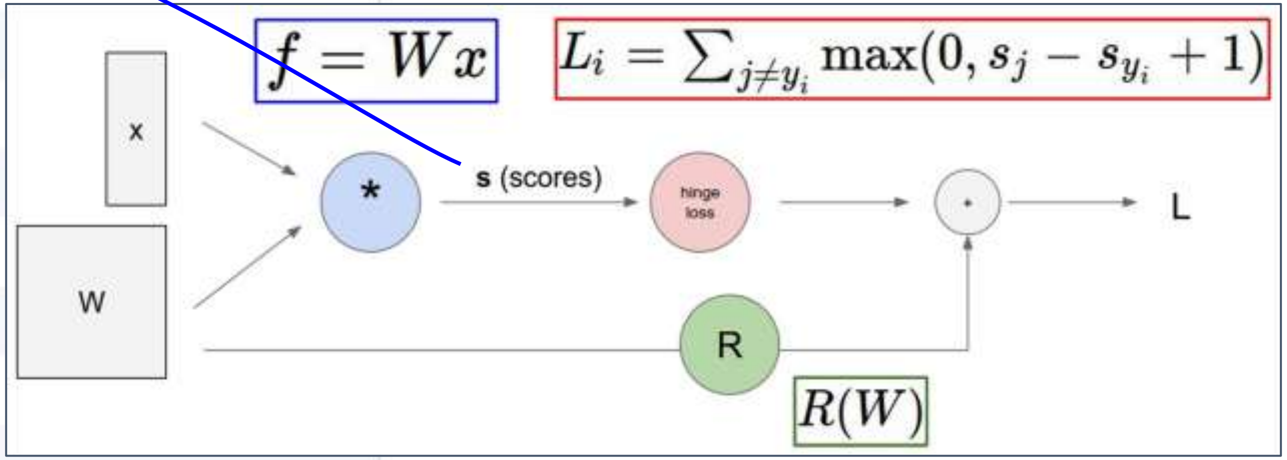
```
def f(w0, x0, w1, x1, w2):
    s0 = w0 * x0
    s1 = w1 * x1
    s2 = s0 + s1
    s3 = s2 + w2
    L = sigmoid(s3)

    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 = #...
```



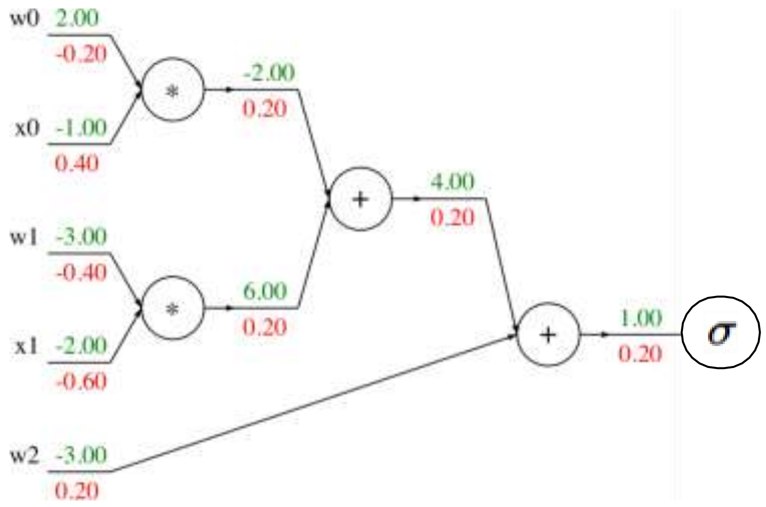
“Flat” Backprop: Do this for Assignment 2!

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 = #...
```

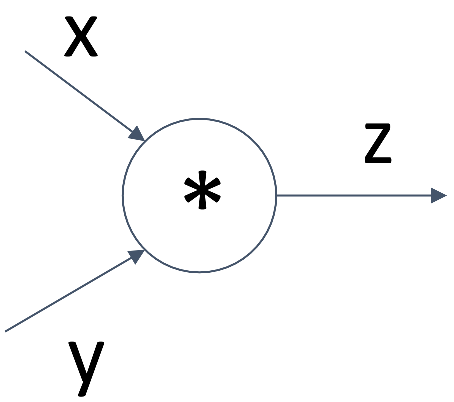
Backprop Implementation: Modular API



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



(x,y,z are scalars)

```python
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
```

Need to stash some values for use in backward

Upstream gradient

Multiply upstream and local gradients

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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Regular derivative:

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

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

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

Derivative is **Gradient**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^N \quad \left(\frac{\partial y}{\partial x}\right)_n = \frac{\partial y}{\partial x_n}$$

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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Derivative is **Gradient**:

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

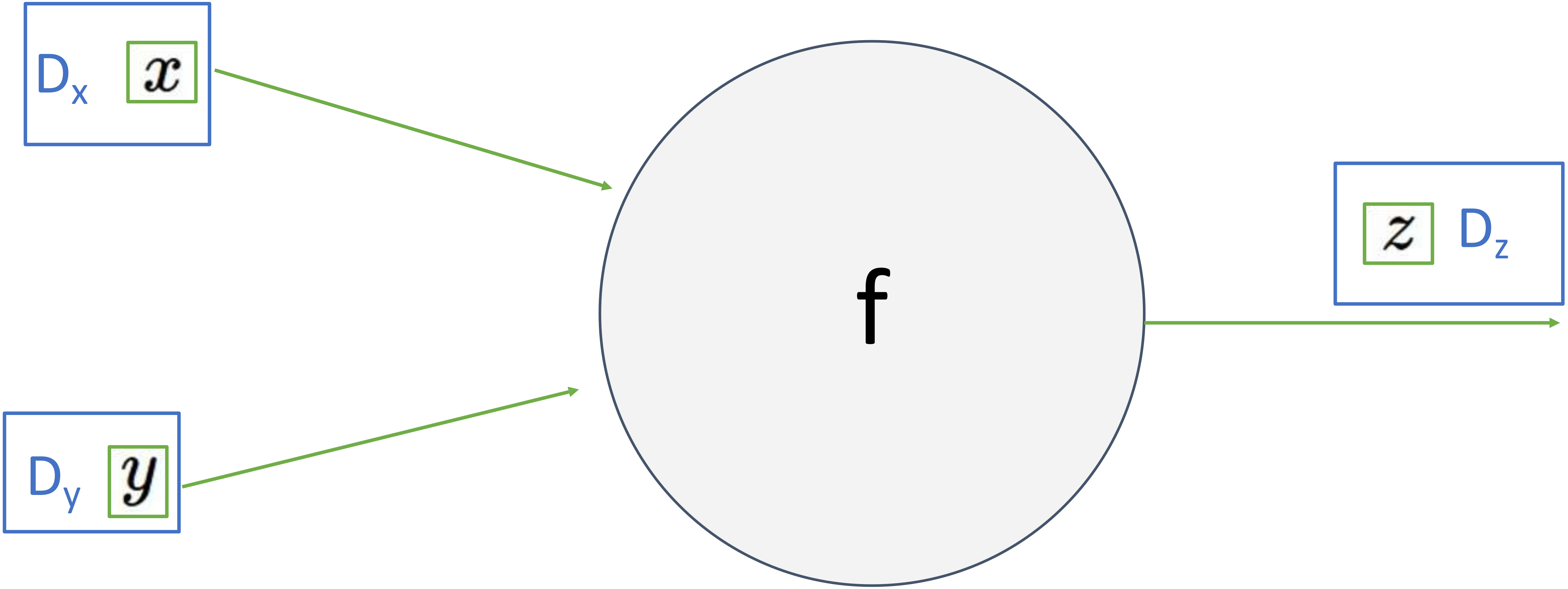
$x \in \mathbb{R}^N, y \in \mathbb{R}^M$

Derivative is **Jacobian**:

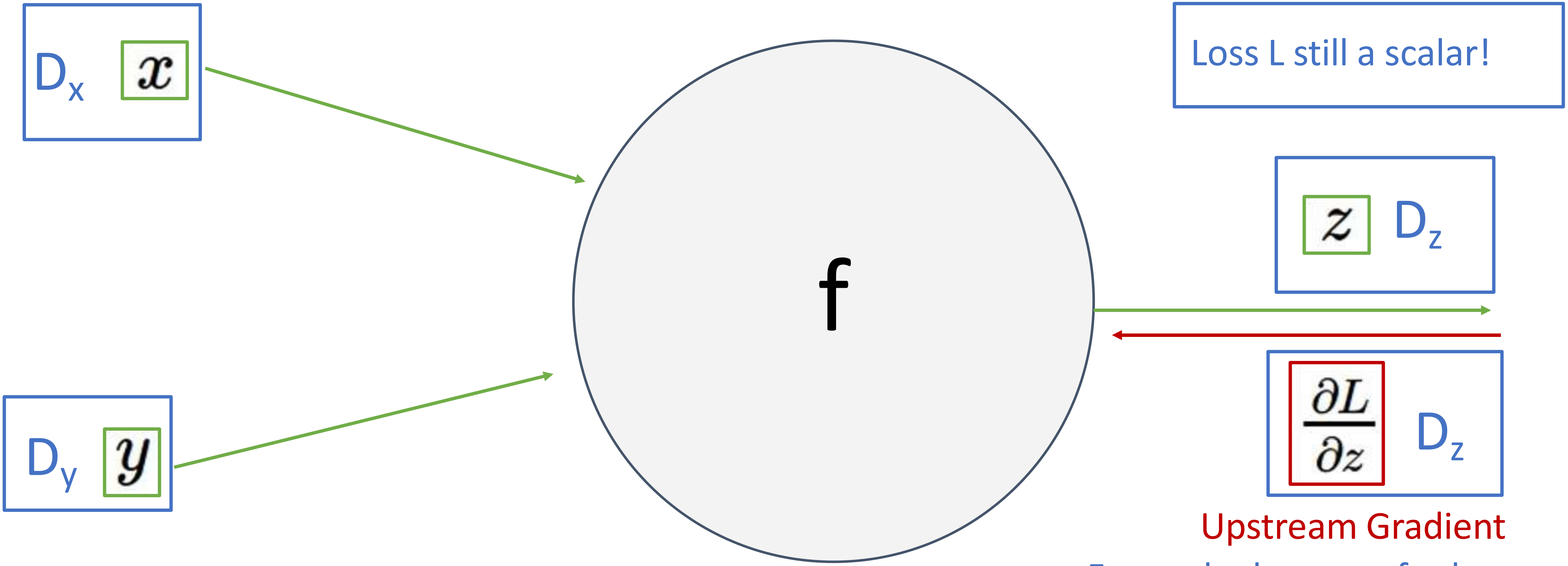
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x}\right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

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

Backprop with Vectors

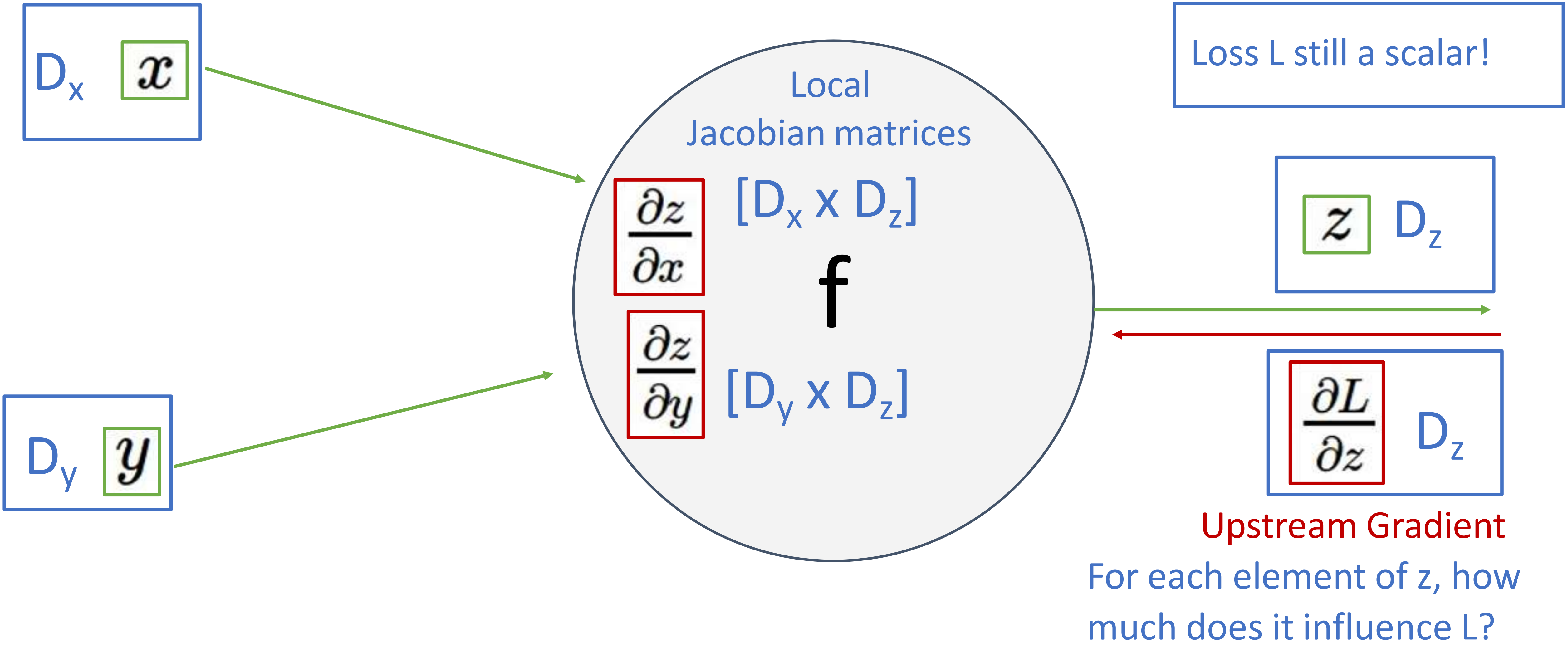


Backprop with Vectors

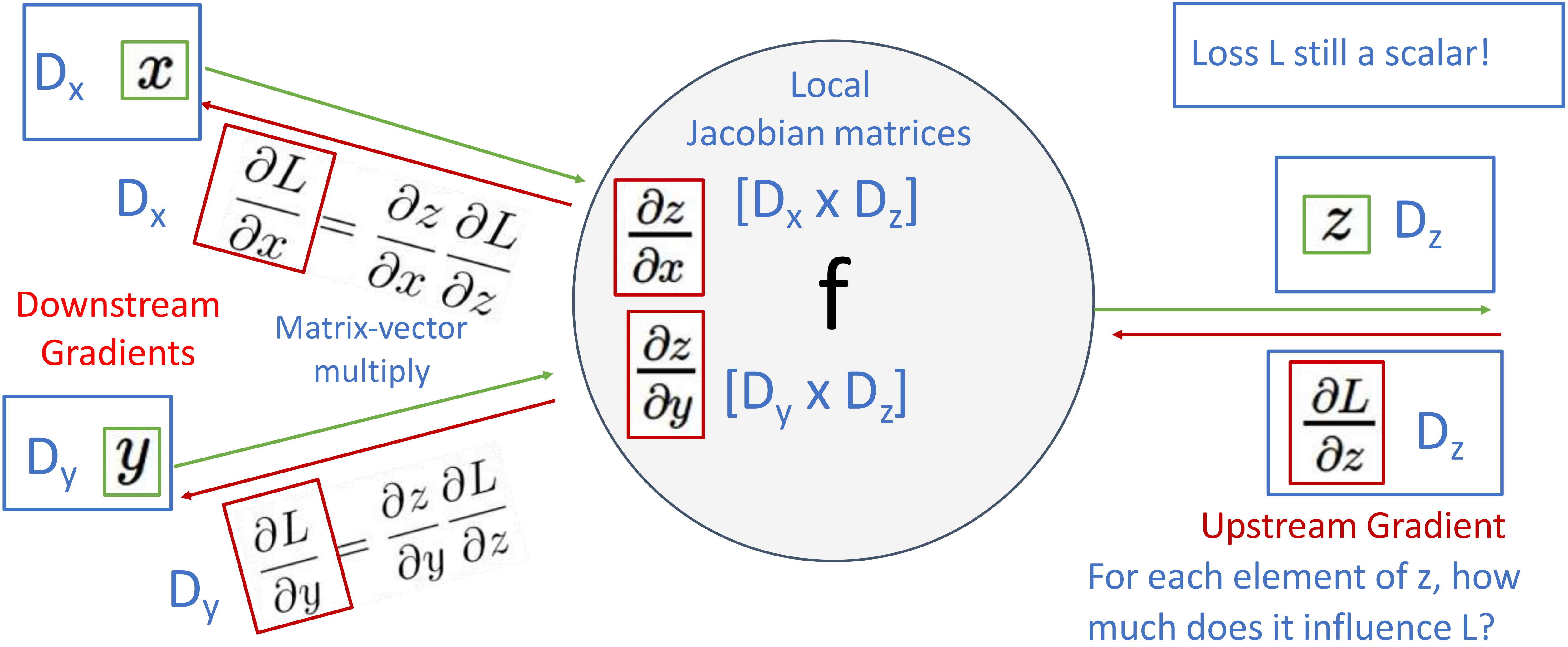


For each element of z, how much does it influence L?

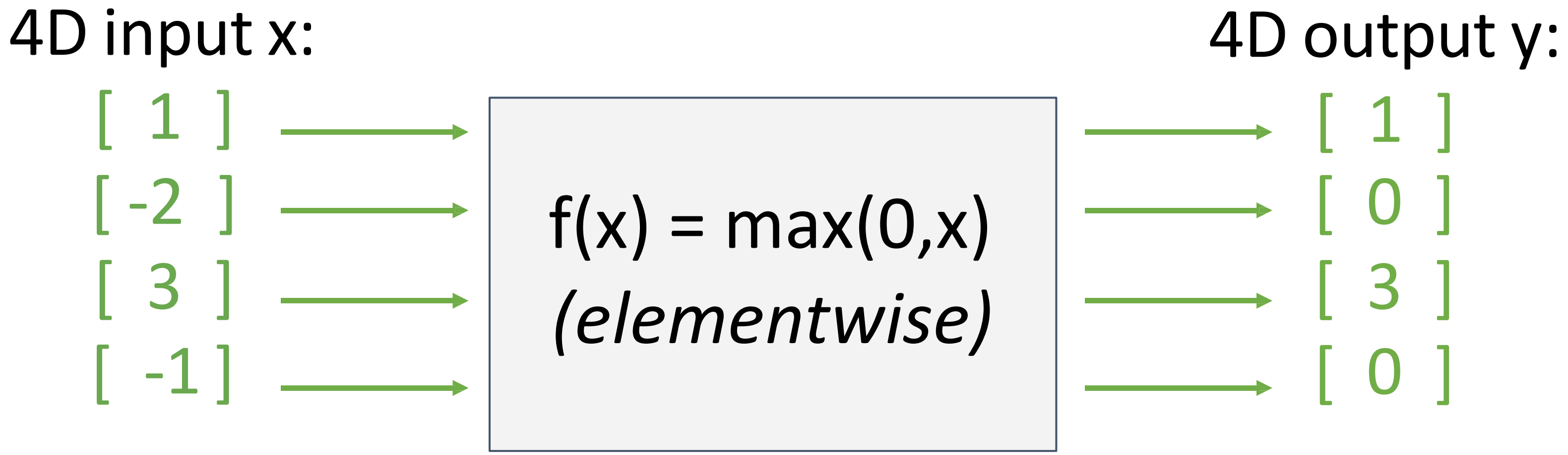
Backprop with Vectors



Backprop with Vectors



Backprop with Vectors



Backprop with Vectors

4D input x:

[1]
[-2]
[3]
[-1]

f(x) = max(0,x)
(elementwise)

4D output y:

[1]
[0]
[3]
[0]

4D dL/dy:

[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Vectors

4D input x:

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

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

(elementwise)

4D output y:

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

Jacobian dy/dx

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

4D dL/dy:

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

Upstream gradient

Backprop with Vectors

4D input x:

[1]
[-2]
[3]
[-1]

$f(x) = \max(0,x)$
(elementwise)

4D output y:

[1]
[0]
[3]
[0]

[dy/dx] [dL/dy]

[1 0 0 0] [4]
[0 0 0 0] [-1]
[0 0 1 0] [5]
[0 0 0 0] [9]

4D dL/dy:

[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Vectors

4D input x:

[1]
[-2]
[3]
[-1]

f(x) = max(0,x)
(elementwise)

4D output y:

[1]
[0]
[3]
[0]

4D dL/dx:

[4]
[0]
[5]
[0]

[dy/dx] [dL/dy]

[1 0 0 0] [4]
[0 0 0 0] [-1]
[0 0 1 0] [5]
[0 0 0 0] [9]

4D dL/dy:

[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Vectors

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

4D input x:

[1]
[-2]
[3]
[-1]

f(x) = max(0,x)
(elementwise)

4D output y:

[1]
[0]
[3]
[0]

4D dL/dx:

[4]
[0]
[5]
[0]

[dy/dx] [dL/dy]

[1 0 0 0] [4]
[0 0 0 0] [-1]
[0 0 1 0] [5]
[0 0 0 0] [9]

4D dL/dy:

[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Vectors

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

4D input x:

[1]
[-2]
[3]
[-1]

f(x) = max(0,x)
(elementwise)

4D output y:

[1]
[0]
[3]
[0]

4D dL/dx:

[4]
[0]
[5]
[0]

[dy/dx] [dL/dy]

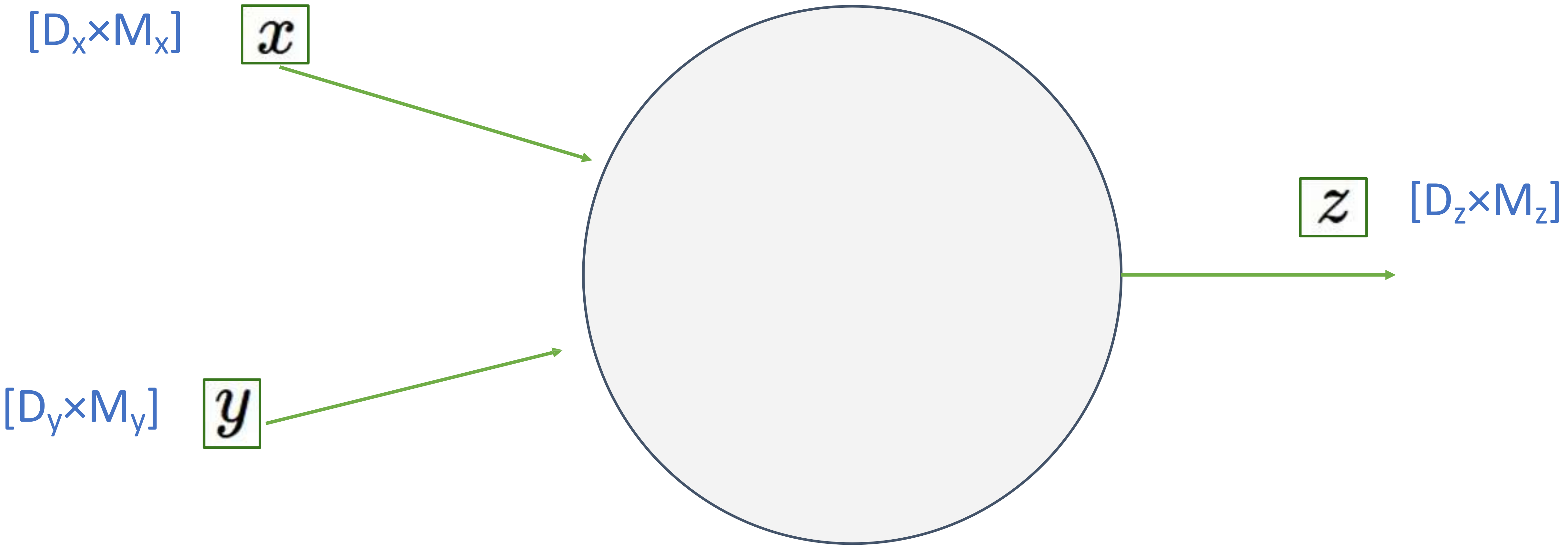
$$\left(\frac{\partial L}{\partial x}\right)_i = \begin{cases} \left(\frac{\partial L}{\partial y}\right)_i & \text{if } x_i > 0 \\ 0 & \text{otherwise} \end{cases}$$

4D dL/dy:

[4]
[-1]
[5]
[9]

Upstream gradient

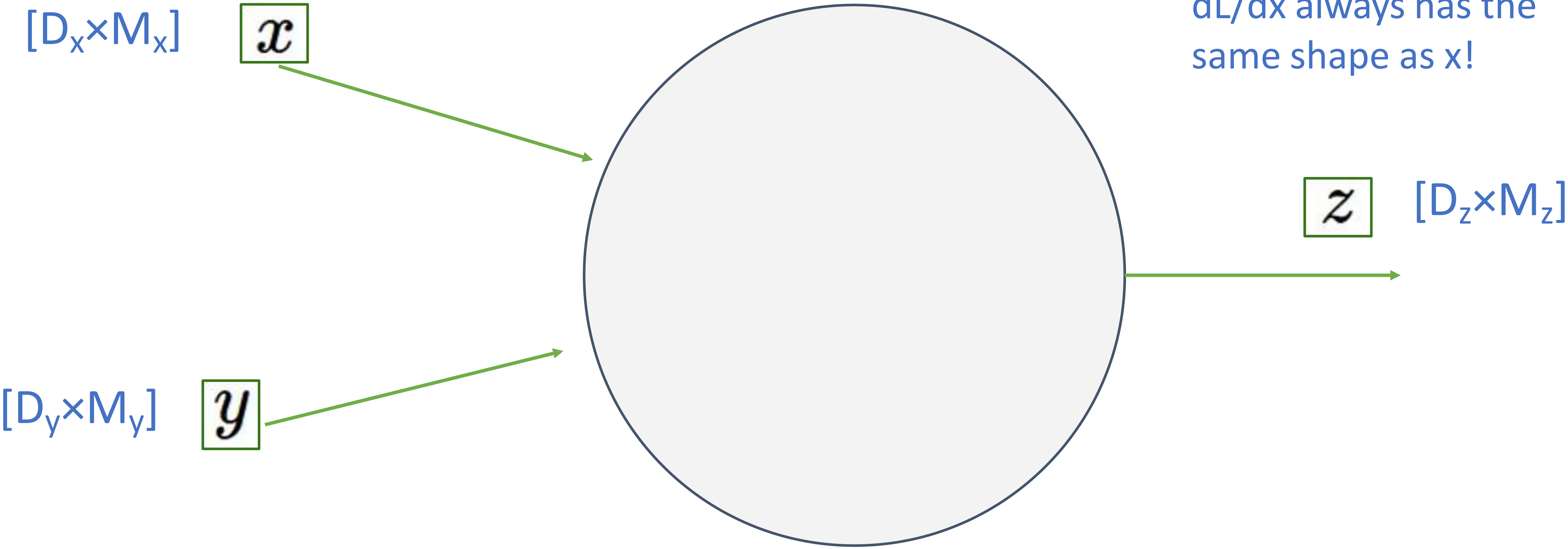
Backprop with Matrices (or Tensors):



Backprop with Matrices (or Tensors):

Loss L still a scalar!

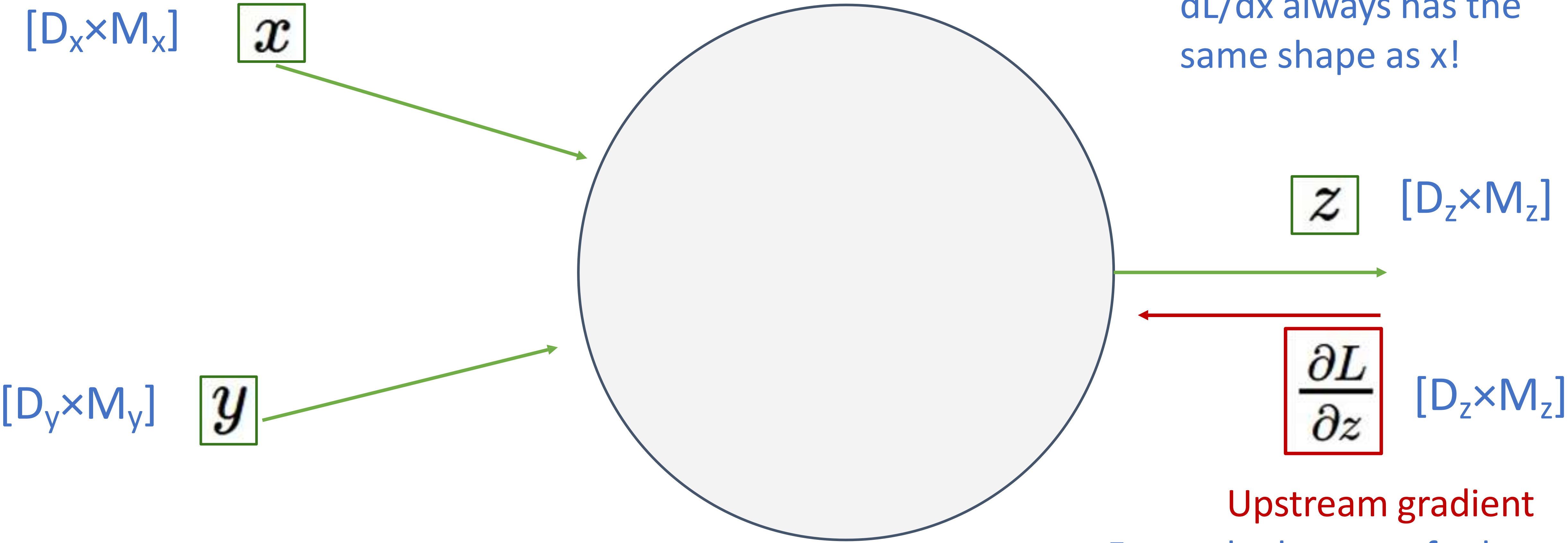
dL/dx always has the same shape as x!



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?

Backprop with Matrices (or Tensors):

Loss L still a scalar!

dL/dx always has the same shape as x!

$[D_x \times M_x]$ $\boxed{x}$

$[D_y \times M_y]$ $\boxed{y}$

Local Jacobian matrices

$\boxed{\frac{\partial z}{\partial x}}$ $[(D_x \times M_x) \times (D_z \times M_z)]$

$\boxed{\frac{\partial z}{\partial y}}$ $[(D_y \times M_y) \times (D_z \times M_z)]$

$\boxed{z}$ $[D_z \times M_z]$

$\boxed{\frac{\partial L}{\partial z}}$ $[D_z \times M_z]$

Upstream gradient

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

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

Backprop with Matrices (or Tensors):

Loss L still a scalar!

dL/dx always has the same shape as x!

$[D_x \times M_x]$ $\boxed{x}$

$[D_x \times M_x]$ $\boxed{\frac{\partial L}{\partial x}} = \frac{\partial z}{\partial x}\frac{\partial L}{\partial z}$

Matrix-vector multiply

$[D_y \times M_y]$ $\boxed{y}$

$[D_y \times M_y]$ $\boxed{\frac{\partial L}{\partial y}} = \frac{\partial z}{\partial y}\frac{\partial L}{\partial z}$

Local Jacobian matrices

$\boxed{\frac{\partial z}{\partial x}}$ $[(D_x \times M_x) \times (D_z \times M_z)]$

$\boxed{\frac{\partial z}{\partial y}}$ $[(D_y \times M_y) \times (D_z \times M_z)]$

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

$\boxed{z}$ $[D_z \times M_z]$

$\boxed{\frac{\partial L}{\partial z}}$ $[D_z \times M_z]$

Upstream gradient

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

Example: Matrix Multiplication

x: [N×D]

[2 1 -3]
[-3 4 2]

w: [D×M]

[3 2 1 -1]
[2 1 3 2]
[3 2 1 -2]

Matrix Multiply $y = xw$

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

[-1 -1 2 6]
[5 2 11 7]

Example: Matrix Multiplication

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y: [N×M]

[-1 -1 2 6]
[5 2 11 7]

dL/dy: [N×M]

[2 3 -3 9]
[-8 1 4 6]

dL/dx: [N×D]

[? ? ?]
[? ? ?]

Example: Matrix Multiplication

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[2 1 -3]
[-3 4 2]

w: [D×M]
[3 2 1 -1]
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$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]
[-1 -1 2 6]
[5 2 11 7]

dL/dy: [N×M]
[2 3 -3 9]
[-8 1 4 6]

dL/dx: [N×D]
[? ? ?]
[? ? ?]

Jacobians:
dy/dx: [(N×D)×(N×M)]
dy/dw: [(D×M)×(N×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×D]

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

w: [D×M]

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

Matrix Multiply *y = xw*

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

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

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

Matrix Multiply *y = xw*

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

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

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

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$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

$dL/dx_{1,1}$

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply $y = xw$

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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

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

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply *y = xw*

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

$dy_{1,2}/dx_{1,1}$

$$\begin{bmatrix} 3 & \boxed{?} & ? & ? \\ ? & ? & ? & ? \end{bmatrix}$$

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

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

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

$dL/dx_{1,1}$

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

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

$dL/dx_{1,1}$

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

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

$\Rightarrow dy_{1,2}/dx_{1,1} = w_{1,2}$

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply $y = xw$

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

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

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$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

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

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

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply $y = xw$

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

$$\begin{array}{rl} dy_{1,2}/dx_{1,1} & \begin{bmatrix} 3 & 2 & 1 & -1 \\ \boxed{0} & ? & ? & ? \end{bmatrix} \end{array}$$

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

$$\Rightarrow dy_{2,1}/dx_{1,1} = 0$$

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply *y = xw*

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply *y = xw*

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply $y = xw$

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

$$\begin{bmatrix} \boxed{0} & ? & ? \\ ? & ? & ? \end{bmatrix}$$

Local Gradient Slice:

$dy/dx_{1,1}$

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$dL/dx_{1,1}$

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

$= (w_{1,:}) \cdot (dL/dy_{1,:})$

$= 3*2 + 2*3 + 1*(-3) + (-1)*9 = 0$

Example: Matrix Multiplication

x: [N×D]

[2 1 -3]
[-3 4 $\boxed{2}$]

w: [D×M]

[3 2 1 -1]
[2 1 3 2]
[$\boxed{3\ 2\ 1\ {-2}}$]

Matrix Multiply $y = xw$

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

[-1 -1 2 6]
[5 2 11 7]

dL/dy: [N×M]

[2 3 -3 9]
[-8 1 4 6]

dL/dx: [N×D]

[0 ? ?]
[? ? $\boxed{-30}$]

Local Gradient Slice:

$dy/dx_{2,3}$

[0 0 0 0]
[$\boxed{3\ 2\ 1\ {-2}}$]

$dL/dx_{2,3}$

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply $y = xw$

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

$$\begin{bmatrix} 0 & ? & ? \\ ? & ? & \boxed{-30} \end{bmatrix}$$

Local Gradient Slice:

$dy/dx_{2,3}$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ \boxed{3 \quad 2 \quad 1 \quad -2} \end{bmatrix}$$

$dL/dx_{2,3}$

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

$= (w_{3,:}) \cdot (dL/dy_{2,:})$

$= 3*(-8) + 2*1 + 1*4 + (-2)*6 = -30$

Example: Matrix Multiplication

x: [N×D]
[2 1 -3]
[-3 4 2]

w: [D×M]
[3 2 1 -1]
[2 1 3 2]
[3 2 1 -2]

Matrix Multiply *y = xw*

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]
[-1 -1 2 6]
[5 2 11 7]

dL/dy: [N×M]
[2 3 -3 9]
[-8 1 4 6]

dL/dx: [N×D]
[0 16 -9]
[-24 9 -30]

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply $y = xw$

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

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

[N x D] [N x M] [M x D]

$dL/dx_{i,j}$

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

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

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

Example: Matrix Multiplication

x: [N×D]
[2 1 -3]
[-3 4 2]

w: [D×M]
[3 2 1 -1]
[2 1 3 2]
[3 2 1 -2]

Matrix Multiply *y = xw*

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]
[-1 -1 2 6]
[5 2 11 7]

dL/dy: [N×M]
[2 3 -3 9]
[-8 1 4 6]

dL/dx: [N×D]
[0 16 -9]
[-24 9 -30]

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

[N x D] [N x M] [M x D]

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

[D x M] [D x N] [N x M]

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

Backpropagation: Another View

$$\underset{D_0}{x_0} \xrightarrow{f_1} \underset{D_1}{x_1} \xrightarrow{f_2} \underset{D_2}{x_2} \xrightarrow{f_3} \underset{D_3}{x_3} \xrightarrow{f_4} \underset{\text{scalar}}{L}$$

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

$$x_0 \xrightarrow{f_1} x_1 \xrightarrow{f_2} x_2 \xrightarrow{f_3} x_3 \xrightarrow{f_4} L$$

D_0 D_1 D_2 D_3 scalar

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

Chain rule

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

$D_0 \times D_1$ $D_1 \times D_2$ $D_2 \times D_3$ D_3

Reverse-Mode Automatic Differentiation

$$\underset{D_0}{x_0} \xrightarrow{f_1} \underset{D_1}{x_1} \xrightarrow{f_2} \underset{D_2}{x_2} \xrightarrow{f_3} \underset{D_3}{x_3} \xrightarrow{f_4} \underset{\text{scalar}}{L}$$

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

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

Reverse-Mode Automatic Differentiation

$$x_0 \xrightarrow{f_1} x_1 \xrightarrow{f_2} x_2 \xrightarrow{f_3} x_3 \xrightarrow{f_4} L$$

D_0 D_1 D_2 D_3 scalar

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

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

$D_0 \times D_1$ $D_1 \times D_2$ $D_2 \times D_3$ D_3

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

What if we want grads of scalar <u>input</u> w/respect to vector <u>outputs</u>?

Forward-Mode Automatic Differentiation

$$\underset{\text{scalar}}{a} \xrightarrow{f_1} \underset{D_0}{x_0} \xrightarrow{f_2} \underset{D_1}{x_1} \xrightarrow{f_3} \underset{D_2}{x_2} \xrightarrow{f_4} \underset{D_3}{x_3}$$

Chain rule

$$\frac{\partial x_3}{\partial a} = \underbrace{\left(\frac{\partial x_0}{\partial a}\right)}_{D_0} \underbrace{\left(\frac{\partial x_1}{\partial x_0}\right)}_{D_0 \text{ x } D_1} \underbrace{\left(\frac{\partial x_2}{\partial x_1}\right)}_{D_1 \text{ x } D_2} \underbrace{\left(\frac{\partial x_3}{\partial x_2}\right)}_{D_2 \text{ x } D_3}$$

Forward-Mode Automatic Differentiation

$$\underset{\text{scalar}}{a} \xrightarrow{f_1} \underset{D_0}{x_0} \xrightarrow{f_2} \underset{D_1}{x_1} \xrightarrow{f_3} \underset{D_2}{x_2} \xrightarrow{f_4} \underset{D_3}{x_3}$$

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

Chain rule

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

Forward-Mode Automatic Differentiation

$$a \xrightarrow{f_1} x_0 \xrightarrow{f_2} x_1 \xrightarrow{f_3} x_2 \xrightarrow{f_4} x_3$$

scalar $\quad D_0 \quad D_1 \quad D_2 \quad D_3$

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

Not implemented in PyTorch / TensorFlow =(

Chain rule

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

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

Backprop: Higher-Order Derivatives

$$x_0 \xrightarrow{f_1} x_1 \xrightarrow{f_2} L$$

D_0 D_1 scalar

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

$D_0 \times D_0$

Hessian matrix
H of second derivatives.

Backprop: Higher-Order Derivatives

$$x_0 \xrightarrow{f_1} x_1 \xrightarrow{f_2} L$$

D_0 D_1 scalar

Hessian / vector multiply

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

D_0 x D_0

Hessian matrix
H of second
derivatives.

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

D_0 x D_0 D_0

Backprop: Higher-Order Derivatives

$$x_0 \xrightarrow{f_1} x_1 \xrightarrow{f_2} L$$

D_0 D_1 scalar

Hessian / vector multiply

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

D_0 x D_0

Hessian matrix
H of second derivatives.

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

D_0 x D_0 D_0

(if v doesn't depend on x_0)

Backprop: Higher-Order Derivatives

$$x_0 \xrightarrow{f_1} x_1 \xrightarrow{f_2} L \xrightarrow{f'_2} dL/dx_1 \xrightarrow{f'_1} dL/dx_0 \xrightarrow{\cdot v} (dL/dx_0) \cdot v$$

D_0 D_1 scalar D_1 D_0 scalar

Hessian / vector multiply

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

D_0 x D_0

Hessian matrix
H of second derivatives.

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

D_0 x D_0 D_0

(if v doesn't depend on x_0)

Backprop: Higher-Order Derivatives

$$\underset{D_0}{x_0} \xrightarrow{f_1} \underset{D_1}{x_1} \xrightarrow{f_2} \underset{\text{scalar}}{L} \xrightarrow{f'_2} \underset{D_1}{dL/dx_1} \xrightarrow{f'_1} \underset{D_0}{dL/dx_0} \xrightarrow{\cdot v} \underset{\text{scalar}}{(dL/dx_0) \cdot v}$$

Backprop!

Hessian / vector multiply

$$\underset{D_0 \times D_0}{\frac{\partial^2 L}{\partial x_0^2}}$$

Hessian matrix
H of second derivatives.

$$\underset{D_0 \times D_0}{\frac{\partial^2 L}{\partial x_0^2}} \underset{D_0}{v} = \frac{\partial}{\partial x_0}\left[\frac{\partial L}{\partial x_0} \cdot v\right]$$

(if v doesn't depend on x_0)

Backprop: Higher-Order Derivatives

$$\underset{D_0}{x_0} \xrightarrow{f_1} \underset{D_1}{x_1} \xrightarrow{f_2} \underset{\text{scalar}}{L} \xrightarrow{f'_2} \underset{D_1}{dL/dx_1} \xrightarrow{f'_1} \underset{D_0}{dL/dx_0} \xrightarrow{\cdot v} \underset{\text{scalar}}{(dL/dx_0) \cdot v}$$

Backprop!

This is implemented in PyTorch / Tensorflow!

Hessian / vector multiply

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

$D_0 \times D_0$

Hessian matrix
H of second derivatives.

$$\underset{D_0 \times D_0}{\frac{\partial^2 L}{\partial x_0^2}} \underset{D_0}{v} = \frac{\partial}{\partial x_0}\left[\frac{\partial L}{\partial x_0} \cdot v\right]$$

(if v doesn't depend on x_0)

Backprop: Higher-Order Derivatives

$$\underset{D_0}{x_0} \xrightarrow{f_1} \underset{D_1}{x_1} \xrightarrow{f_2} \underset{\text{scalar}}{L} \xrightarrow{f'_2} \underset{D_1}{dL/dx_1} \xrightarrow{f'_1} \underset{D_0}{dL/dx_0} \xrightarrow{\text{norm}} \underset{\text{scalar}}{|dL/dx_0|^2}$$

Backprop!

This is implemented in PyTorch / Tensorflow!

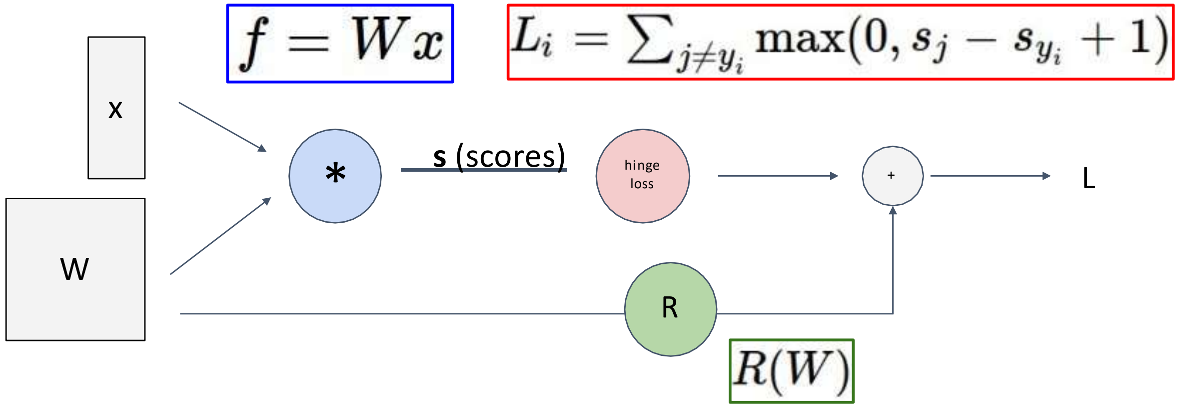
Example: Regularization to penalize the norm of the gradient

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

Gulrajani et al, “Improved Training of Wasserstein GANs”, NeurIPS 2017

Summary

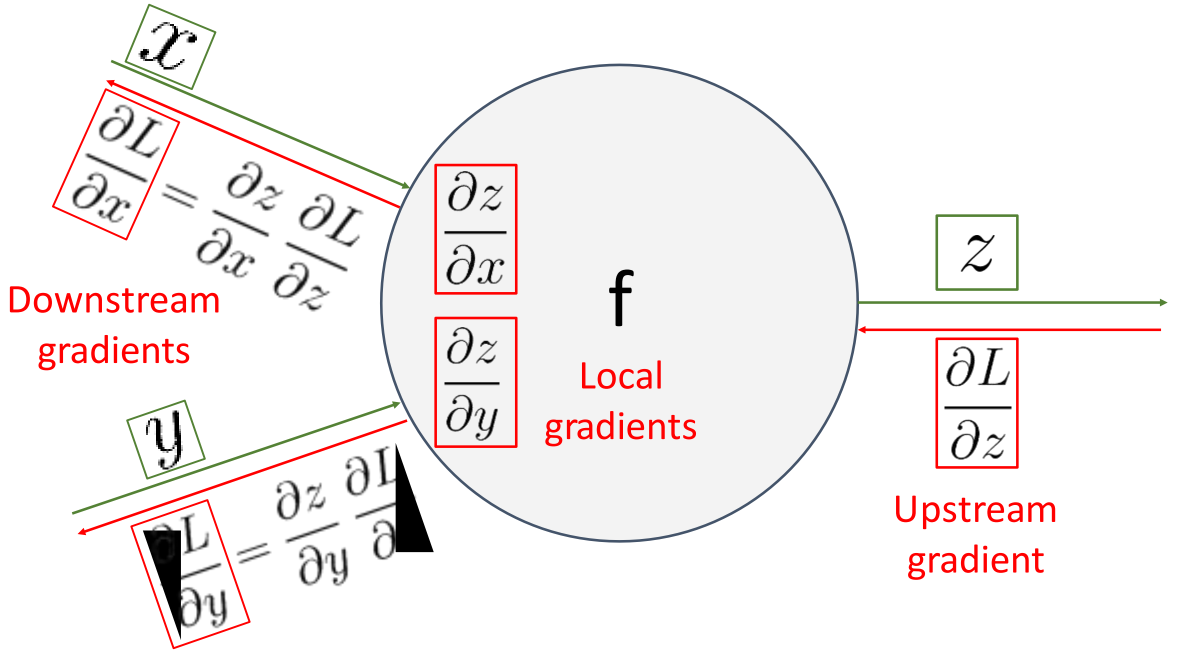
Represent complex expressions as **computational graphs**



Forward pass computes outputs

Backward pass computes gradients

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!)

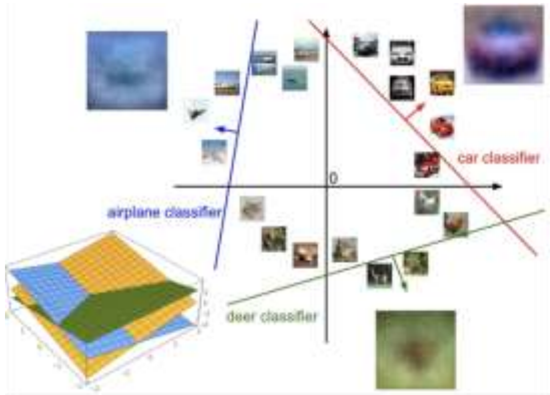
```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)

  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
```

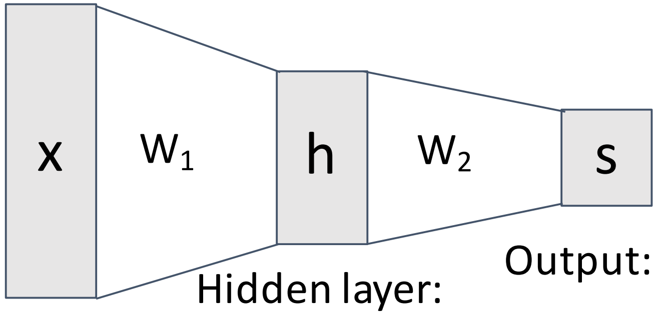
Backprop can be implemented with a modular API, as a set of paired forward/backward functions (We will do this on A3!)

```
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
```

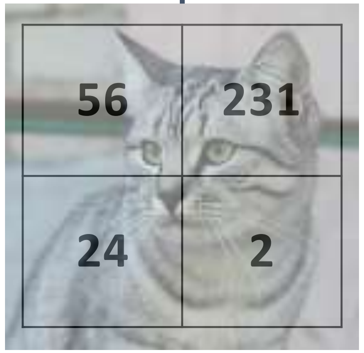
f(x,W) = Wx



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

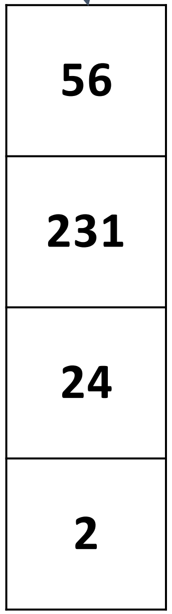


Stretch pixels into column



Input image
(2, 2)

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



(4,)

Next time:
Convolutional Neural Networks