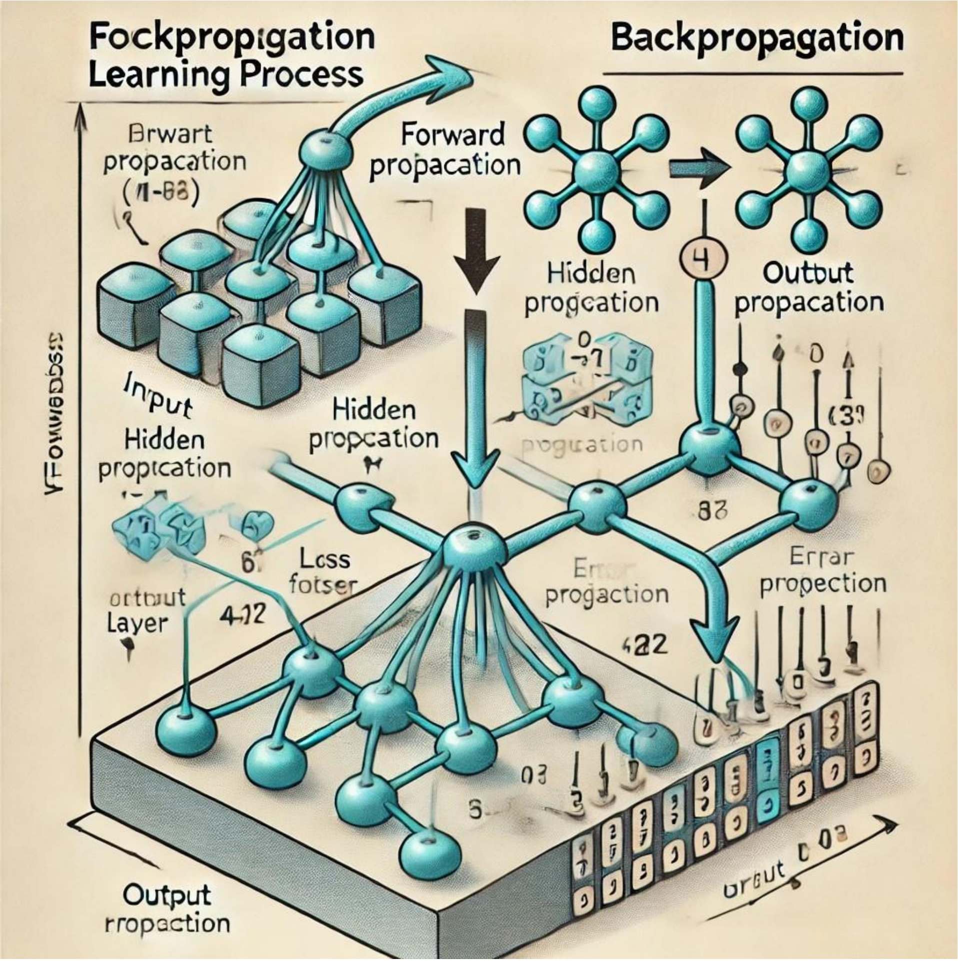
Back Propagation



AI604 Deep Learning for Computer Vision

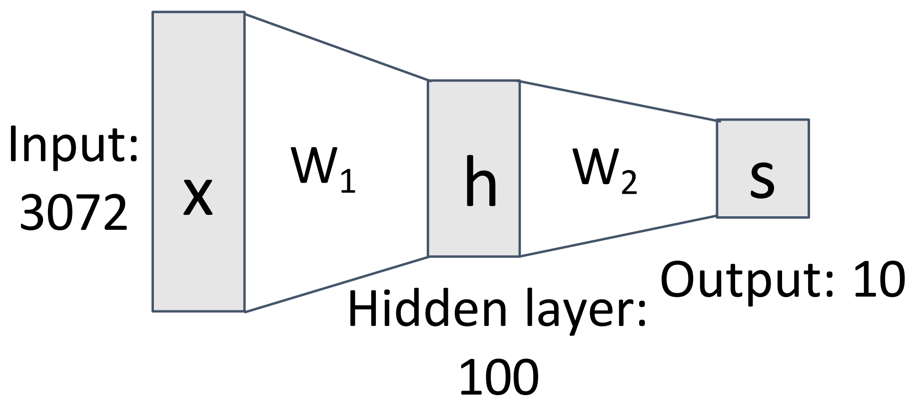
Prof. Hyunjung Shim

Slide credit: Justin Johnson, Fei-Fei Li, Ehsan Adeli

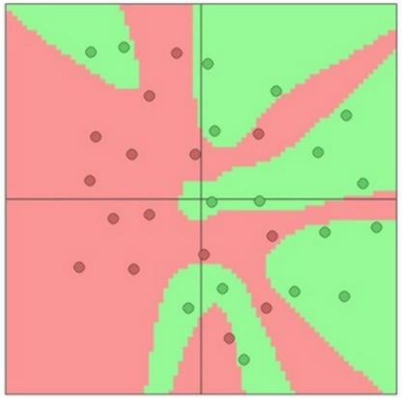
Recap: Classification/Loss/Optimizer

From linear classifiers to fully-connected networks

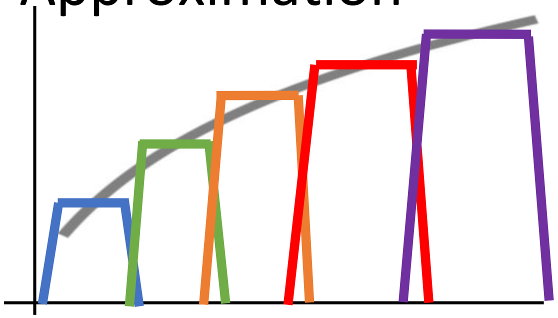
$$f = W_2 \max(0, W_1 x)$$



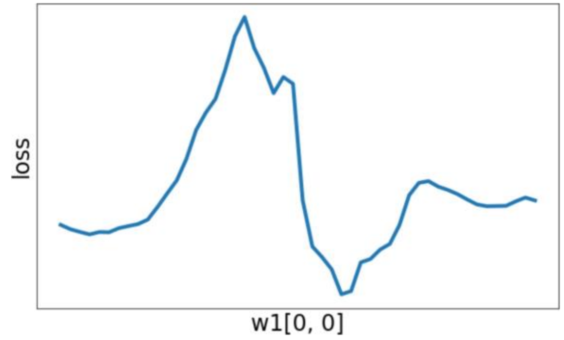
Space Warping



Universal Approximation



Nonconvex



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

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

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

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

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

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

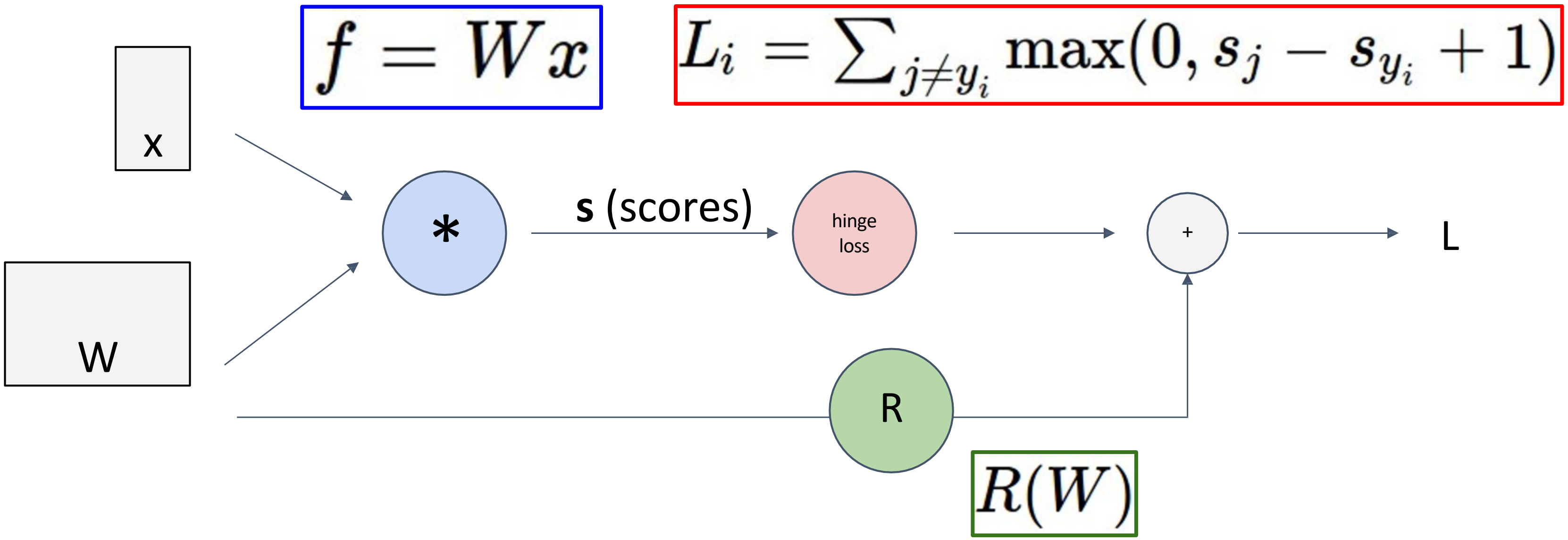
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

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

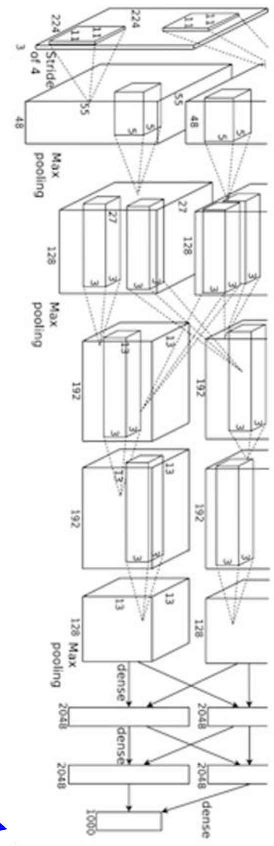


Deep Network (AlexNet)

input image

weights

loss



Neural Turing Machine

input image

loss

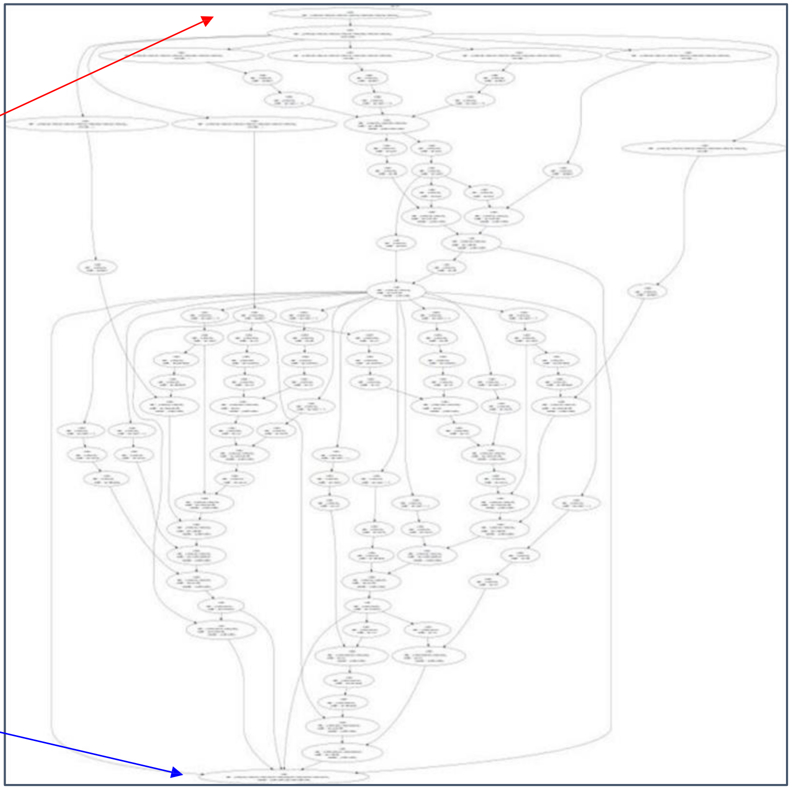


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

Neural Turing Machine

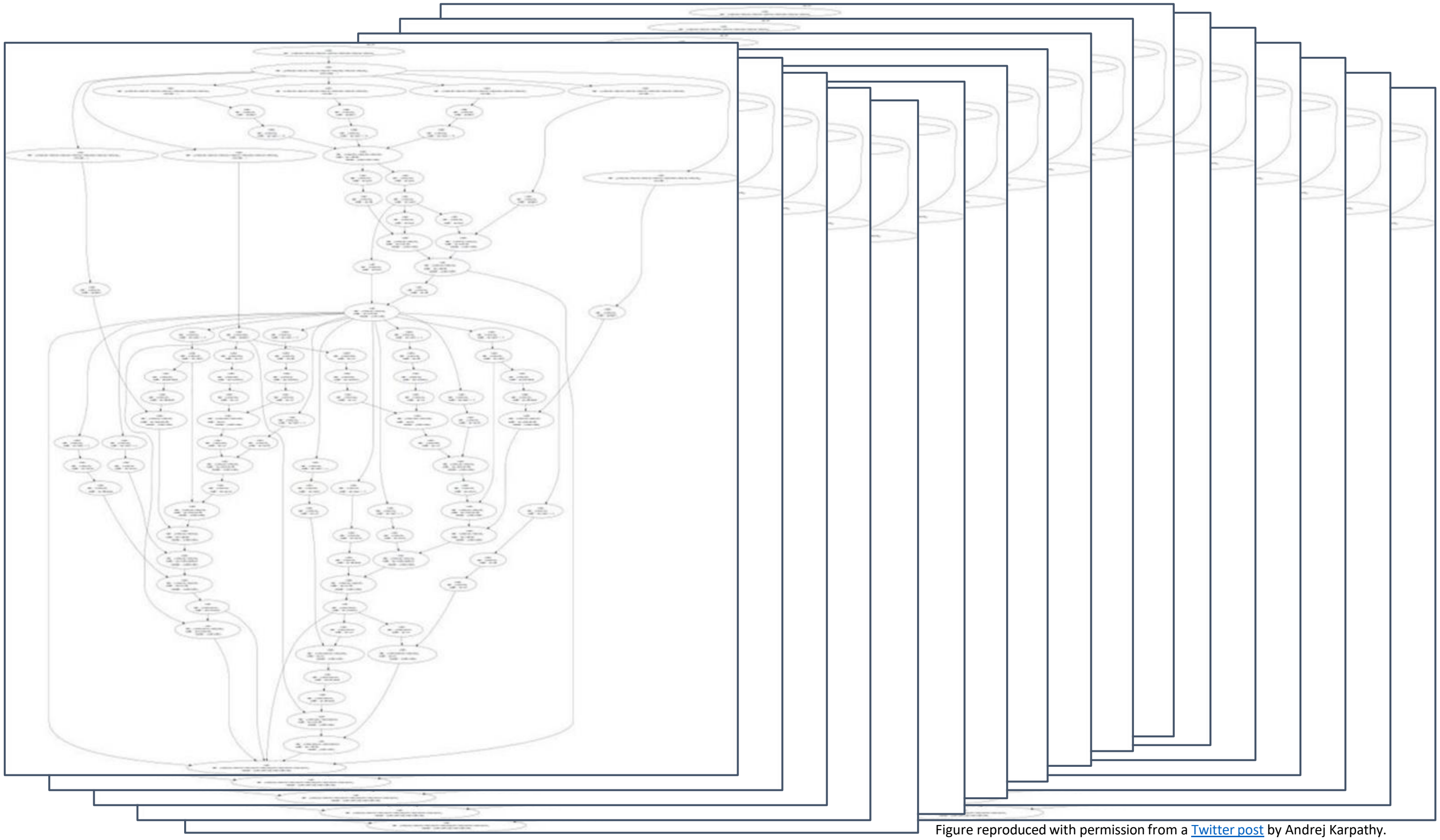
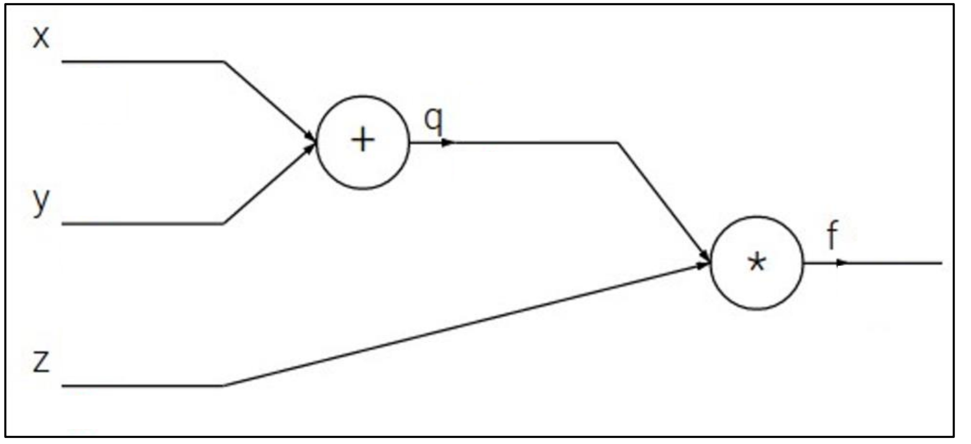


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

Backpropagation: Simple Example

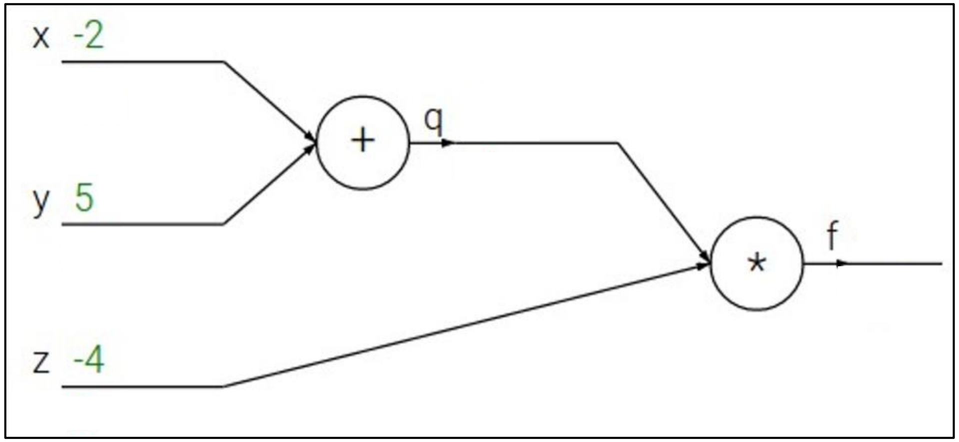
$$f(x, y, z) = (x + y)z$$



Backpropagation: Simple Example

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

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



Backpropagation: Simple Example

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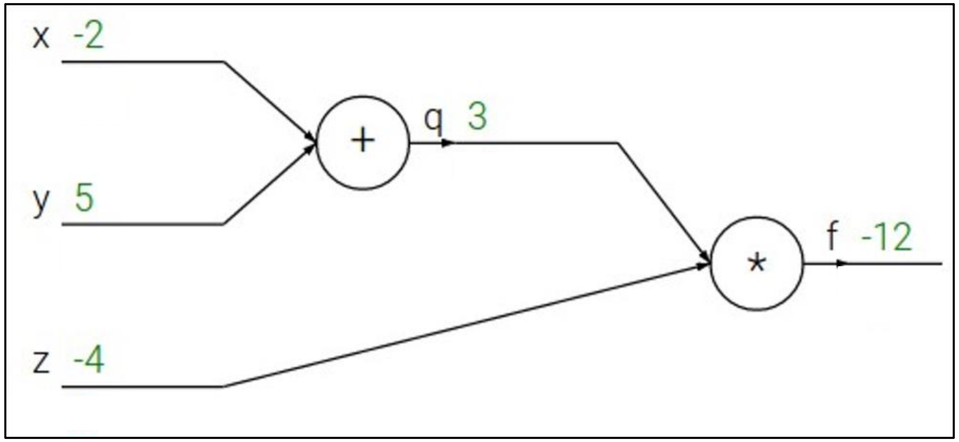
1. Forward pass: Compute outputs

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



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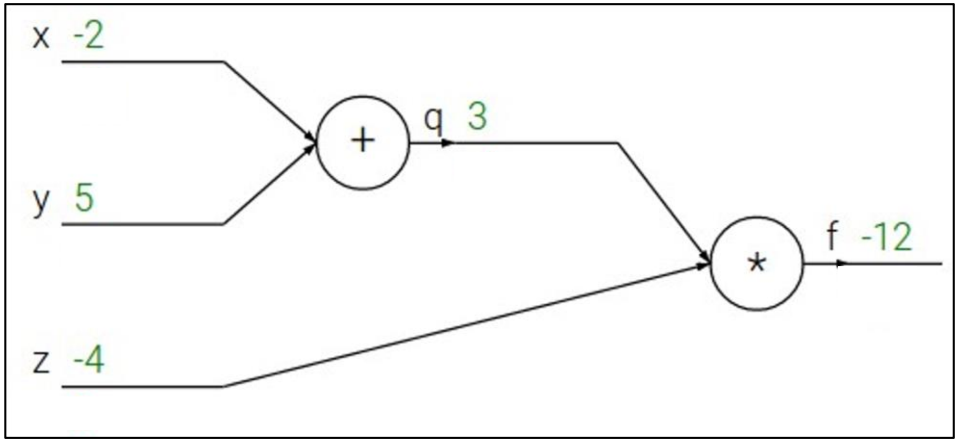


1. Forward pass: Compute outputs

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

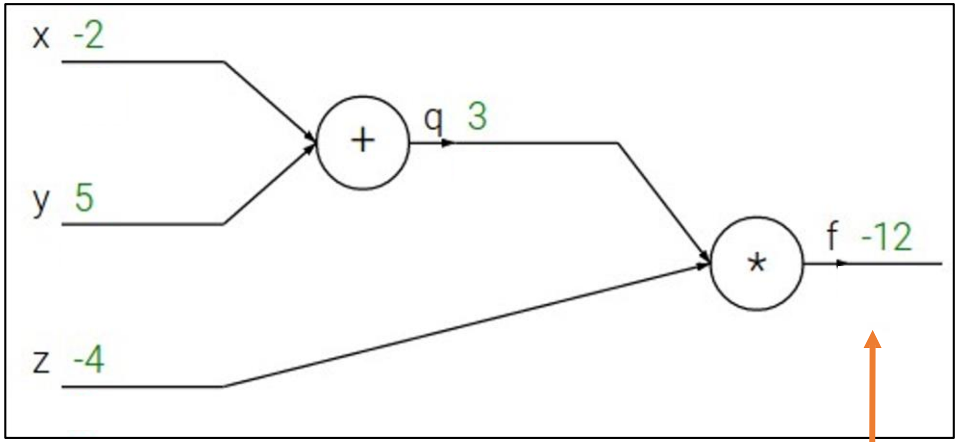
2 . Backward pass: Compute derivatives

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

Backpropagation: Simple Example

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

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



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

1. Forward pass: Compute outputs

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

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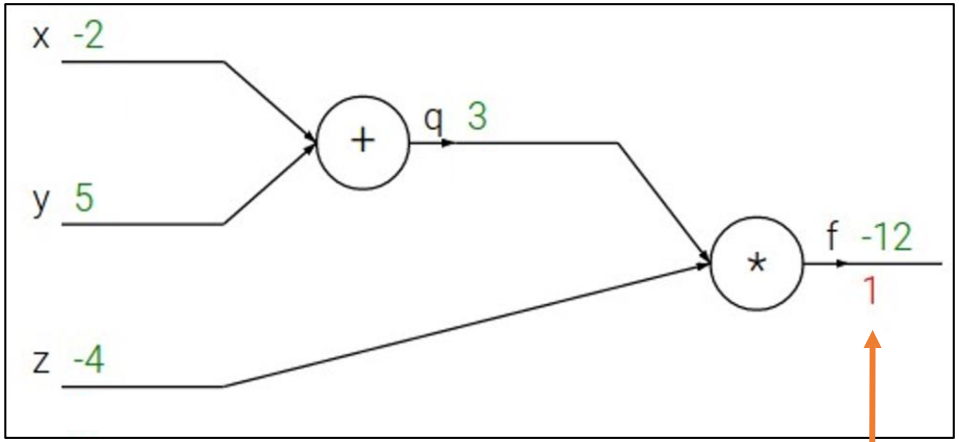

$$\boxed{\frac{\partial f}{\partial f}}$$

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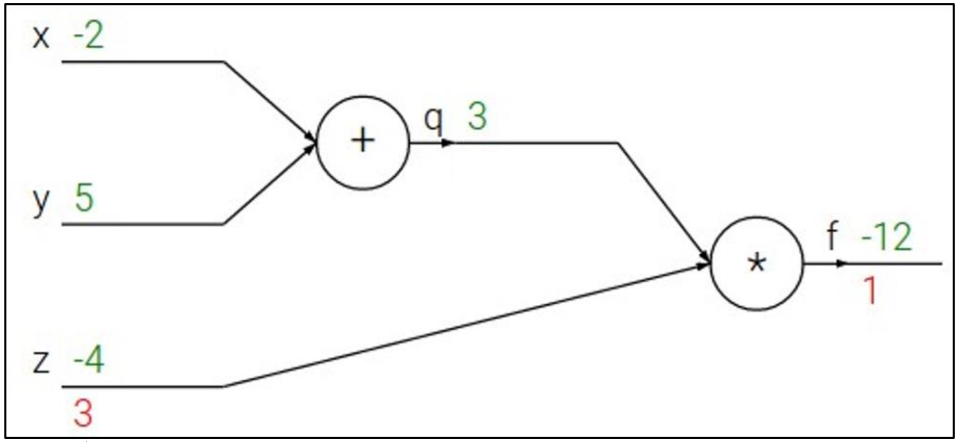

1. Forward pass: Compute outputs

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

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

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

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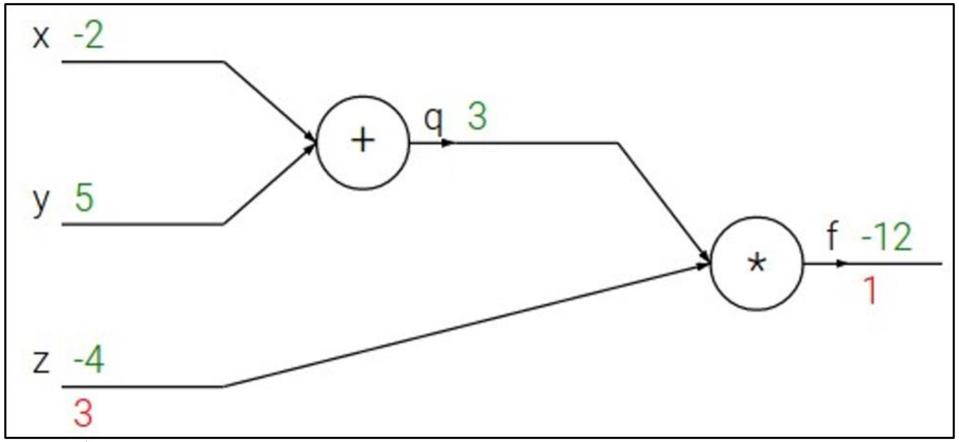


1. Forward pass: Compute outputs

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

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

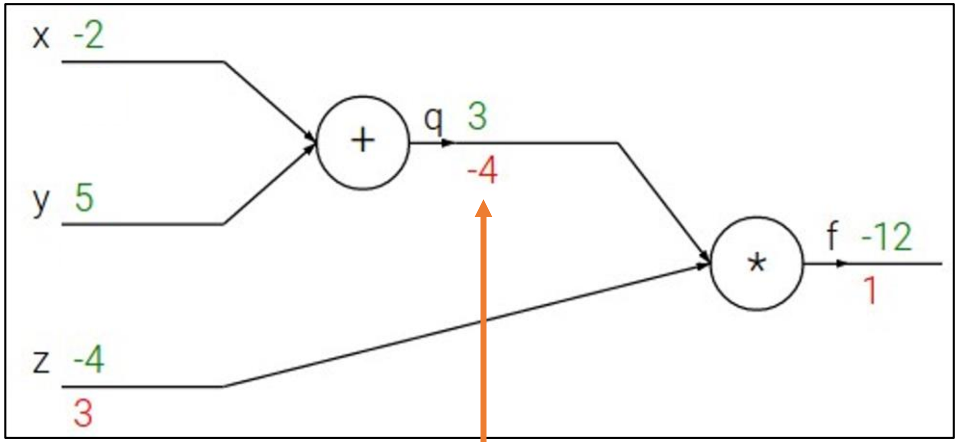
2 . Backward pass: Compute derivatives

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

Backpropagation: Simple Example

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

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



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

1. Forward pass: Compute outputs

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

2 . Backward pass: Compute derivatives

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

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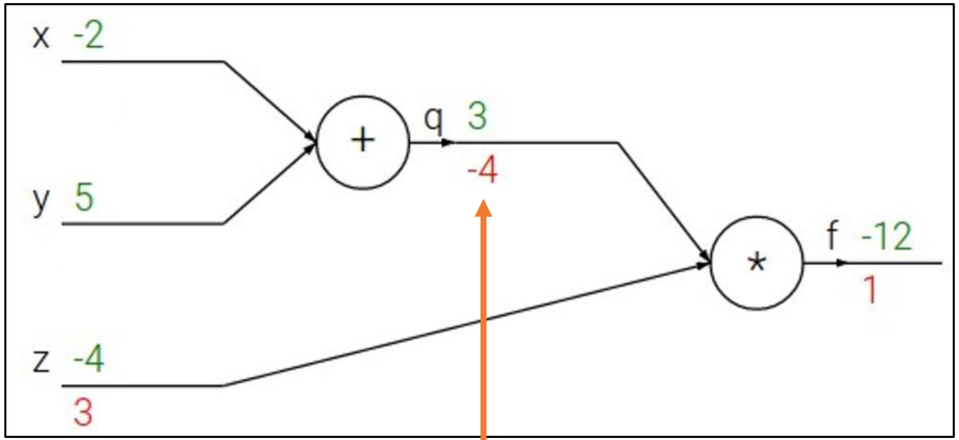


1. Forward pass: Compute outputs

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

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

2 . Backward pass: Compute derivatives

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

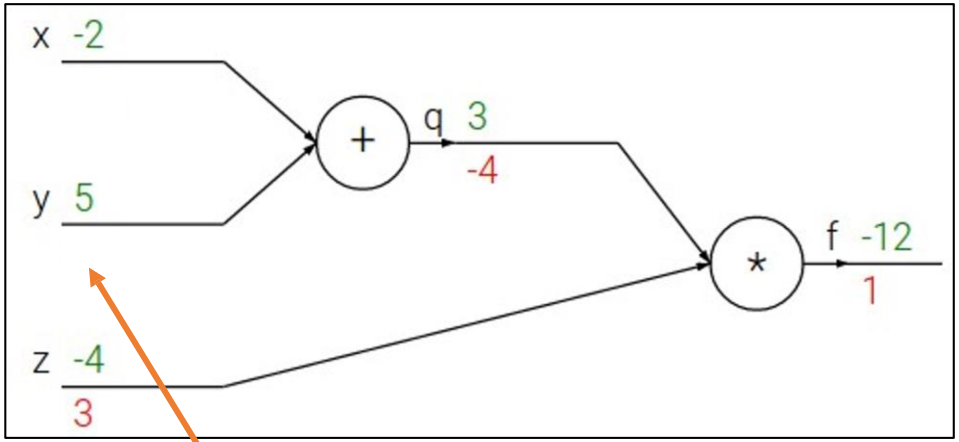
Backpropagation: Simple Example

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

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

1. Forward pass: Compute outputs

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



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

2 . Backward pass: Compute derivatives

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

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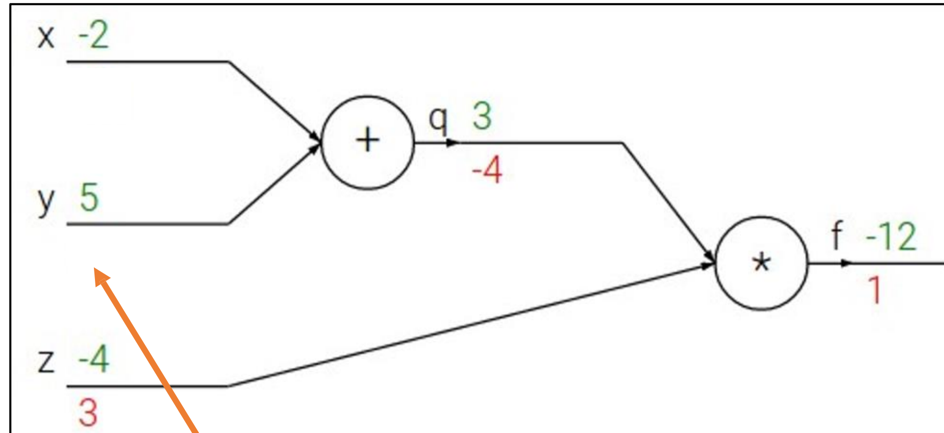
$$f(x, y, z) = (x + y)z$$

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



1. Forward pass: Compute outputs

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

Chain Rule

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

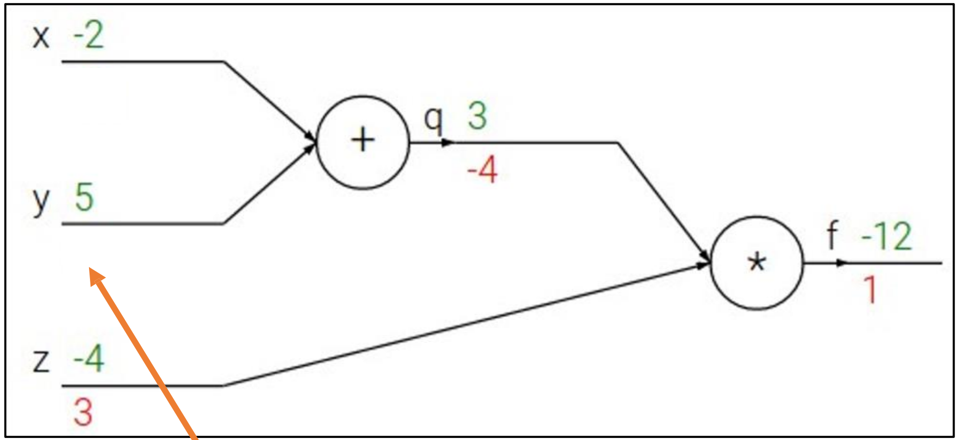
2 . Backward pass: Compute derivatives

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

Backpropagation: Simple Example

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

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



1. Forward pass: Compute outputs

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

2 . Backward pass: Compute derivatives

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

Chain Rule

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

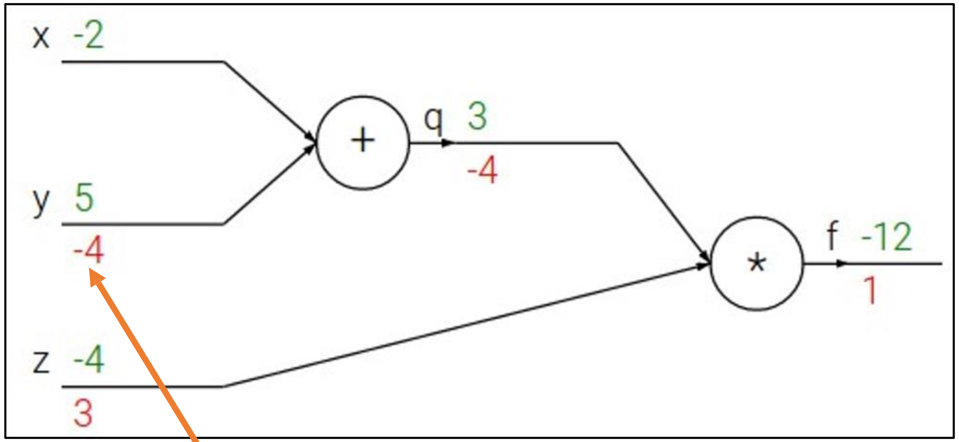
Downstream Gradient **Local Gradient** **Upstream Gradient**

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

Backpropagation: Simple Example

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

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



1. Forward pass: Compute outputs

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

Chain Rule

$$\boxed{\frac{\partial f}{\partial y} = \frac{\partial q}{\partial y} \frac{\partial f}{\partial q}} \qquad \boxed{\frac{\partial q}{\partial y} = 1}$$

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

2 . Backward pass: Compute derivatives

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

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

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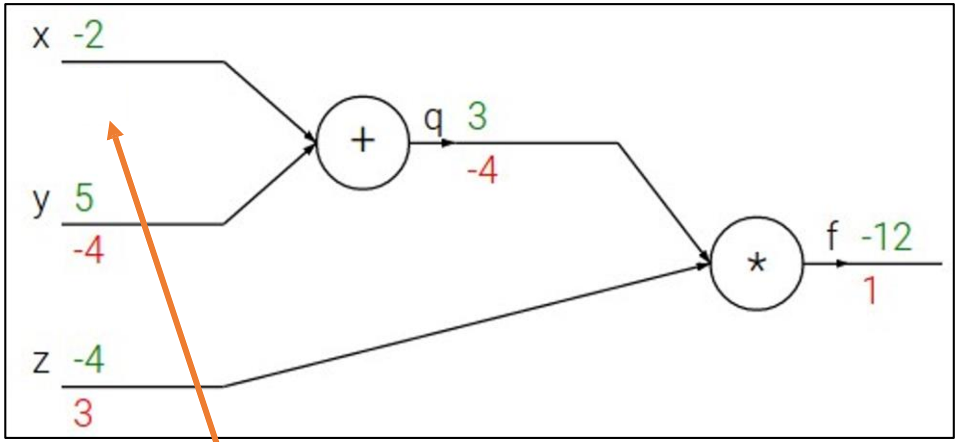

1. Forward pass: Compute outputs

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

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$$\boxed{\frac{\partial f}{\partial x} = \frac{\partial q}{\partial x}\frac{\partial f}{\partial q}} \qquad \boxed{\frac{\partial q}{\partial x} = 1}$$

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

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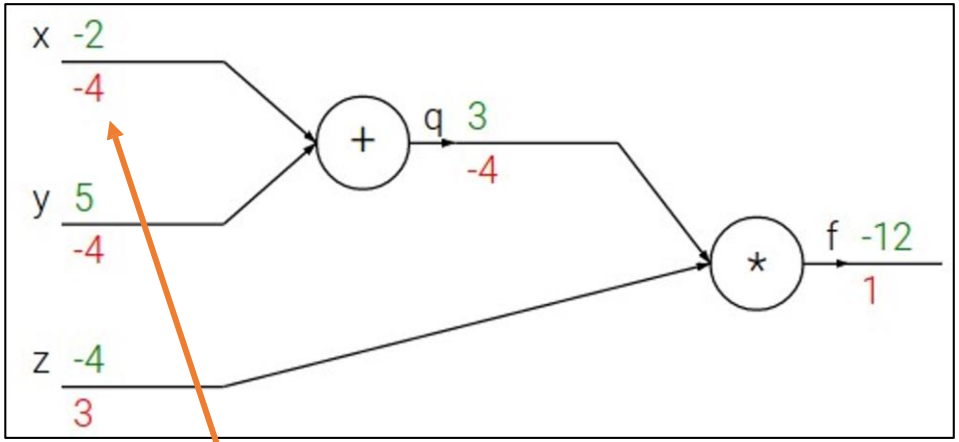


1. Forward pass: Compute outputs

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

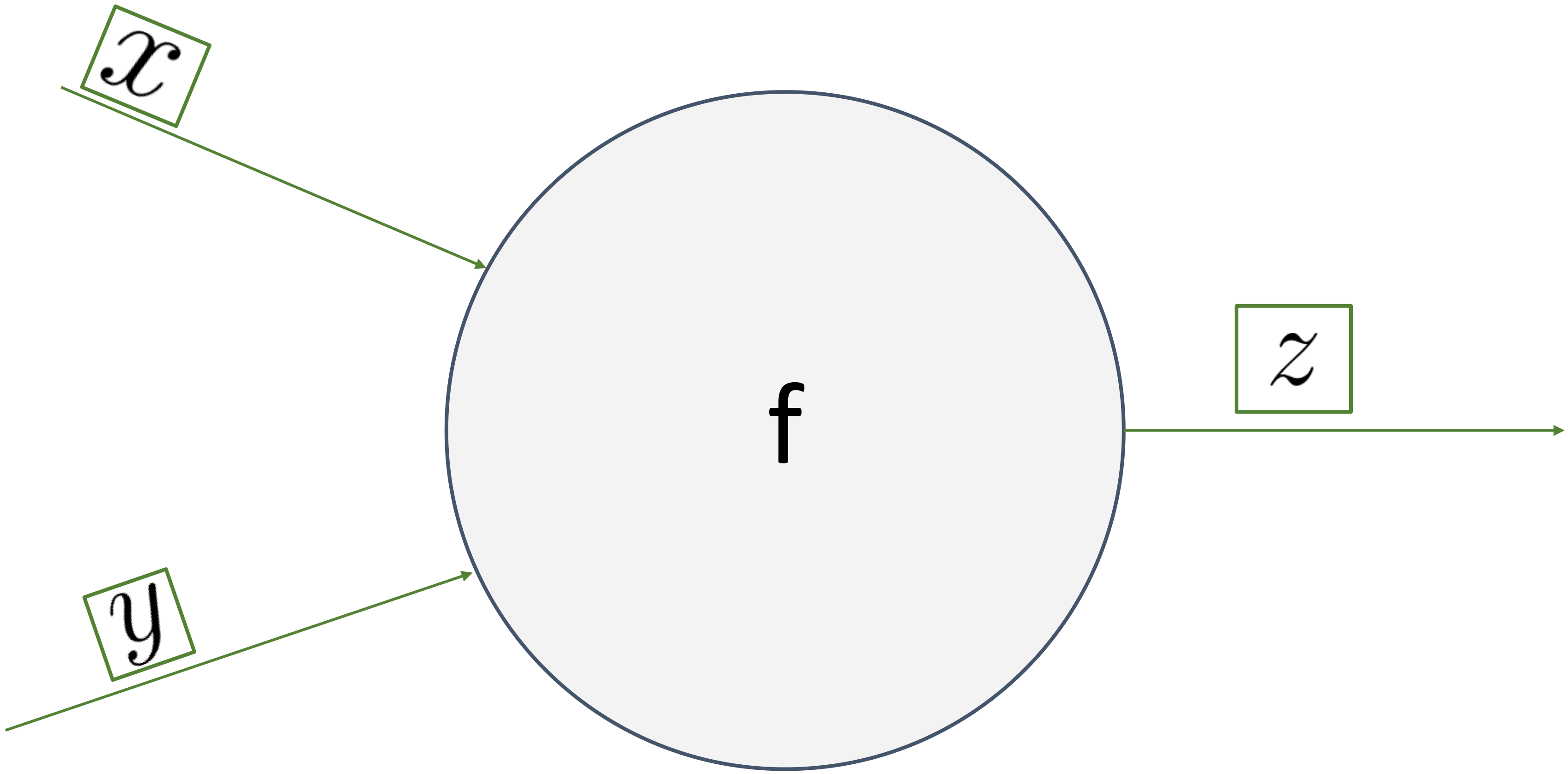
Chain Rule

$$\boxed{\frac{\partial f}{\partial x} = \frac{\partial q}{\partial x}\frac{\partial f}{\partial q}} \qquad \boxed{\frac{\partial q}{\partial x} = 1}$$

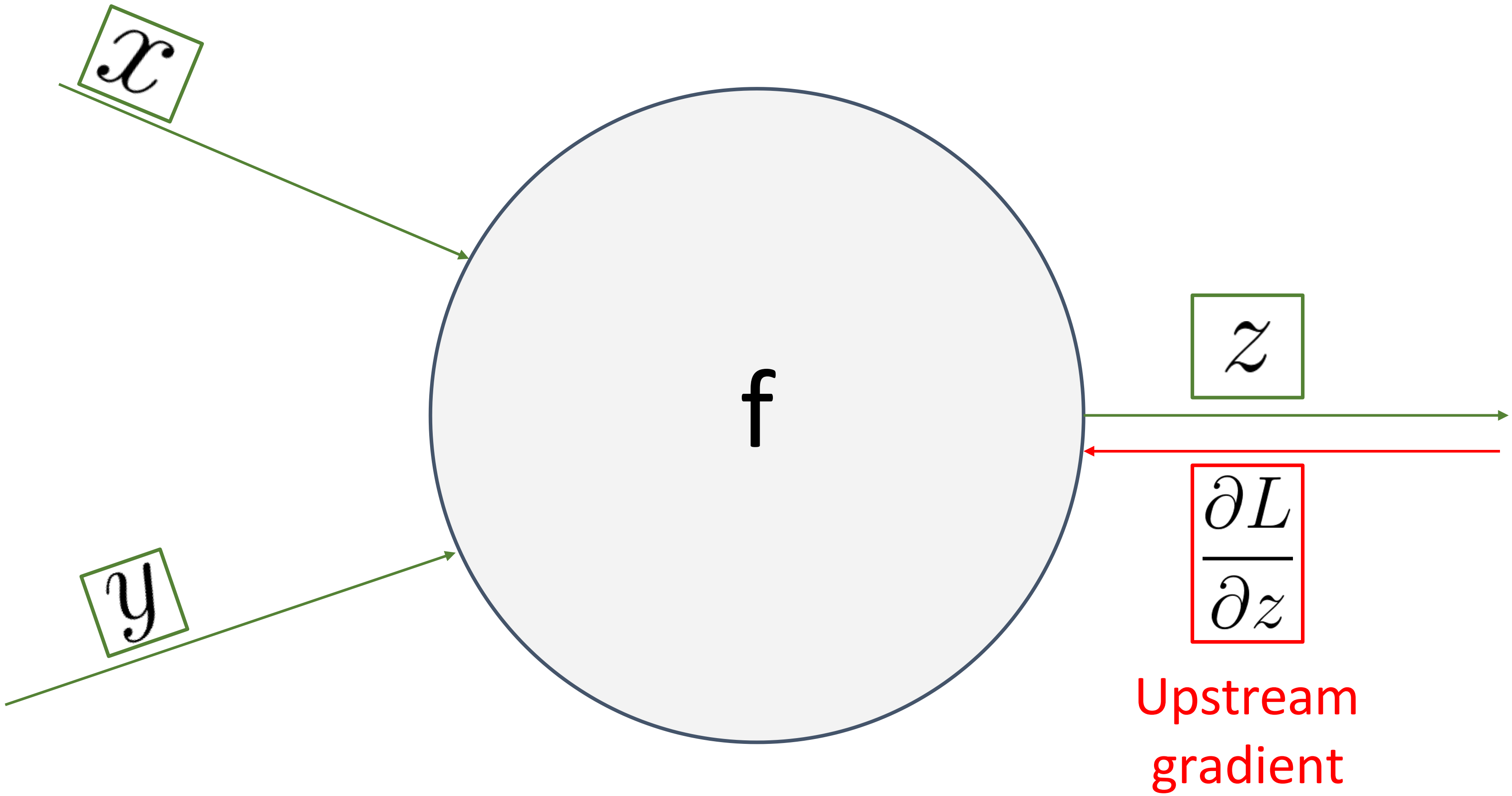
Downstream Gradient **Local Gradient** **Upstream Gradient**

2 . Backward pass: Compute derivatives

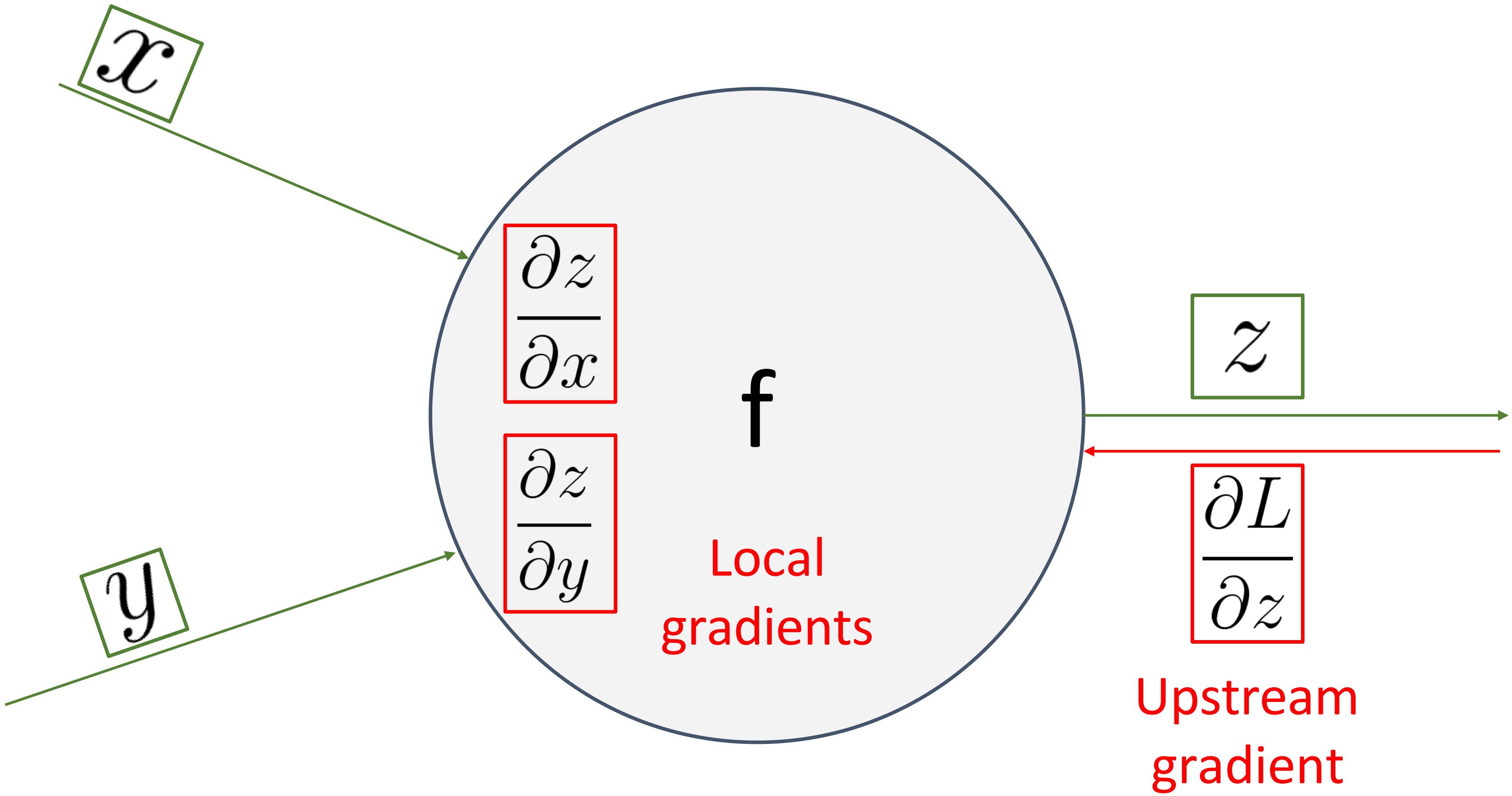
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

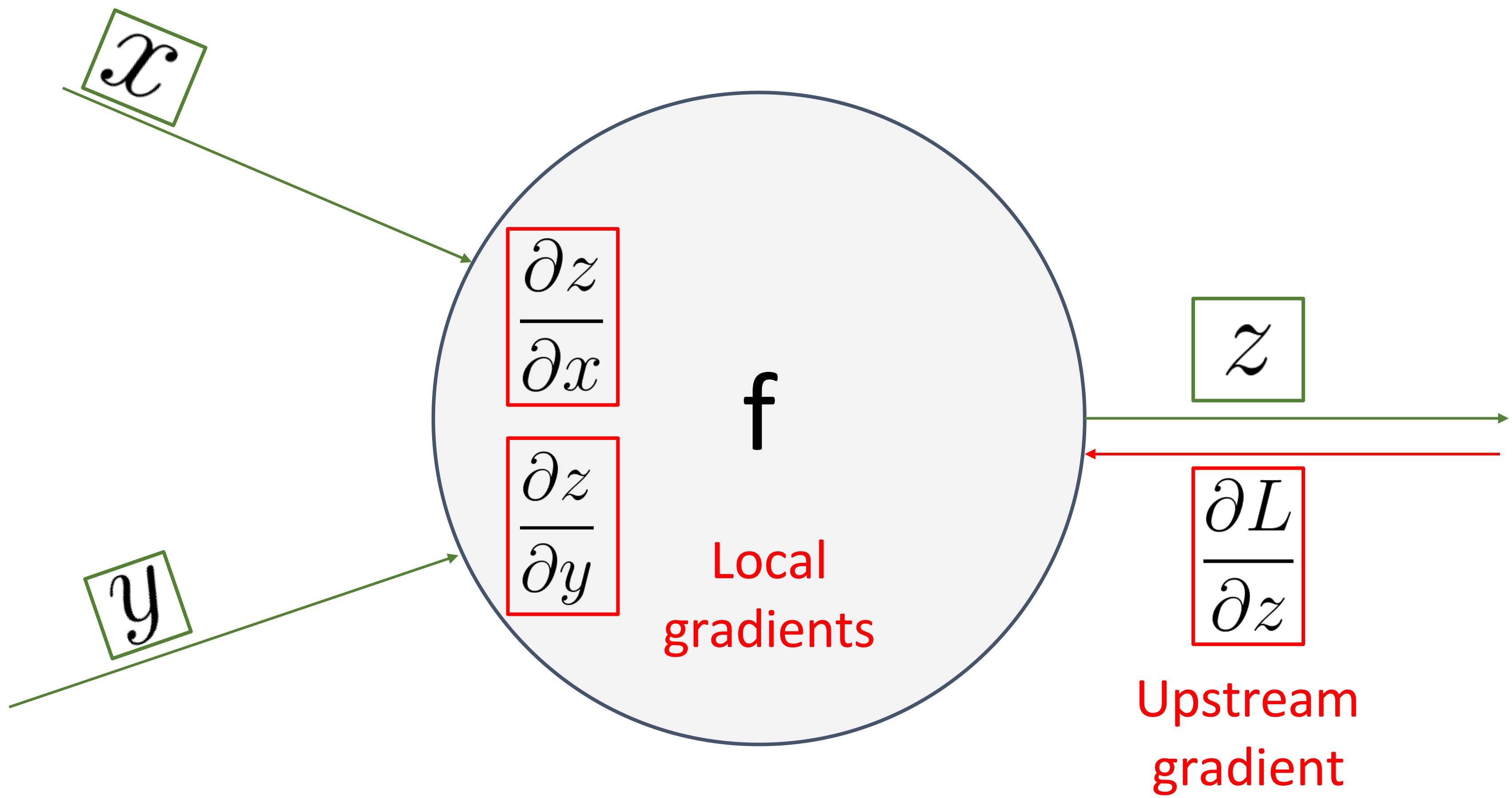


x
y
f
z

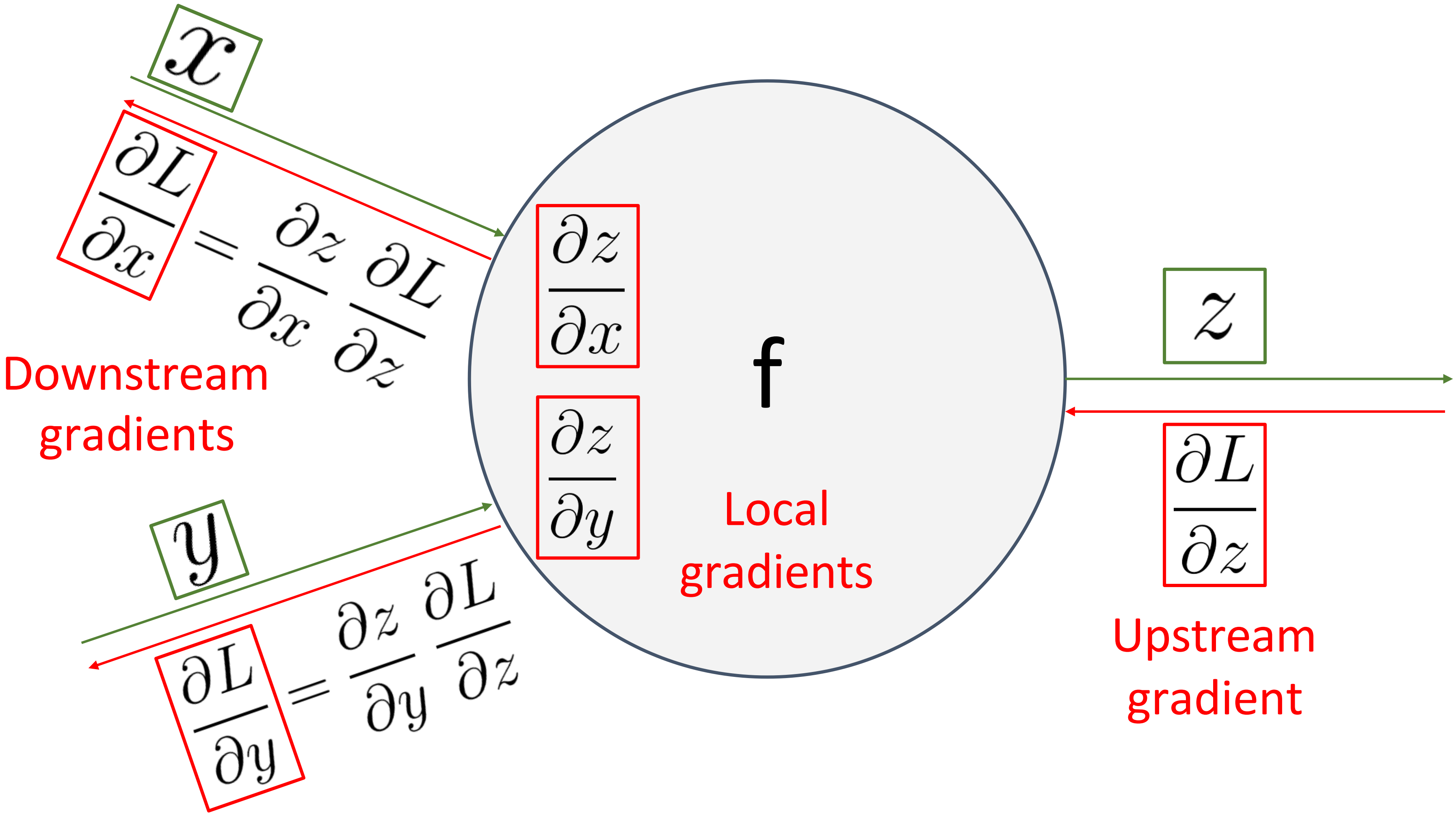


x
y
f
z
$\frac{\partial L}{\partial z}$
Upstream gradient

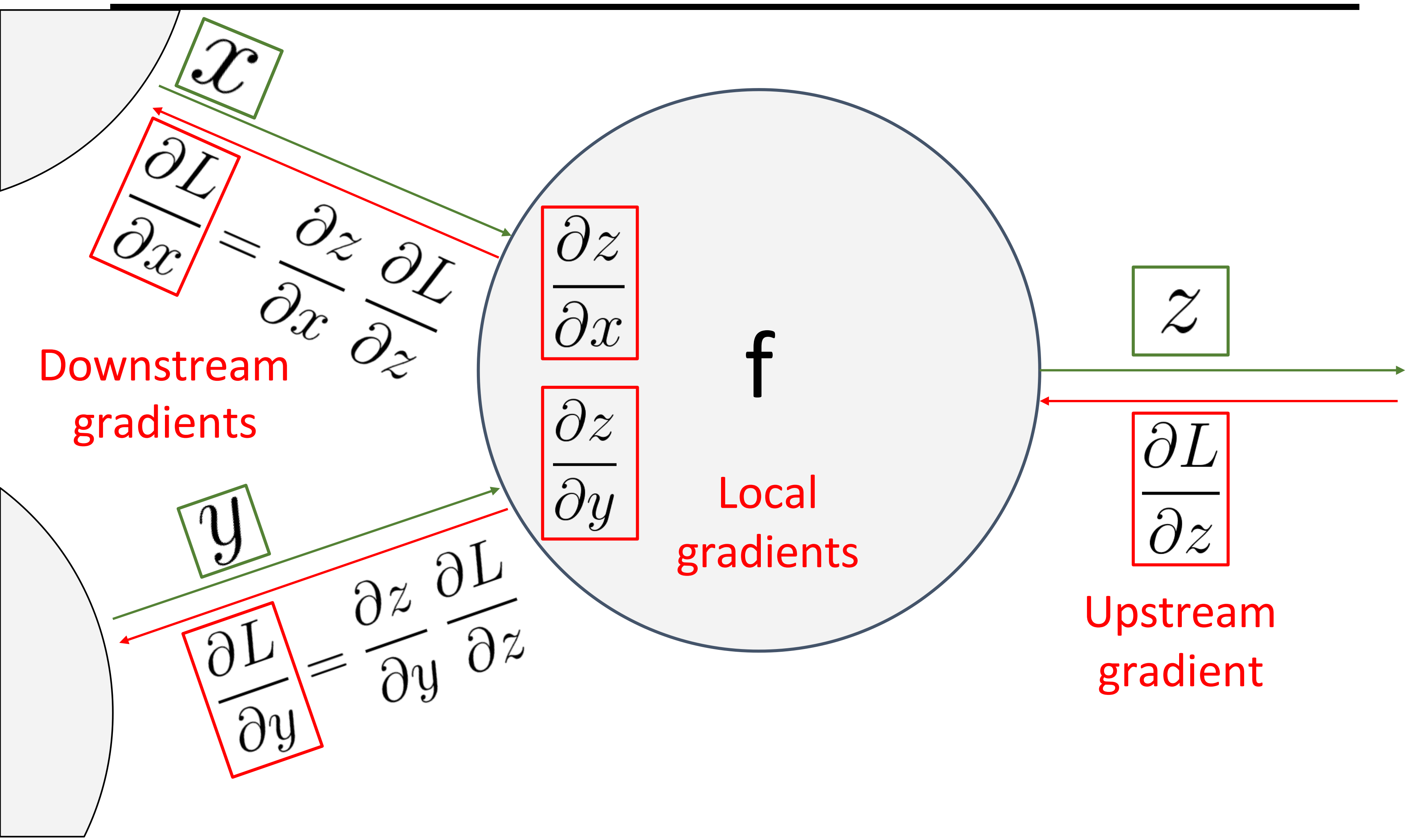

x
y
z
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
Local gradients
$\frac{\partial L}{\partial z}$
Upstream gradient



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



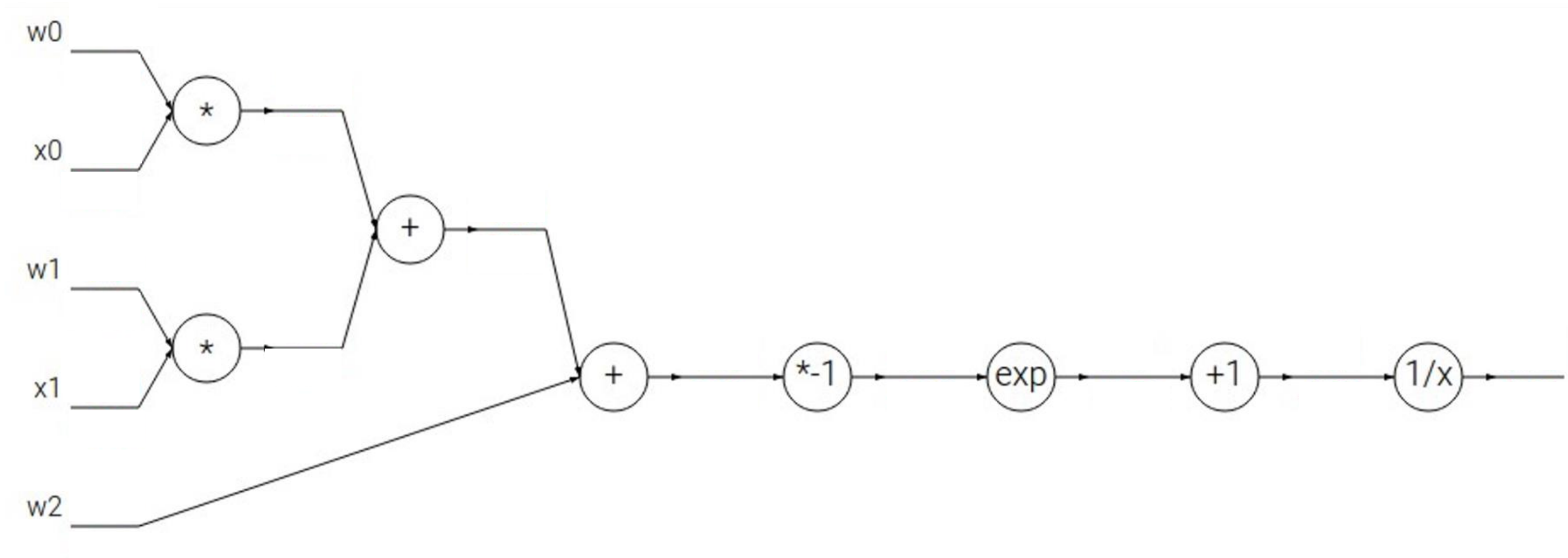
x
$\frac{\partial L}{\partial x} = \frac{\partial z}{\partial x}\frac{\partial L}{\partial z}$
Downstream gradients
y
$\frac{\partial L}{\partial y} = \frac{\partial z}{\partial y}\frac{\partial L}{\partial z}$
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
Local gradients
z
$\frac{\partial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

Another Example

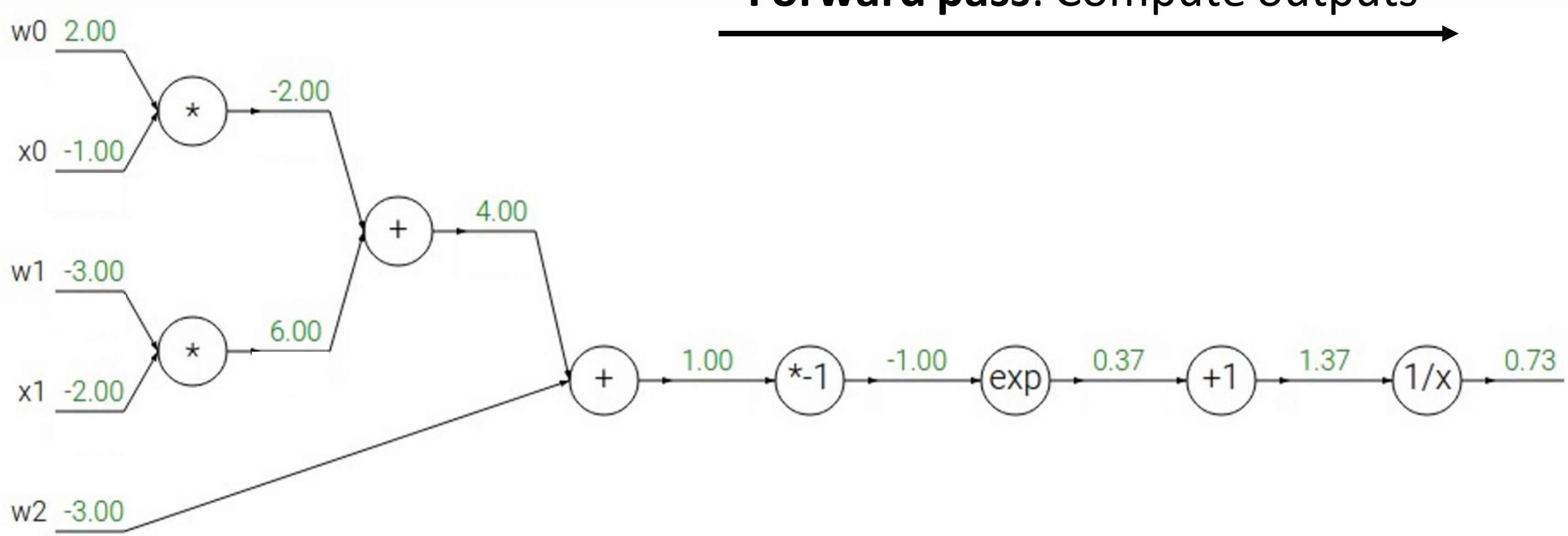
$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



Another Example

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

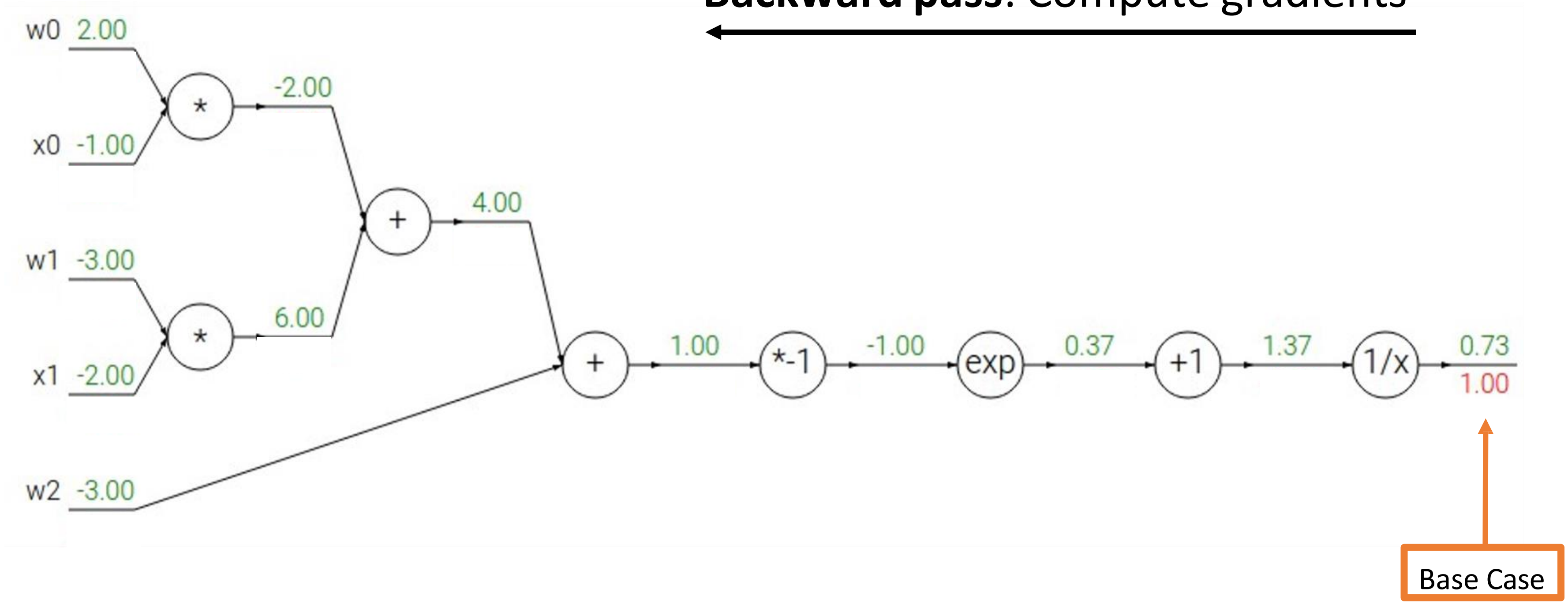
Forward pass: Compute outputs



Another Example

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

Backward pass: Compute gradients



Another Example

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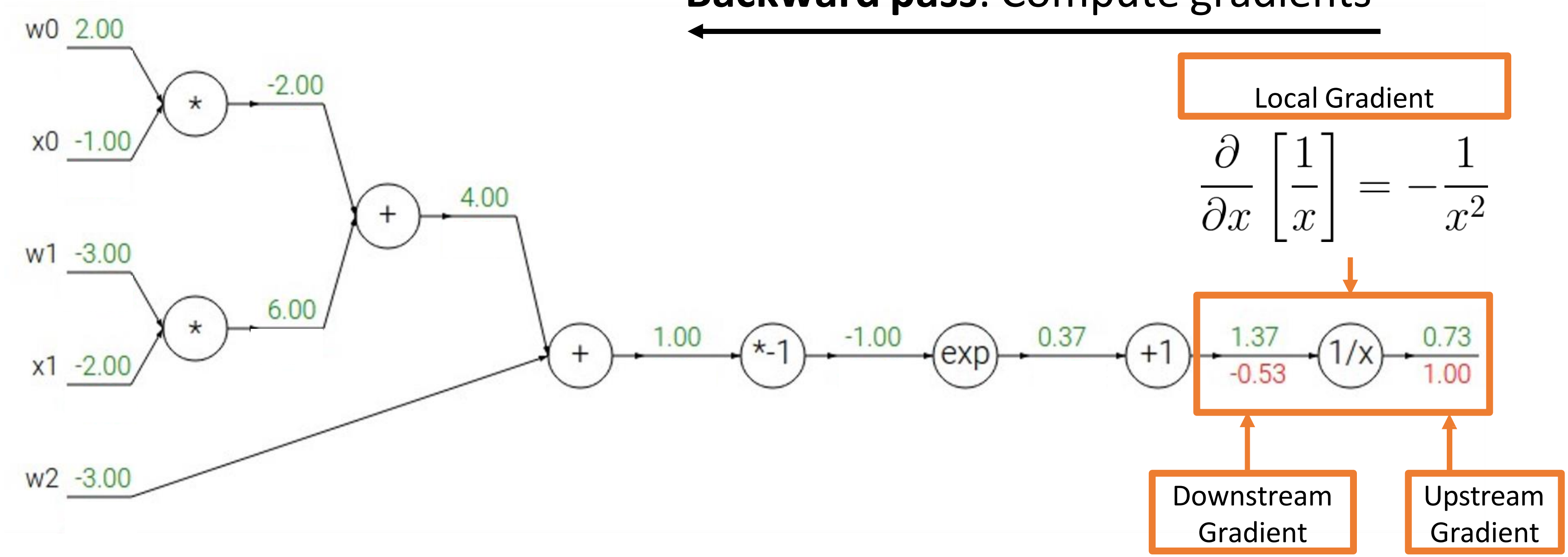
Backward pass: Compute gradients

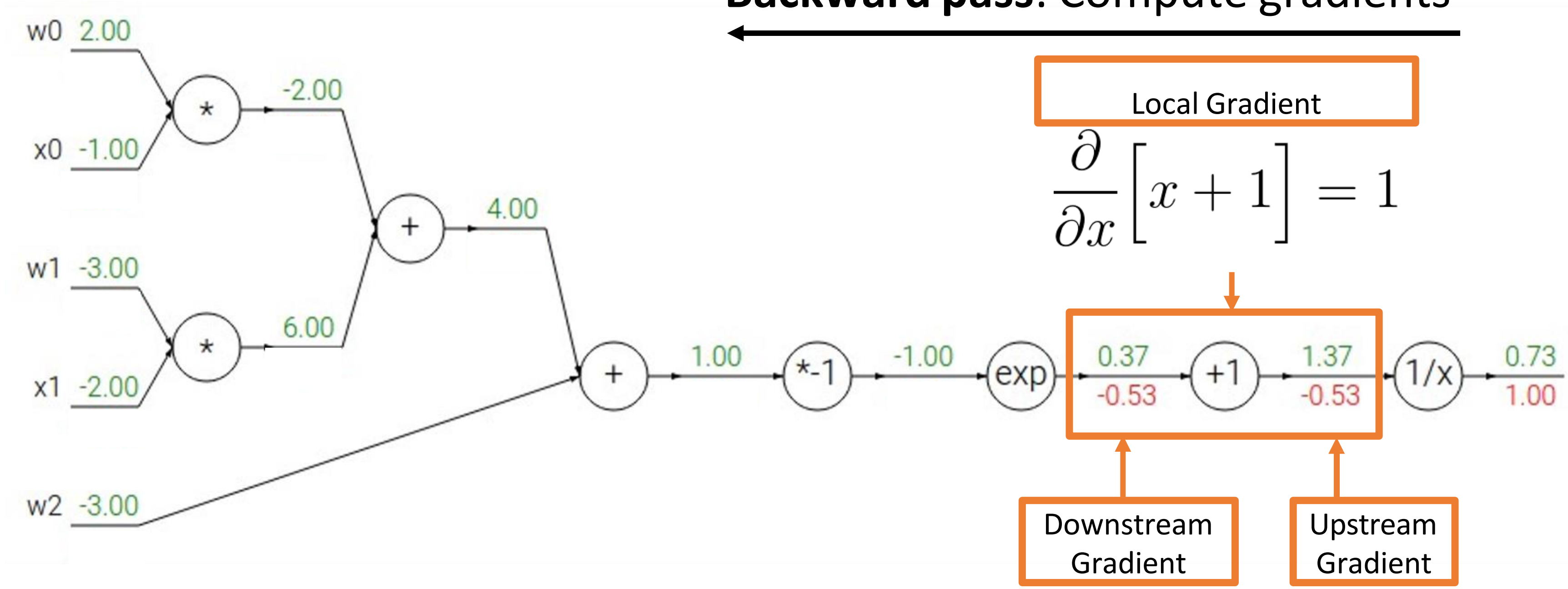


$$\frac{\partial}{\partial x}\left[\frac{1}{x}\right] = -\frac{1}{x^2}$$

Another Example

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

Backward pass: Compute gradients



$$\frac{\partial}{\partial x}\left[x+1\right] = 1$$

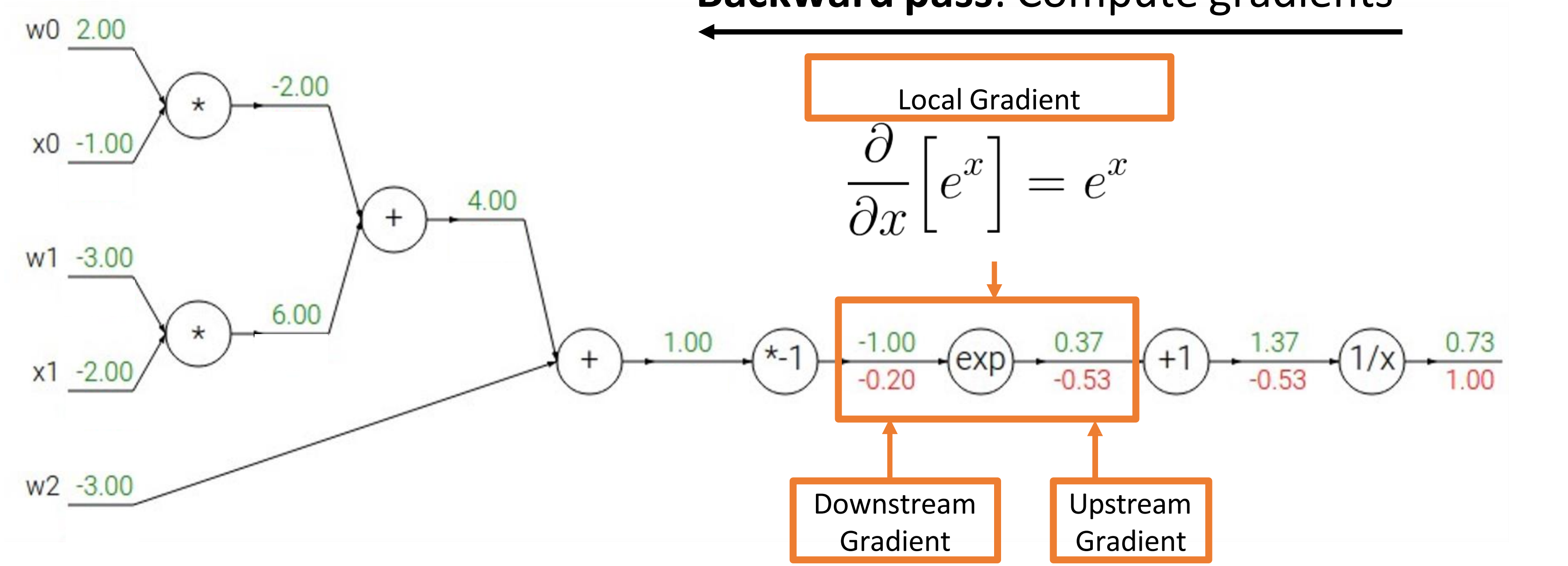
Another Example

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

Backward pass: Compute gradients

Local Gradient

$$\frac{\partial}{\partial x}\left[e^x\right] = e^x$$

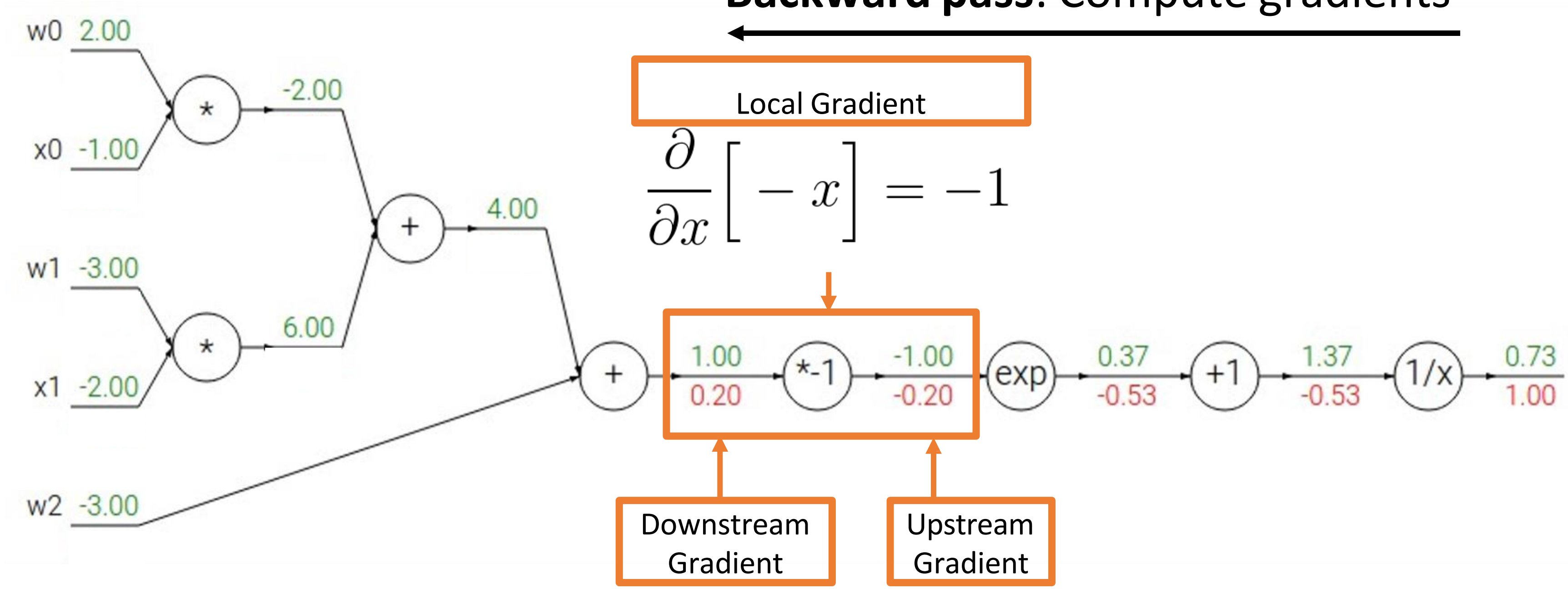


Another Example

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

Backward pass: Compute gradients

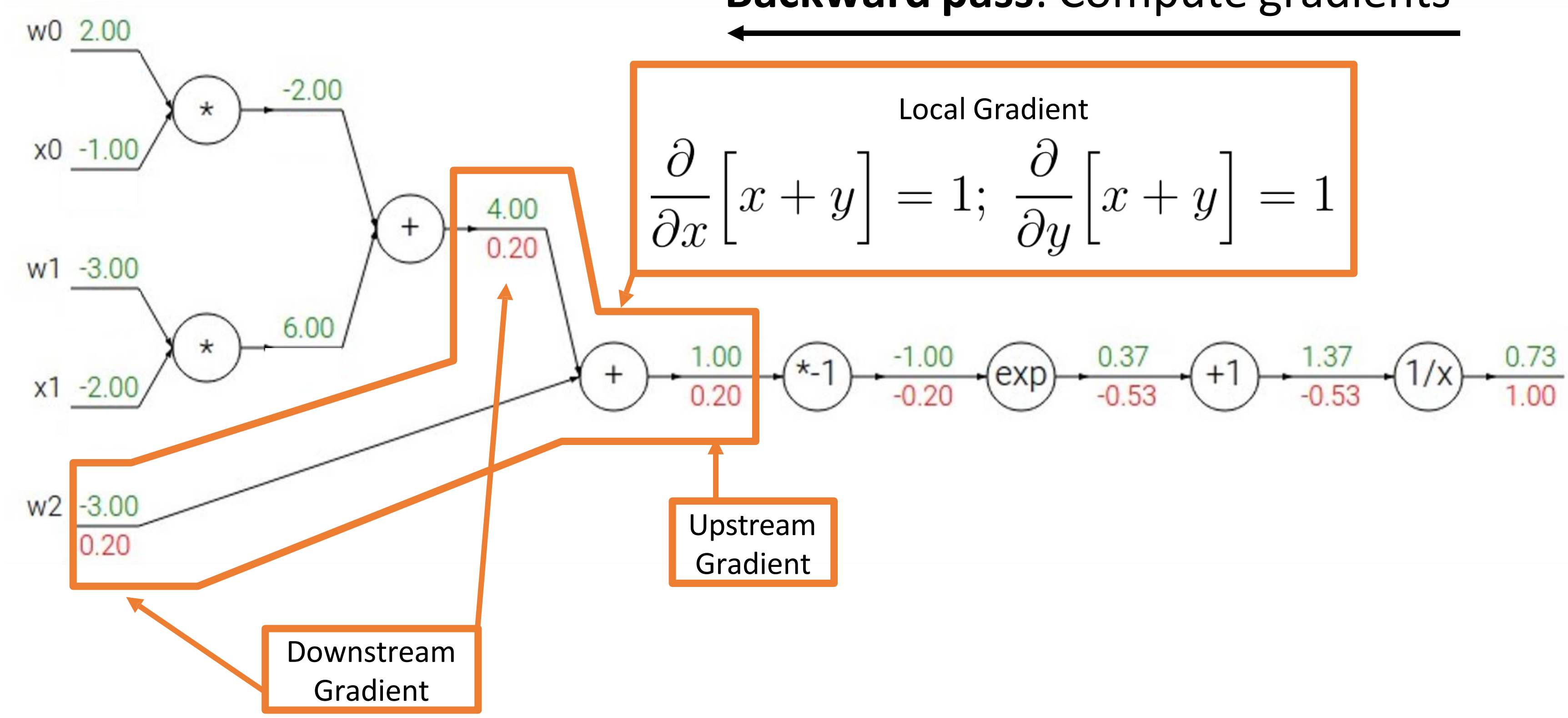
$$\frac{\partial}{\partial x}\left[-x\right] = -1$$



Another Example

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

Backward pass: Compute gradients



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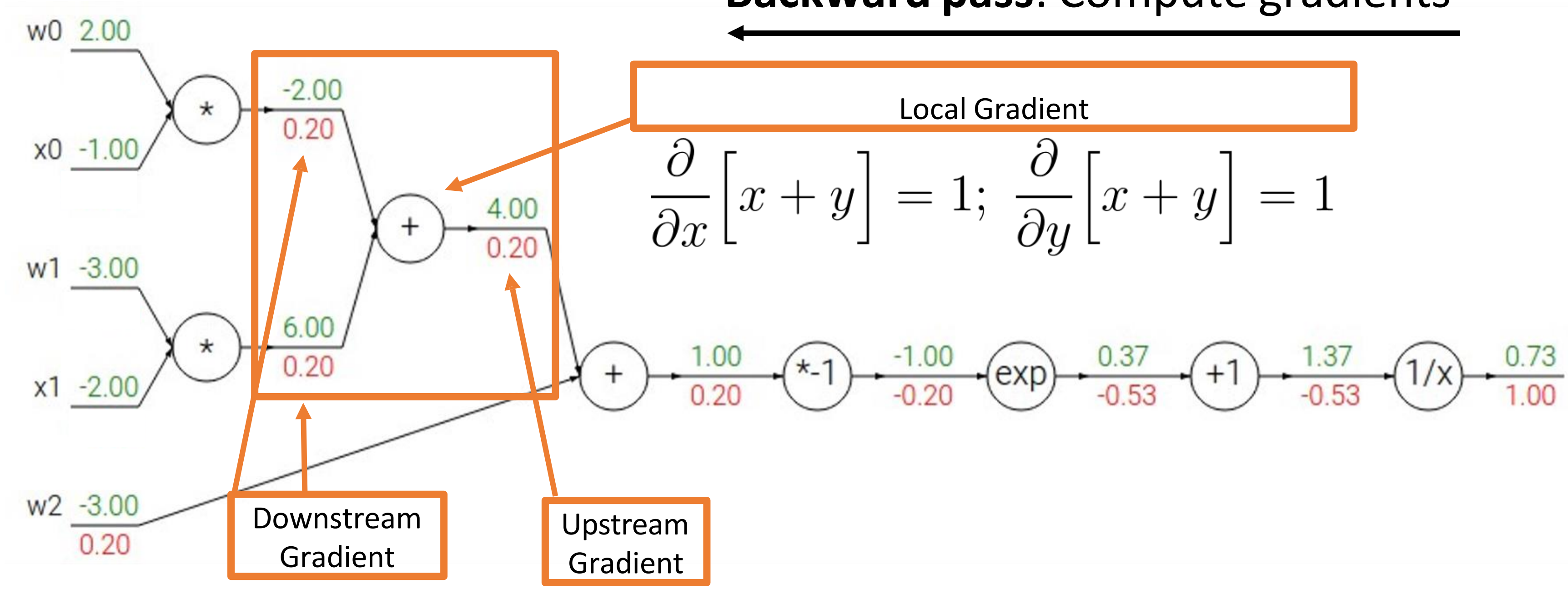
Backward pass: Compute gradients

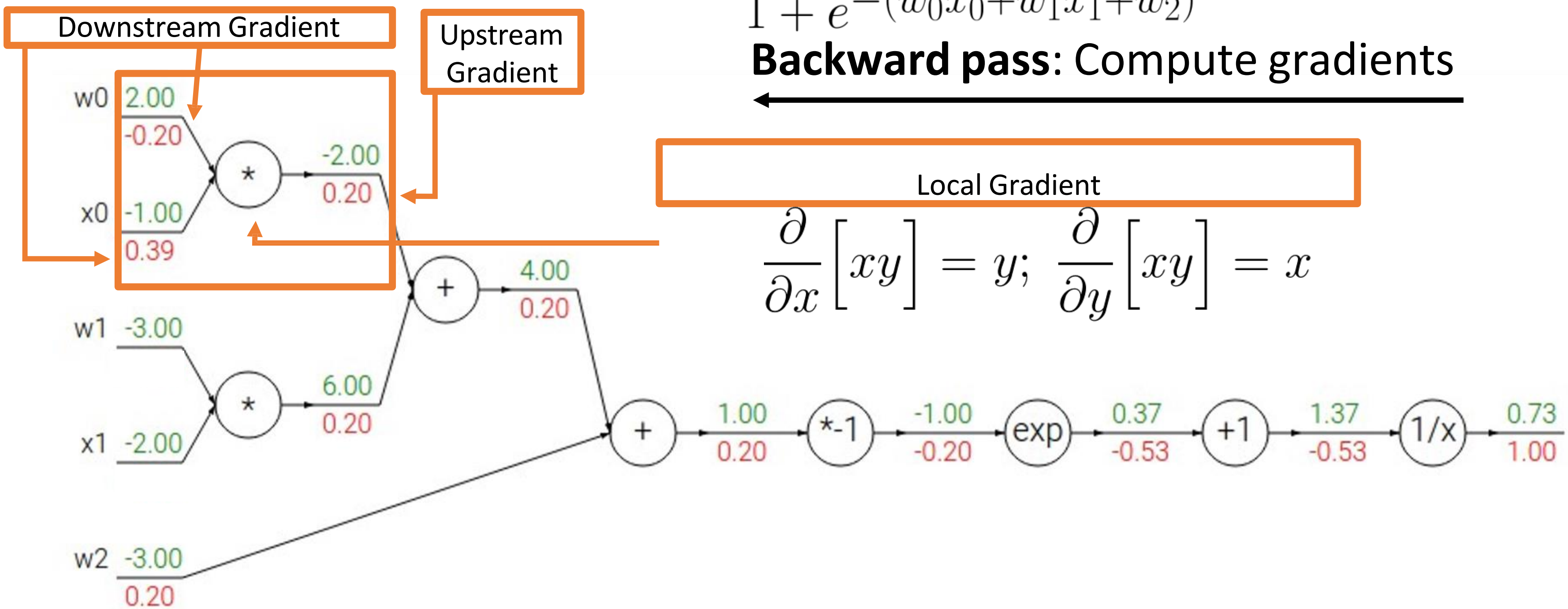


$$\frac{\partial}{\partial x}\left[x+y\right] = 1; \ \frac{\partial}{\partial y}\left[x+y\right] = 1$$

Another Example

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

Backward pass: Compute gradients

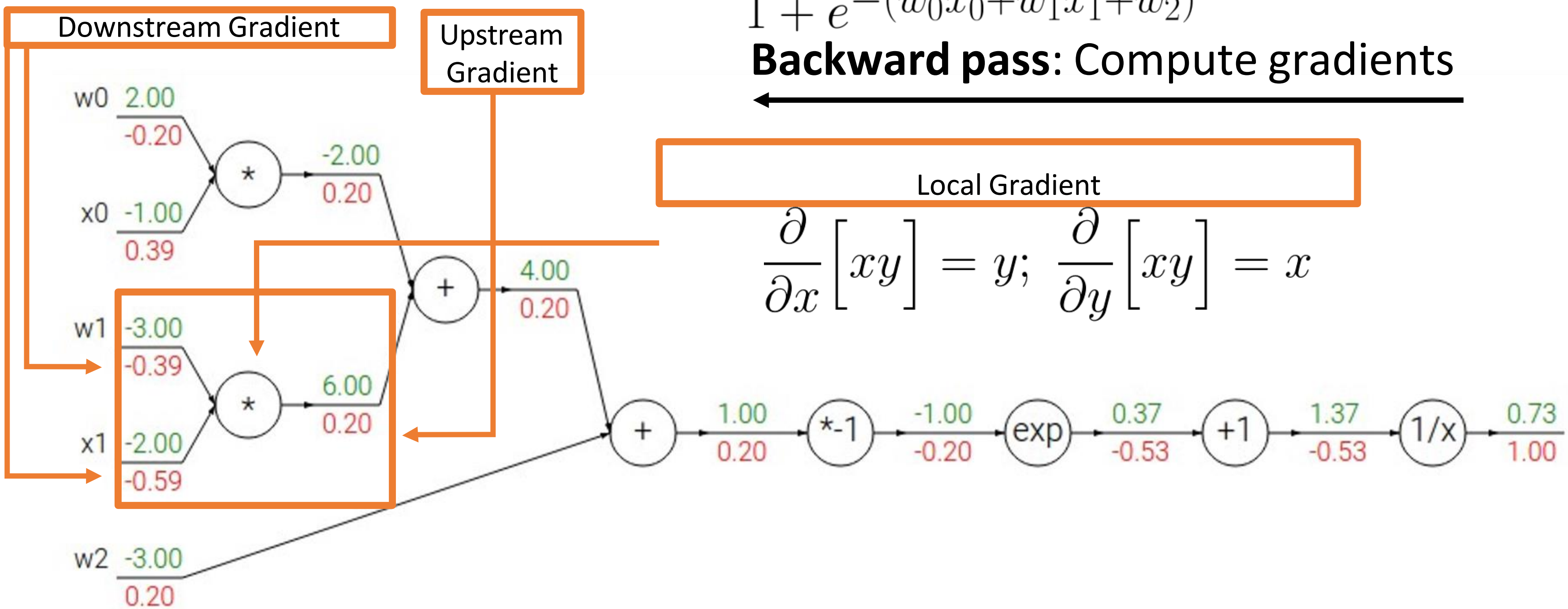


$$\frac{\partial}{\partial x}\left[xy\right] = y; \quad \frac{\partial}{\partial y}\left[xy\right] = x$$

Another Example

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

Backward pass: Compute gradients



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

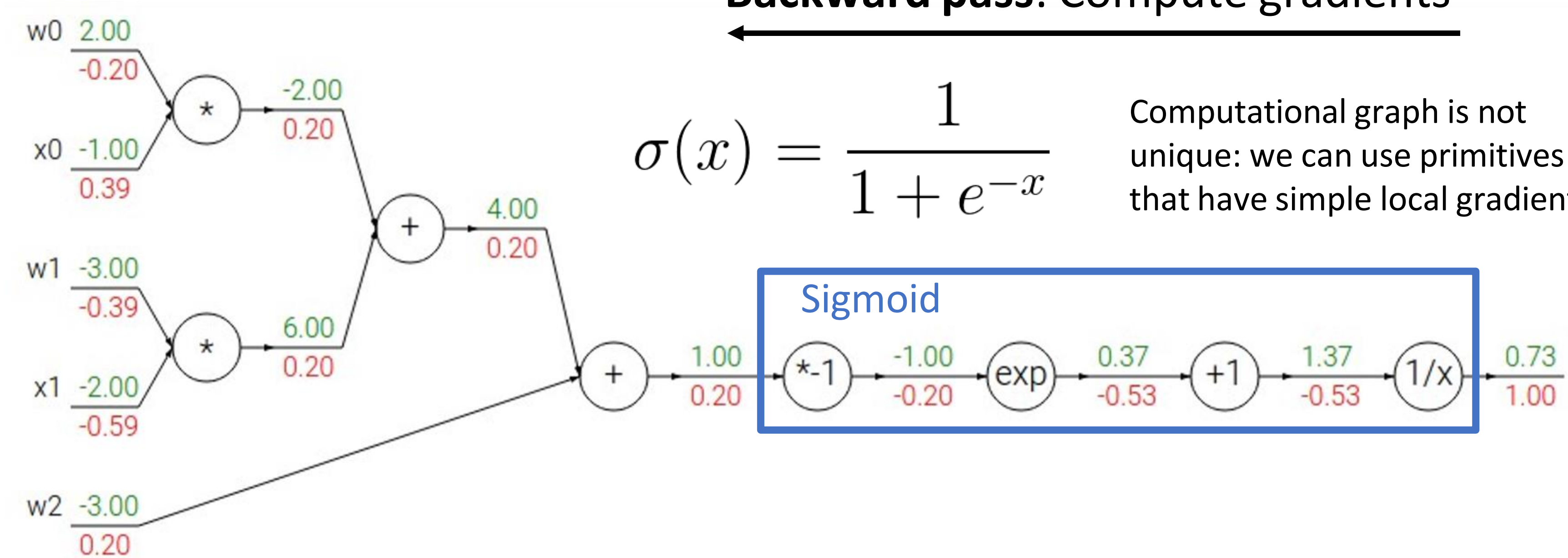
Another Example

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

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

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

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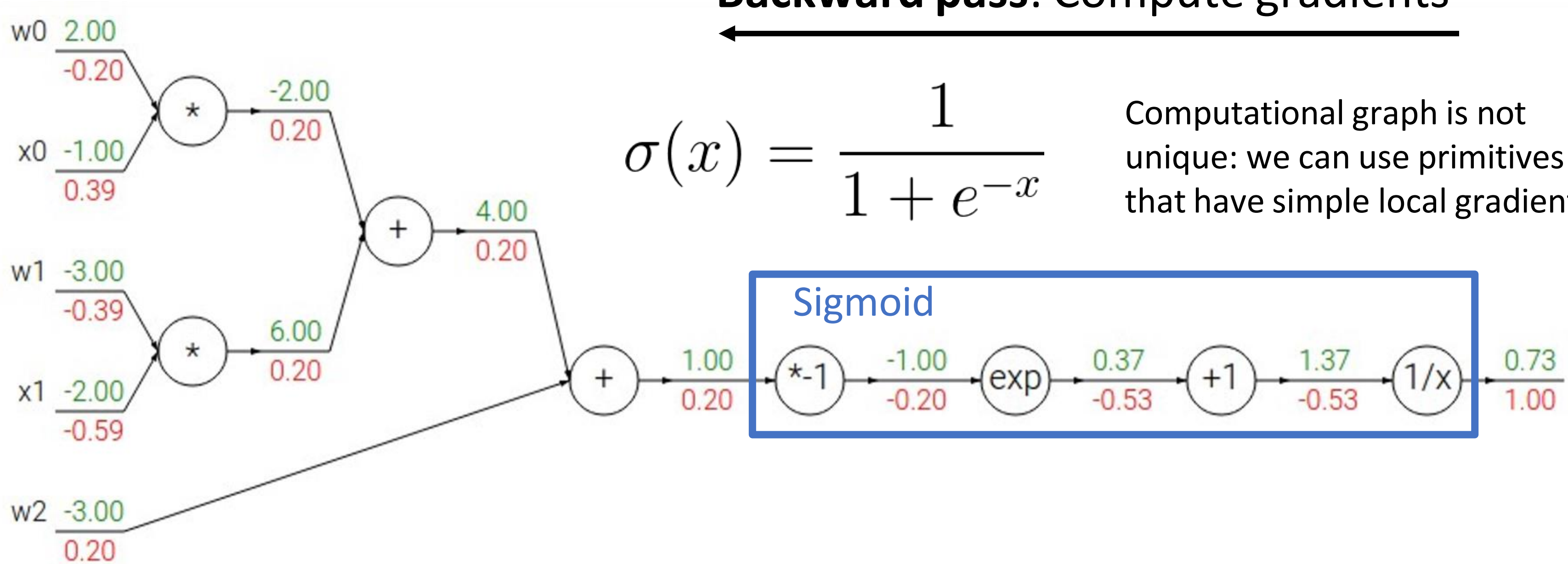

Sigmoid local gradient:

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

Another Example

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

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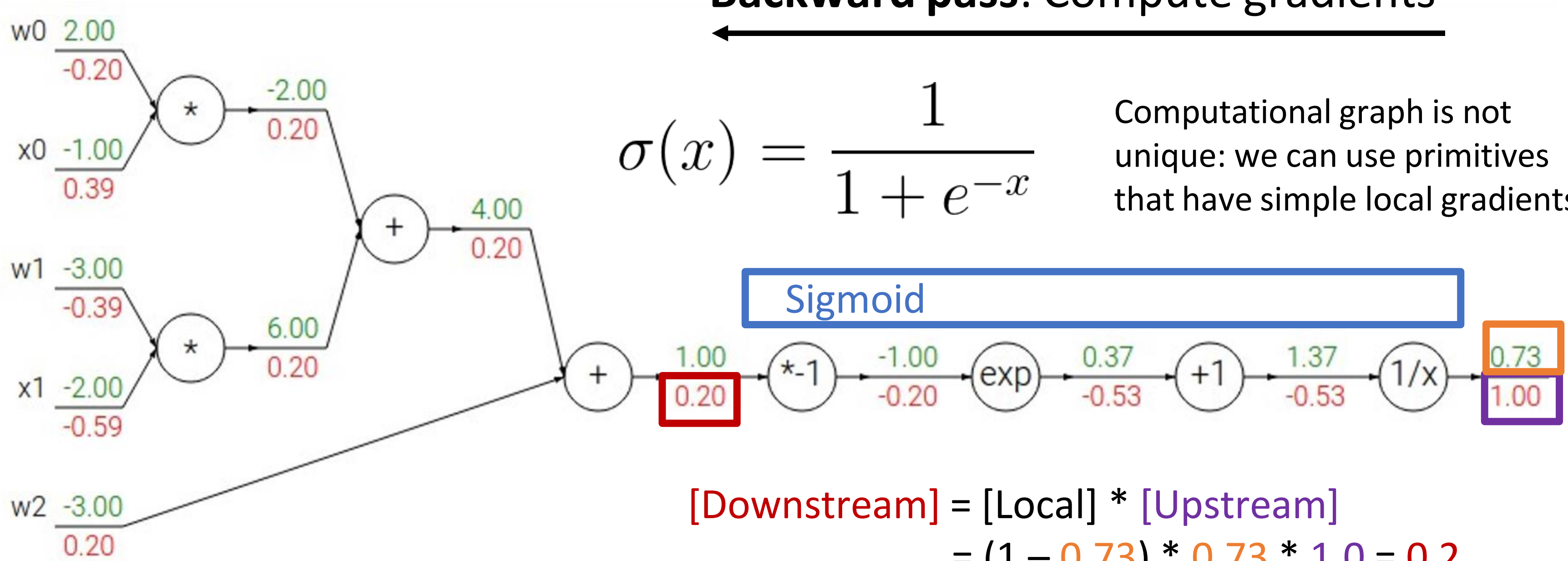


[Downstream] = [Local] * [Upstream]

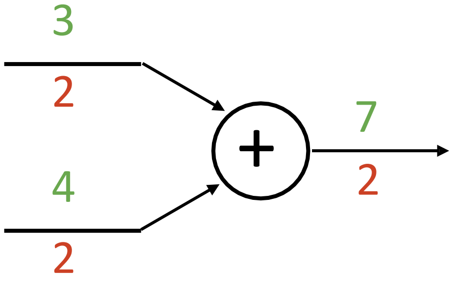
= (1 – 0.73) * 0.73 * 1.0 = 0.2

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



Patterns in Gradient Flow

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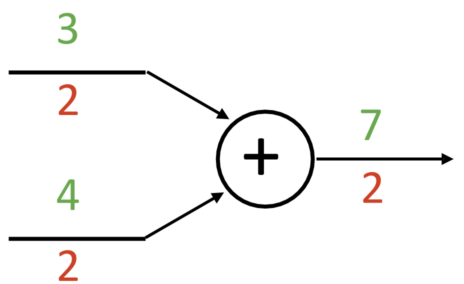
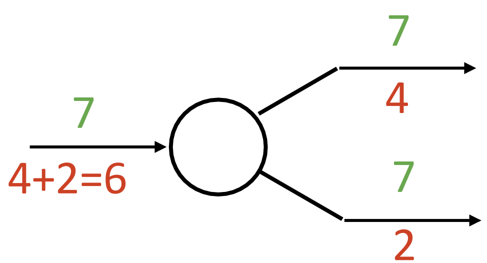


copy gate: gradient adder



Patterns in Gradient Flow

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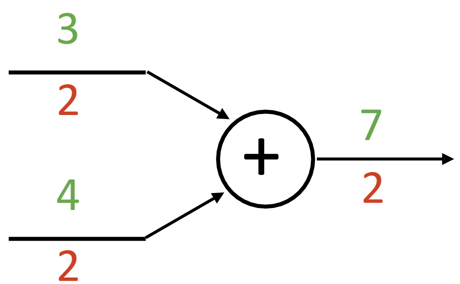
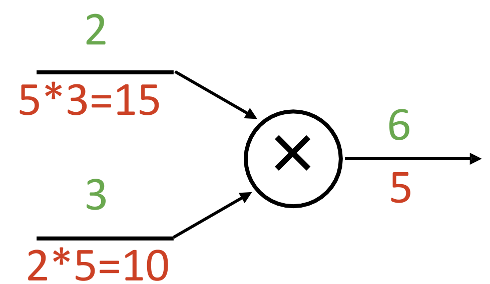


mul gate: “swap multiplier”



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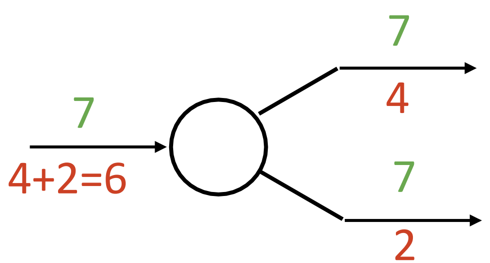

Patterns in Gradient Flow

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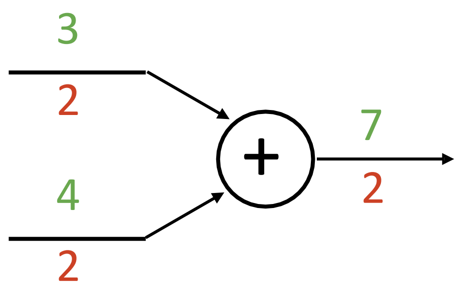

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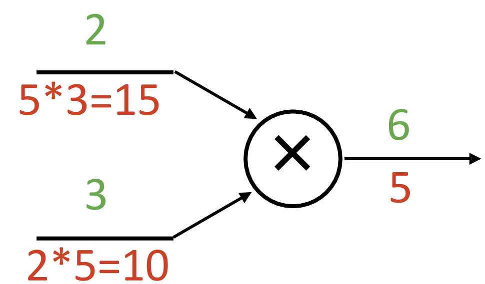
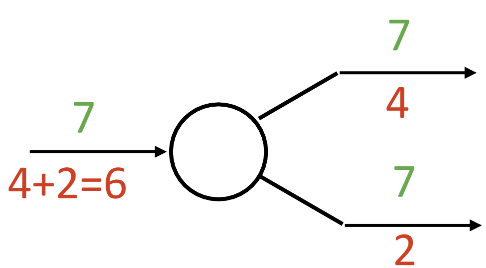
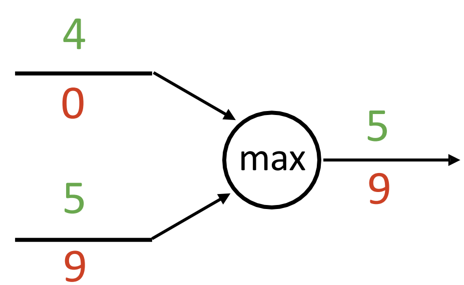


copy gate: gradient adder

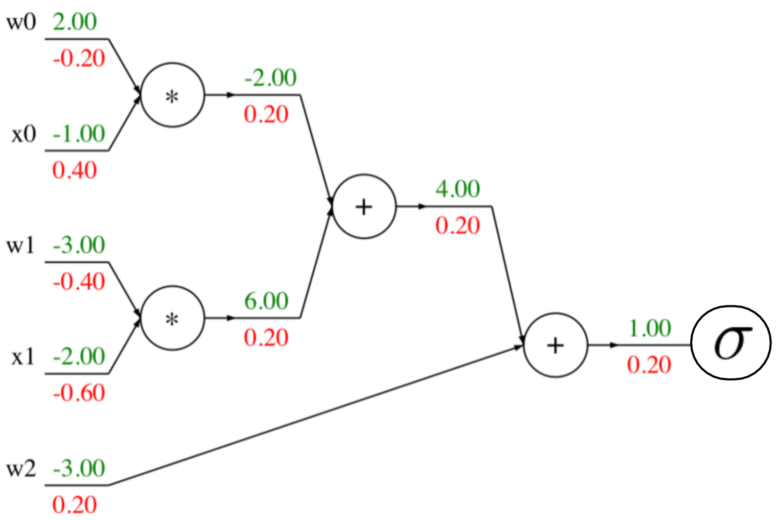


max gate: gradient router



Backprop Implementation:

"Flat" gradient code:

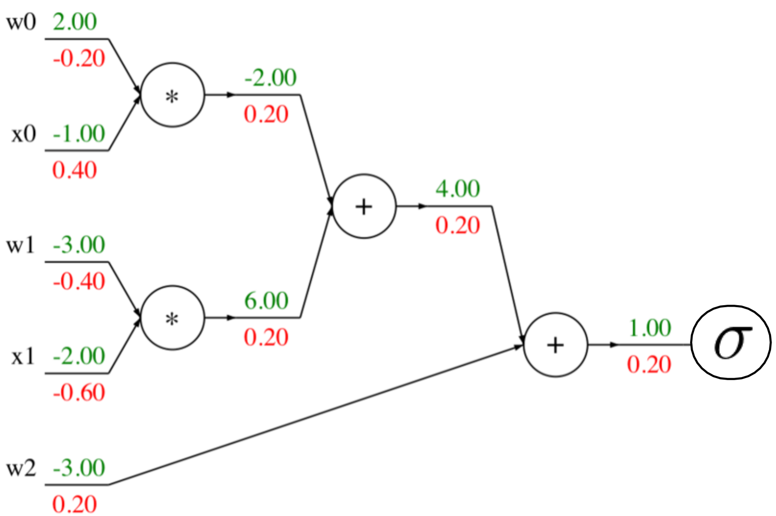


Forward pass:
Compute output

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

Backprop Implementation:

”Flat” gradient code:




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

Forward pass:
Compute output

```
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
```

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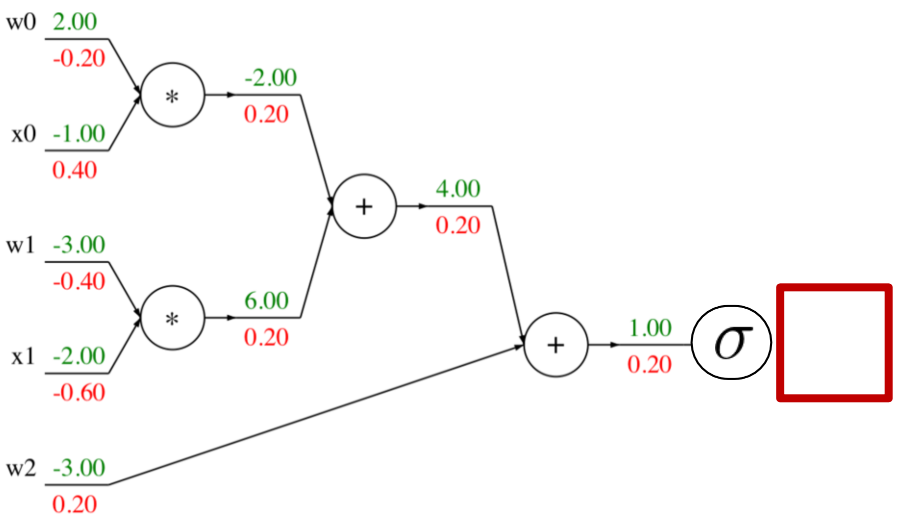

Forward pass: Compute output

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
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```

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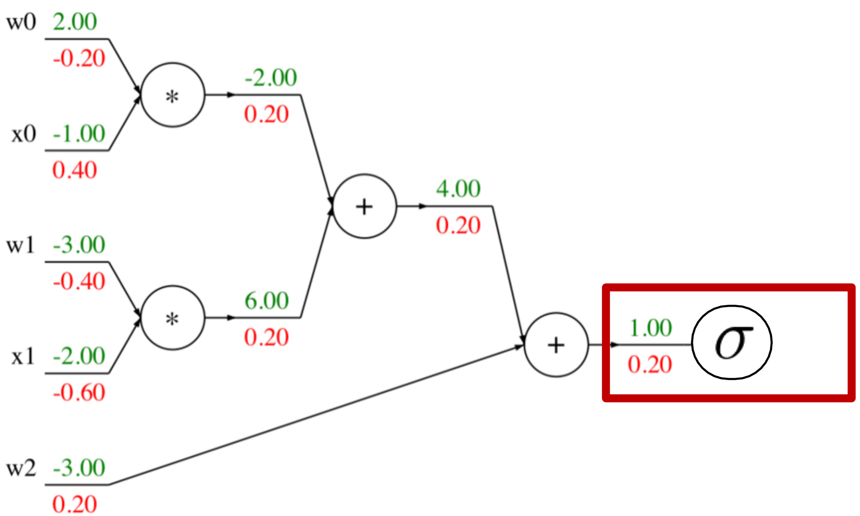

Forward pass:
Compute output

Sigmoid

```
def f(w0, x0, w1, x1, w2):
    s0 = w0 * x0
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    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
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    grad_w0 = grad_s0 * x0
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```

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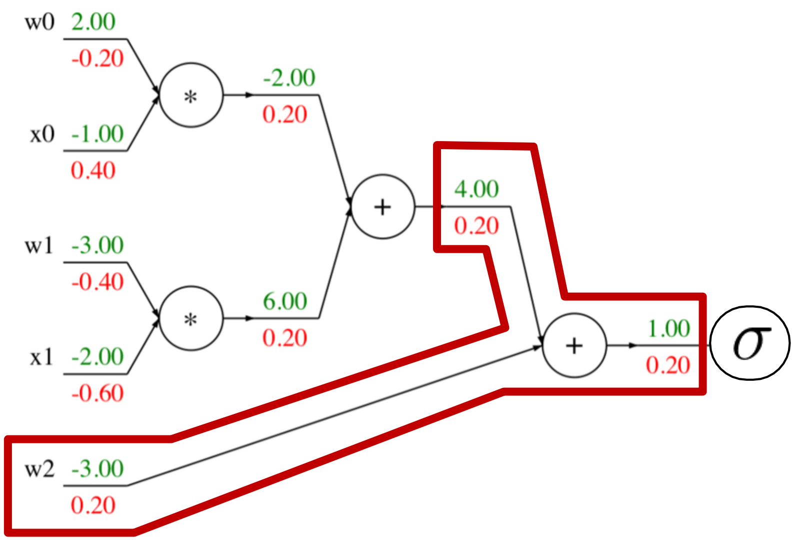

Forward pass:
Compute output

Add

```
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
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  grad_s2 = grad_s3
  grad_s0 = grad_s2
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```

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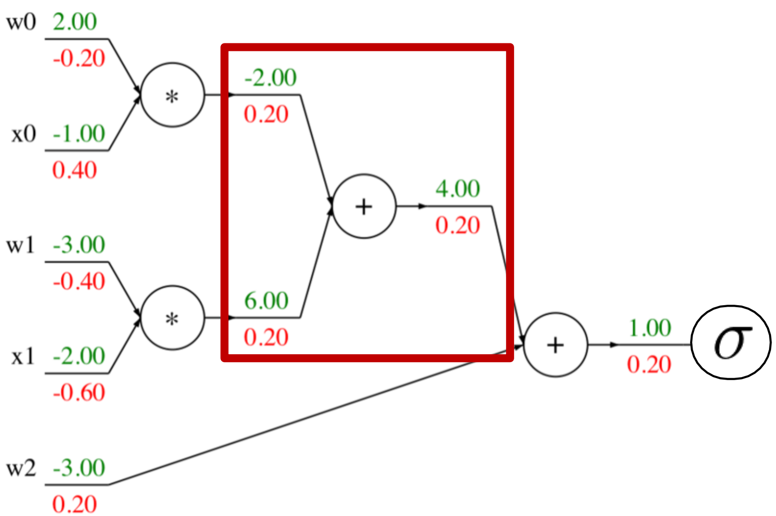
"Flat" gradient code:




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

Forward pass:
Compute output

```
    s0 = w0 * x0
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```

Add

```
    grad_L = 1.0
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    grad_w2 = grad_s3
    grad_s2 = grad_s3
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```

Backprop Implementation:

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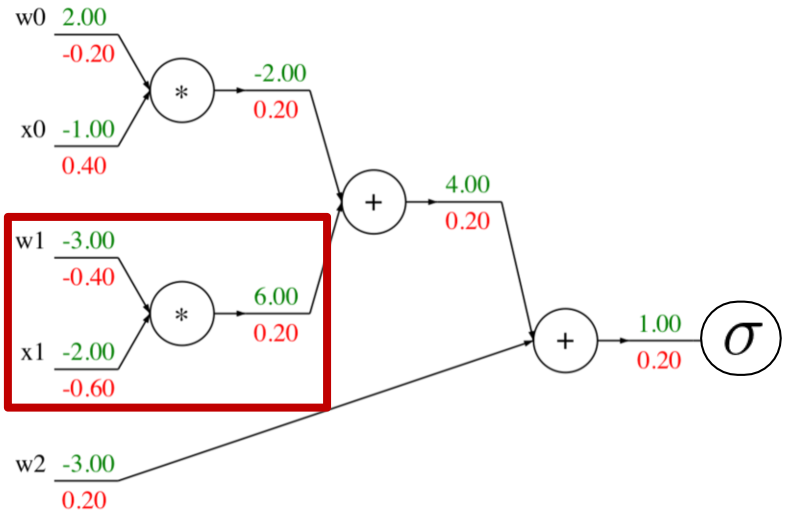

Forward pass:
Compute output

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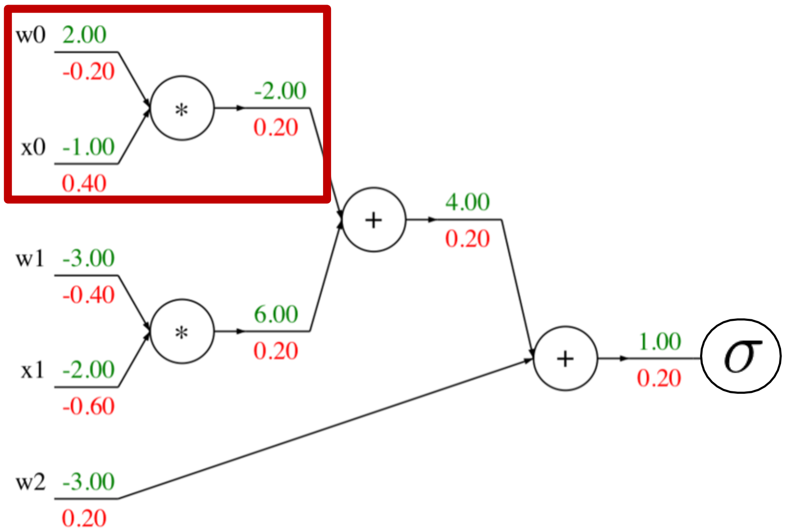
```

Multiply

Backprop Implementation:

”Flat” gradient code:



Forward pass:
Compute output

```
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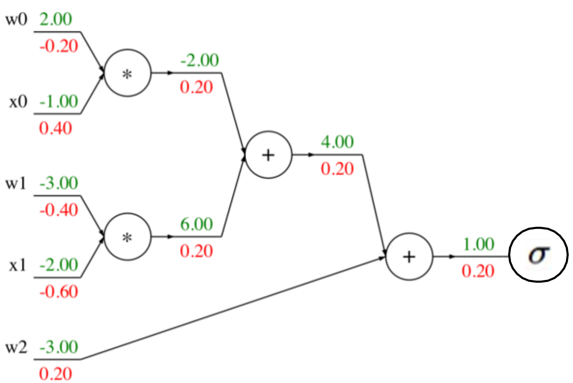
    grad_x0 = grad_s0 * w0
```

Multiply

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
```

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

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?

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

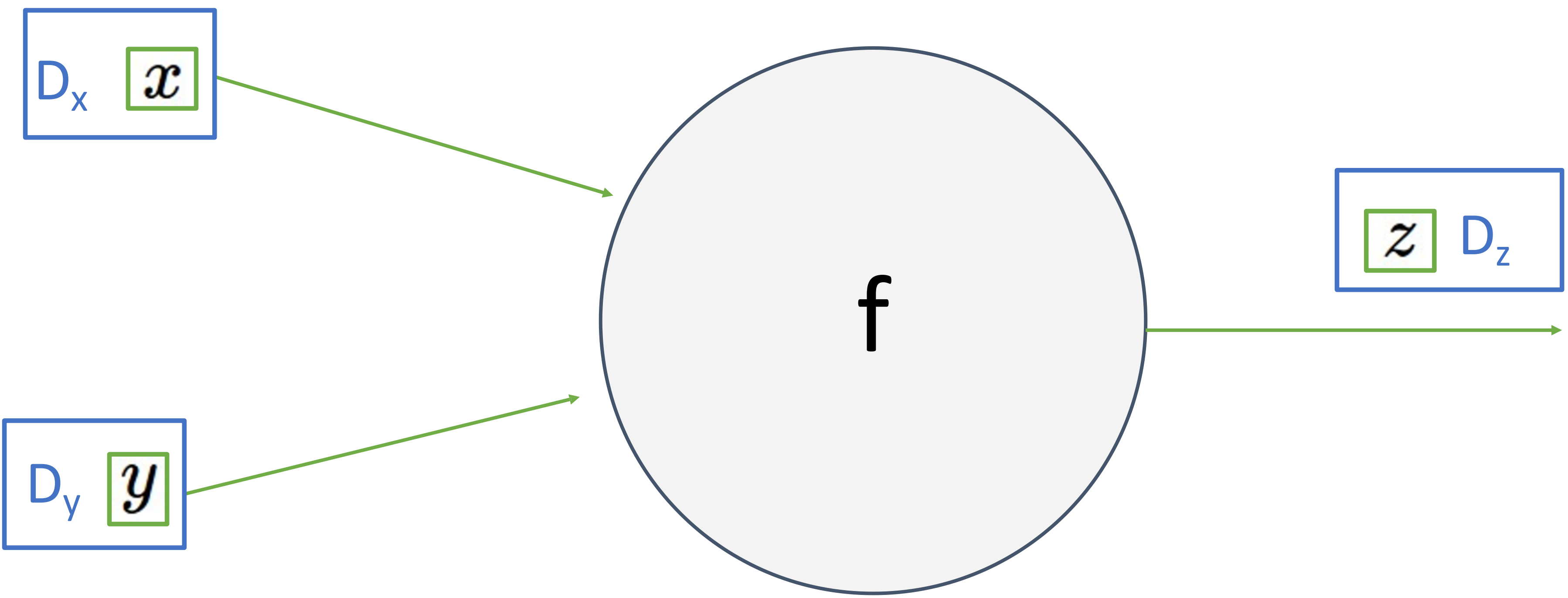
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

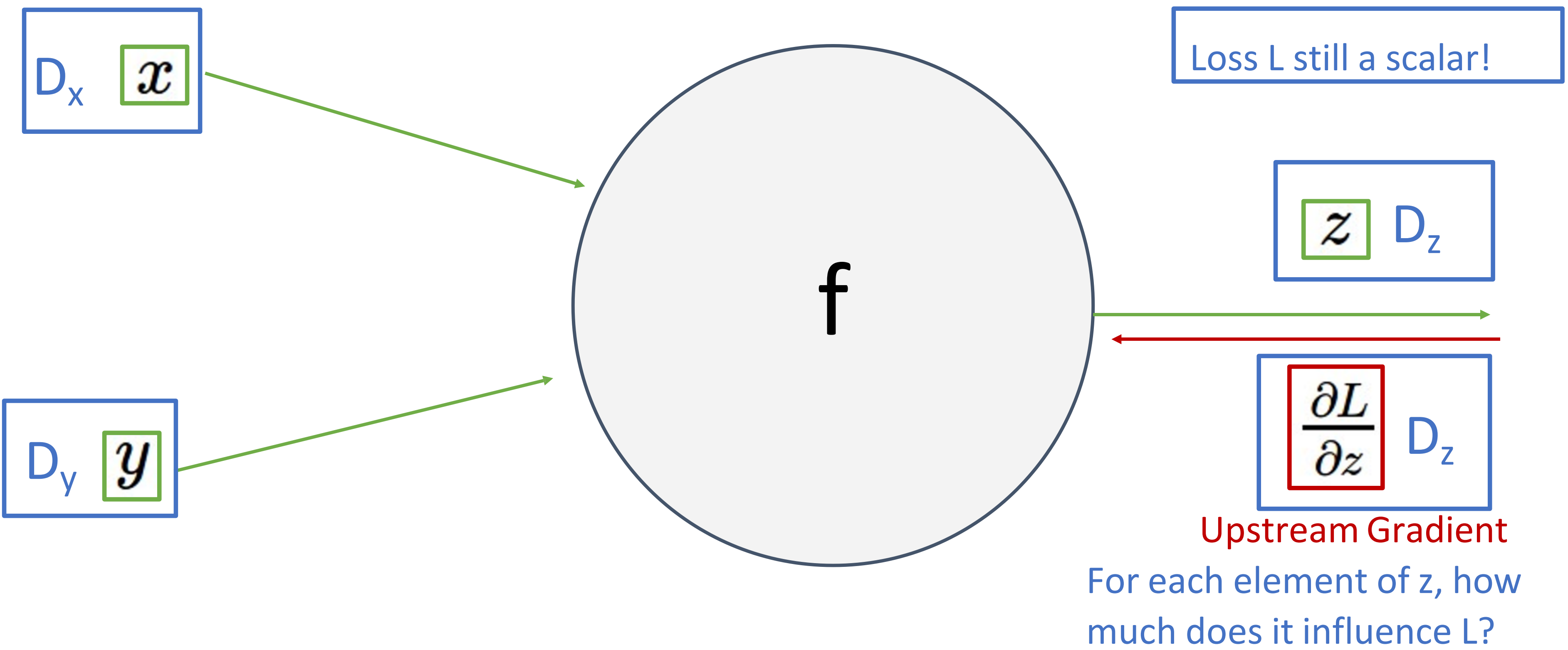
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x}\right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

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



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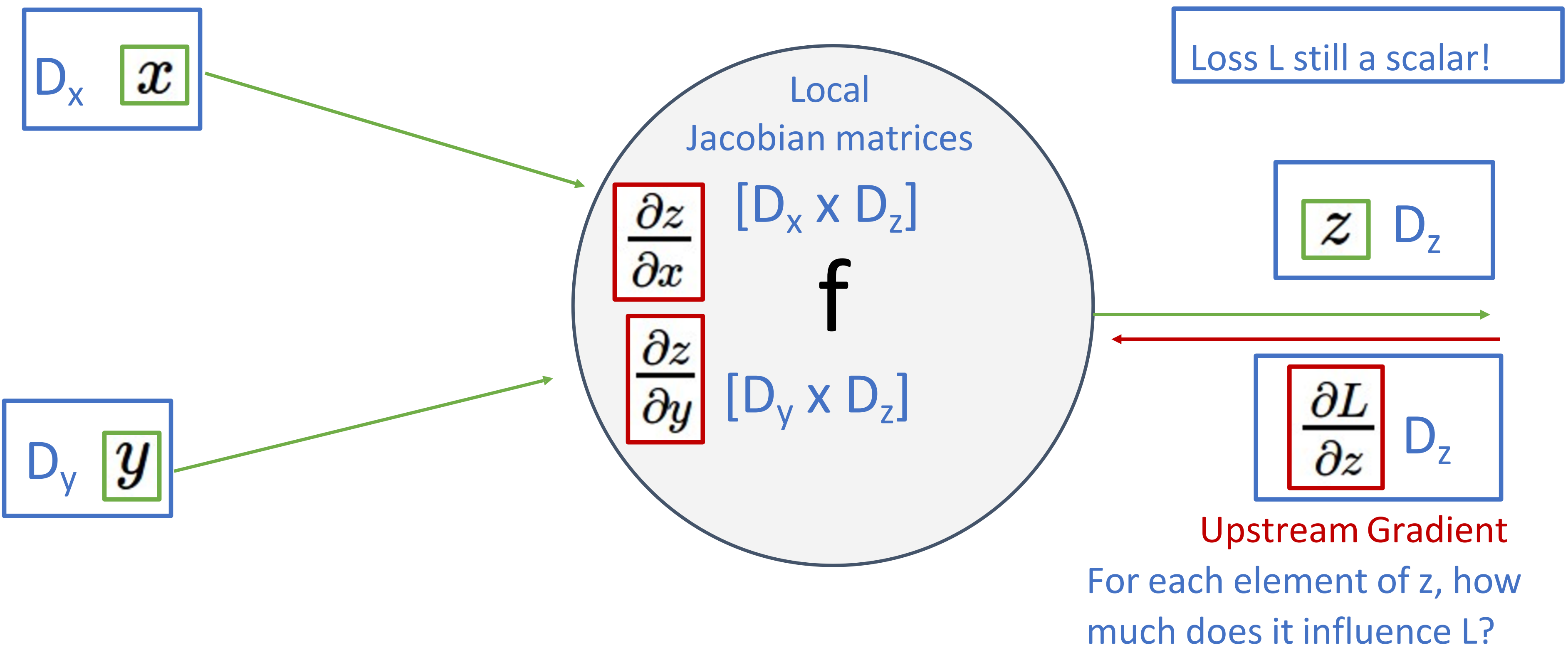

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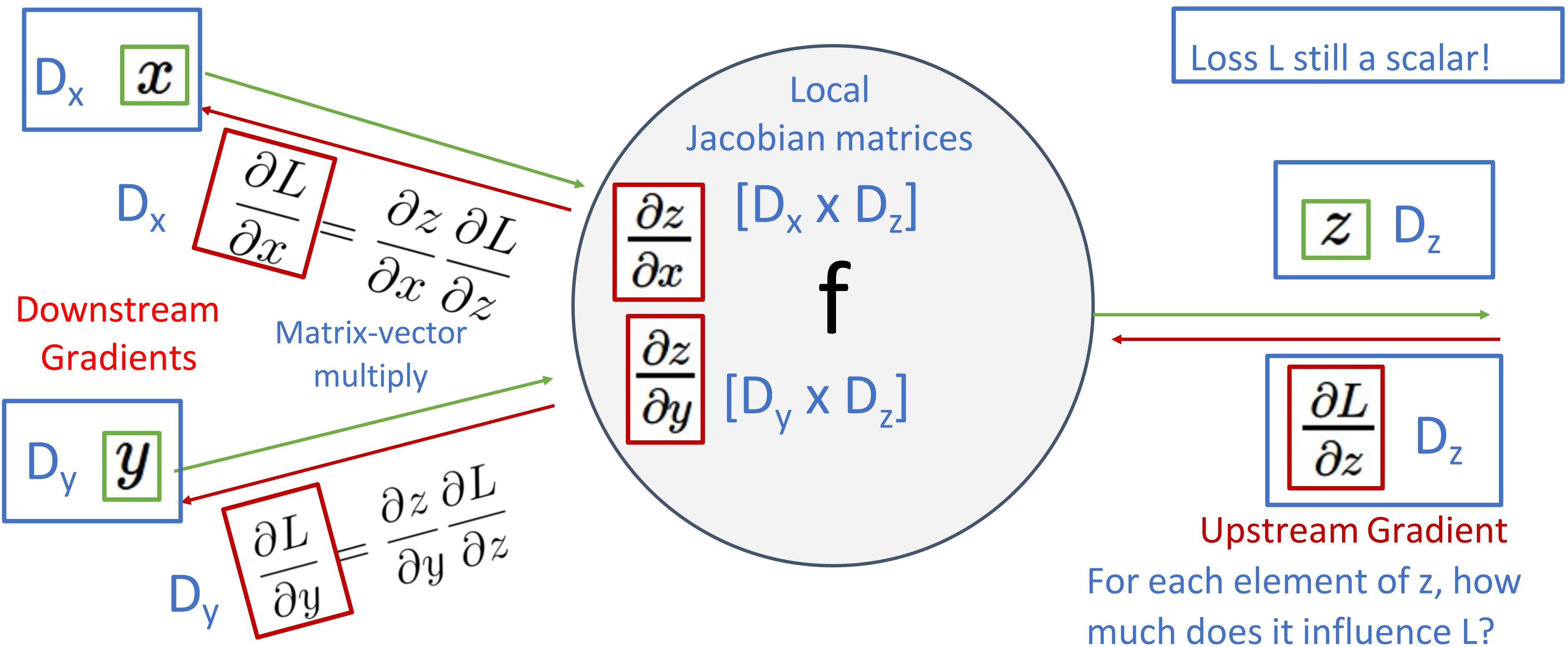

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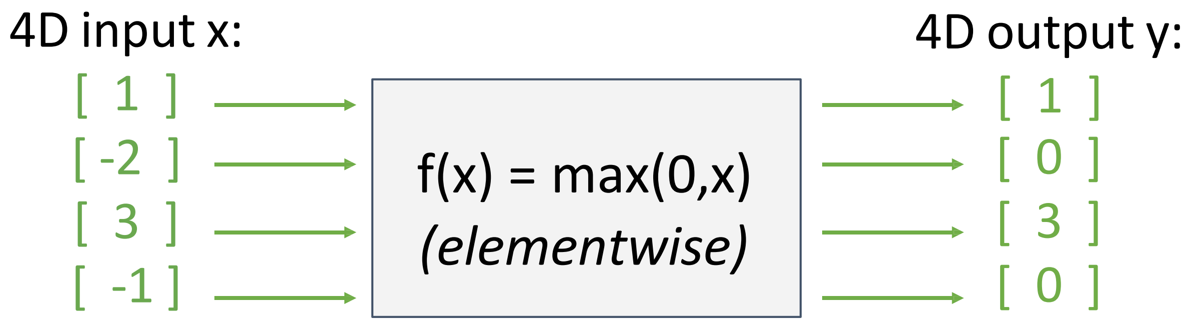

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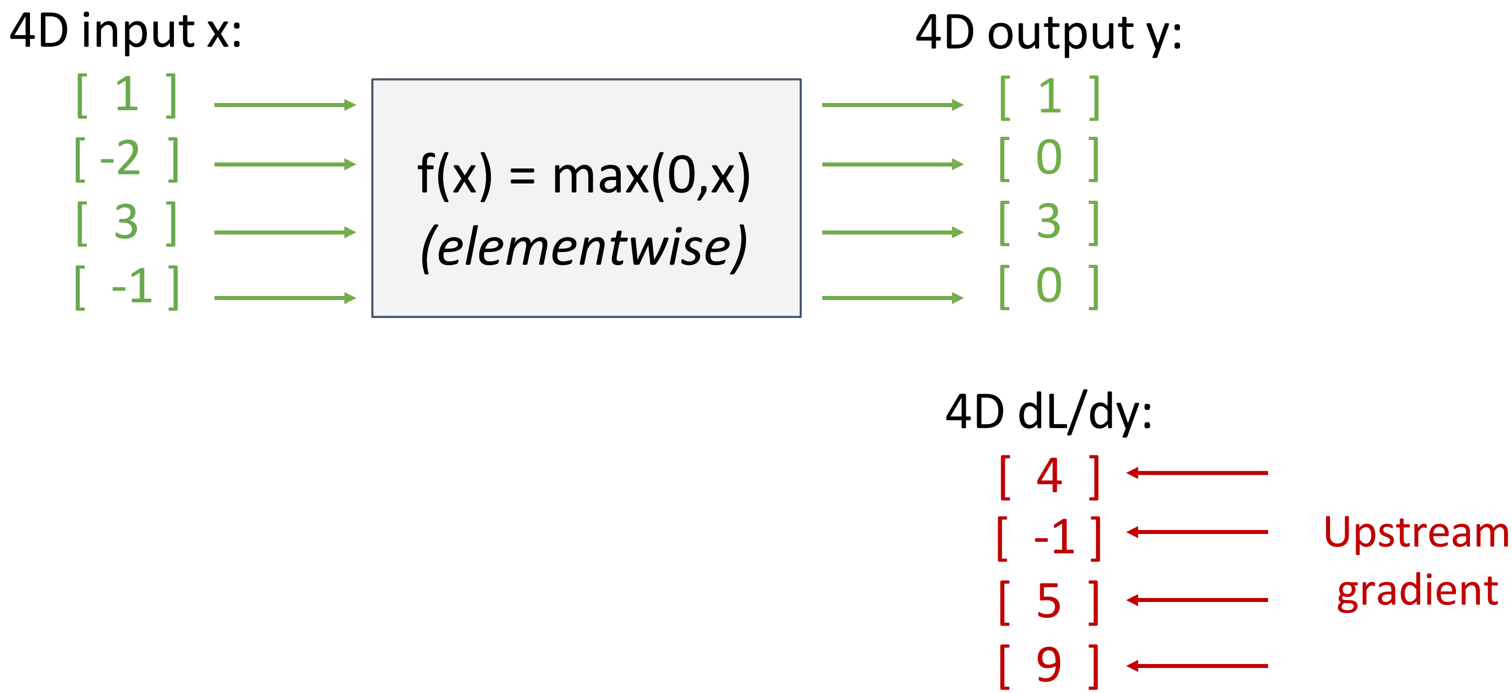
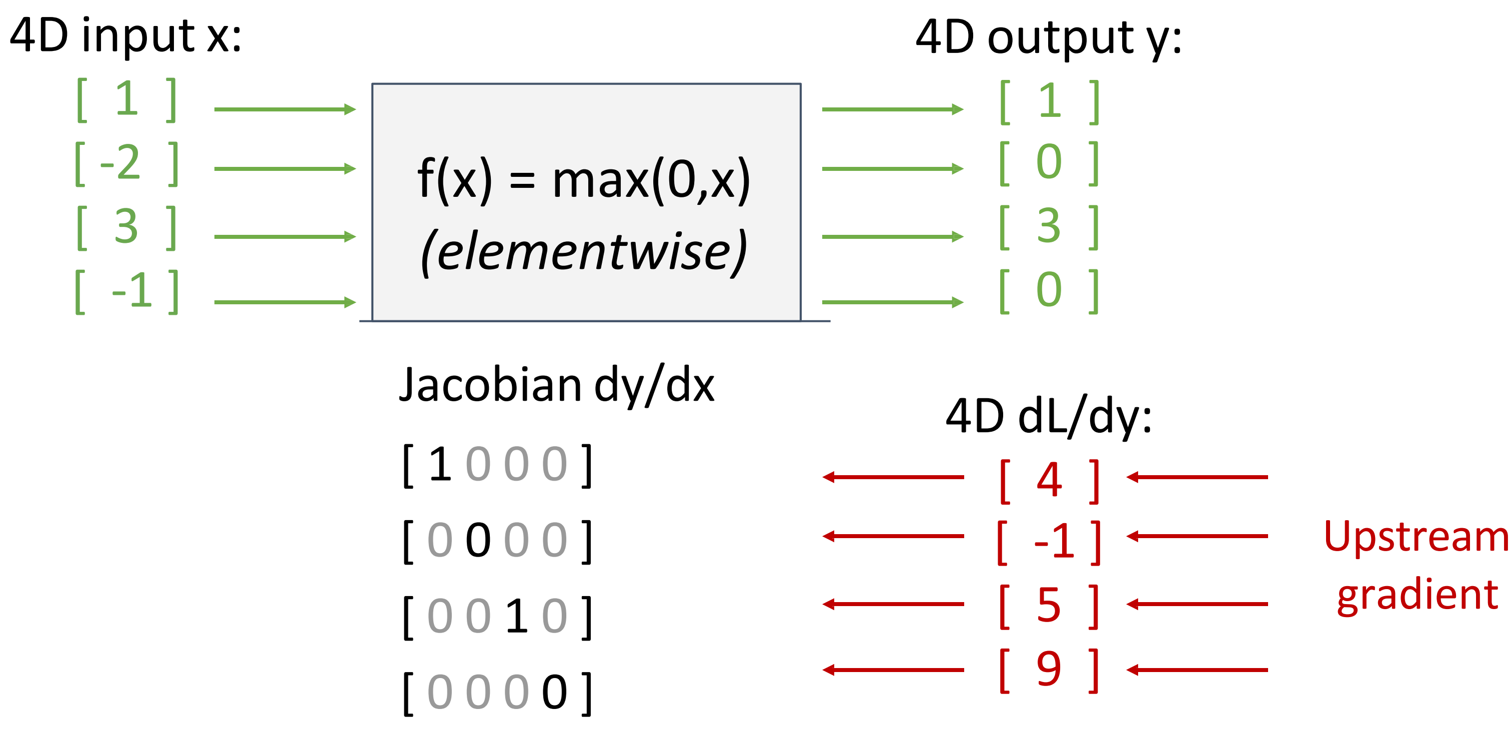
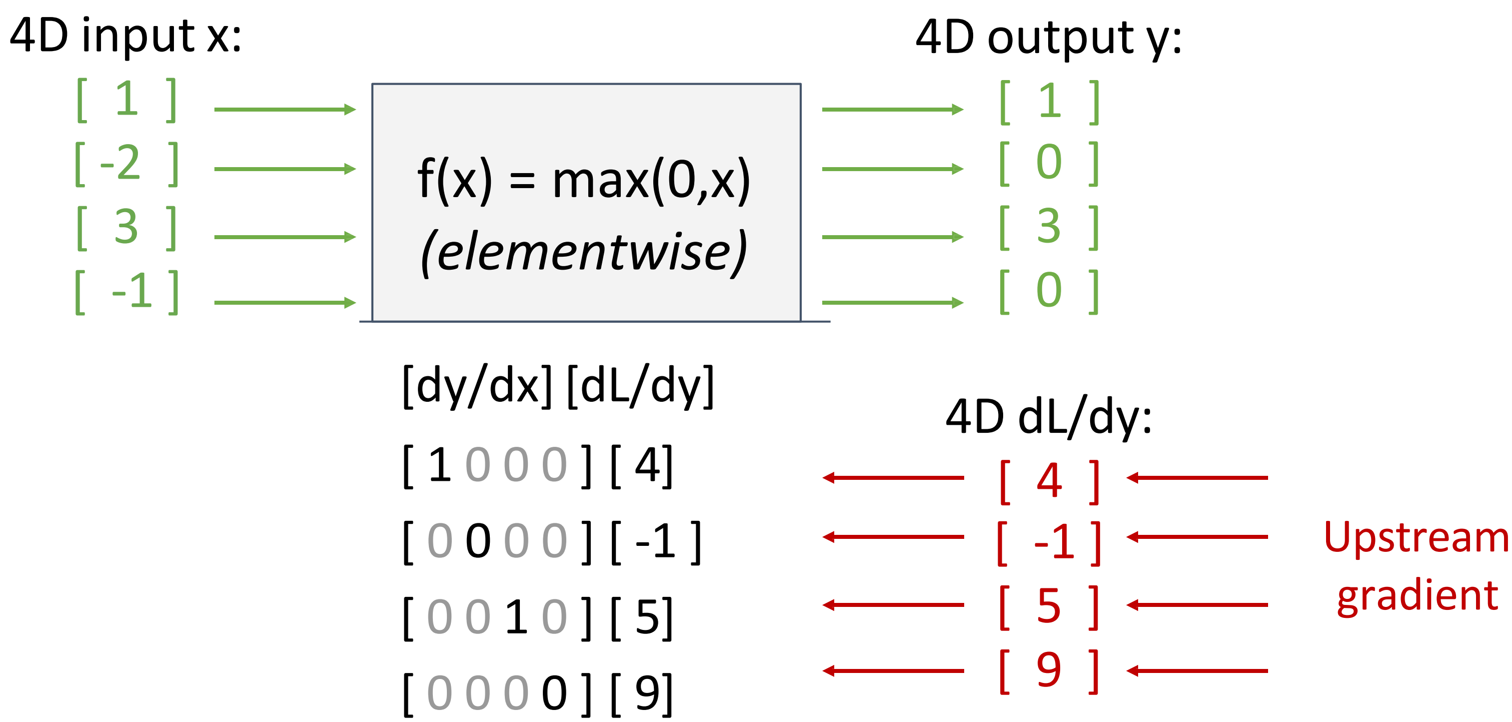


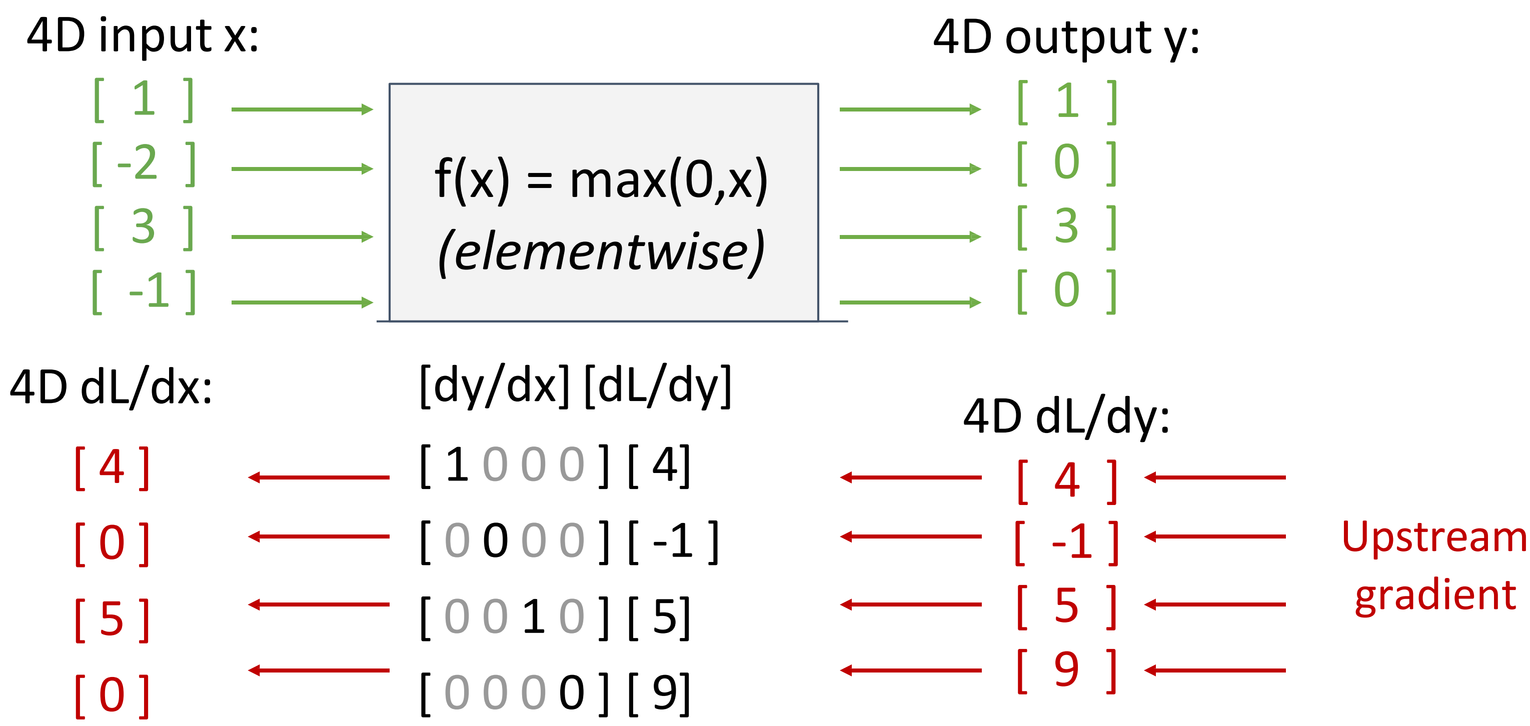
Backprop with Vectors



Backprop with Vectors



Backprop with Vectors



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

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[1]
[-2]
[3]
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f(x) = max(0,x)
(elementwise)

4D output y:

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

4D dL/dx:

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

[dy/dx] [dL/dy]

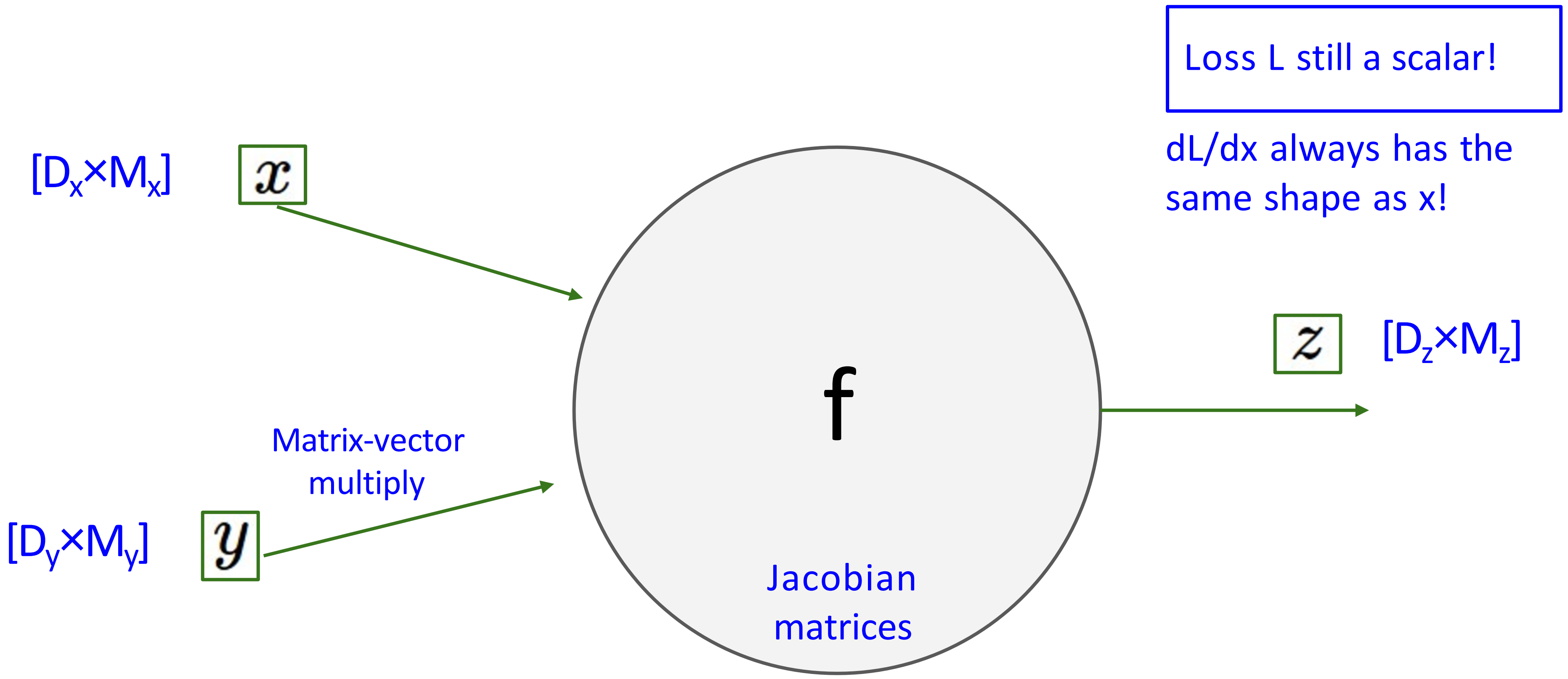
$$\left(\frac{\partial L}{\partial x}\right)_i = \begin{cases} \left(\frac{\partial L}{\partial y}\right)_i & \text{if } x_i > 0 \\ 0 & \text{otherwise} \end{cases}$$

4D dL/dy:

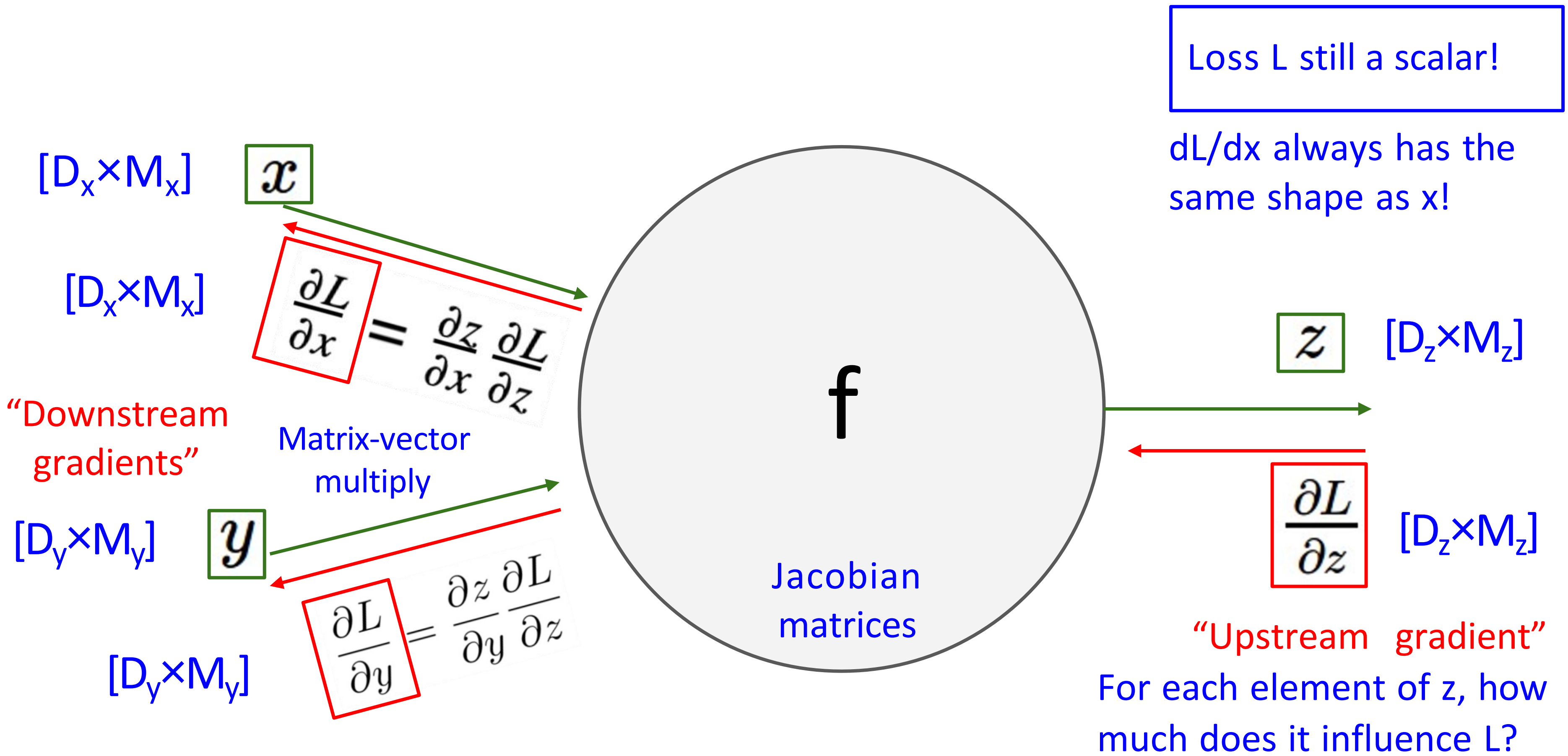
[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Matrices (or Tensors):



Backprop with Matrices (or Tensors):



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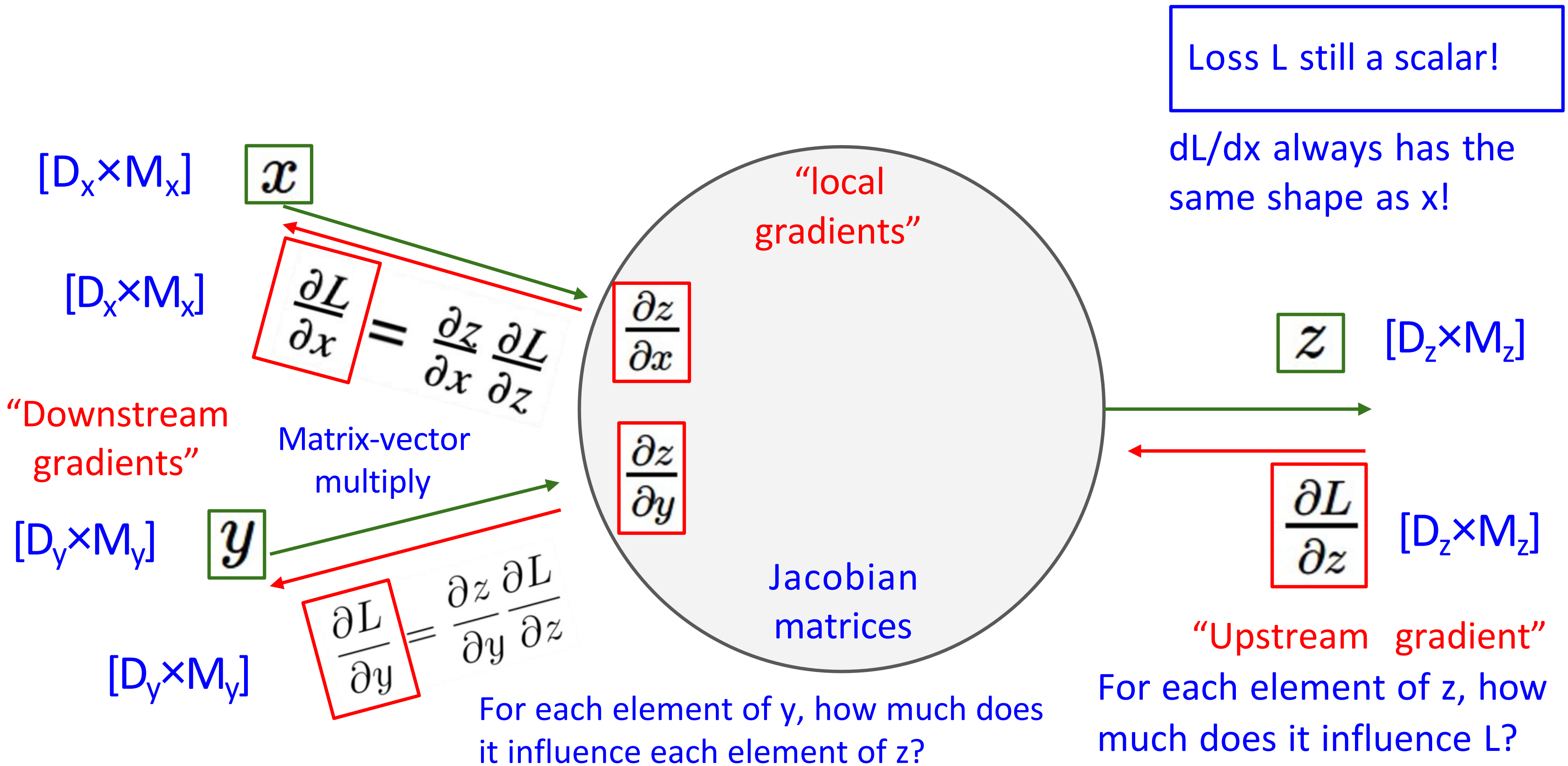
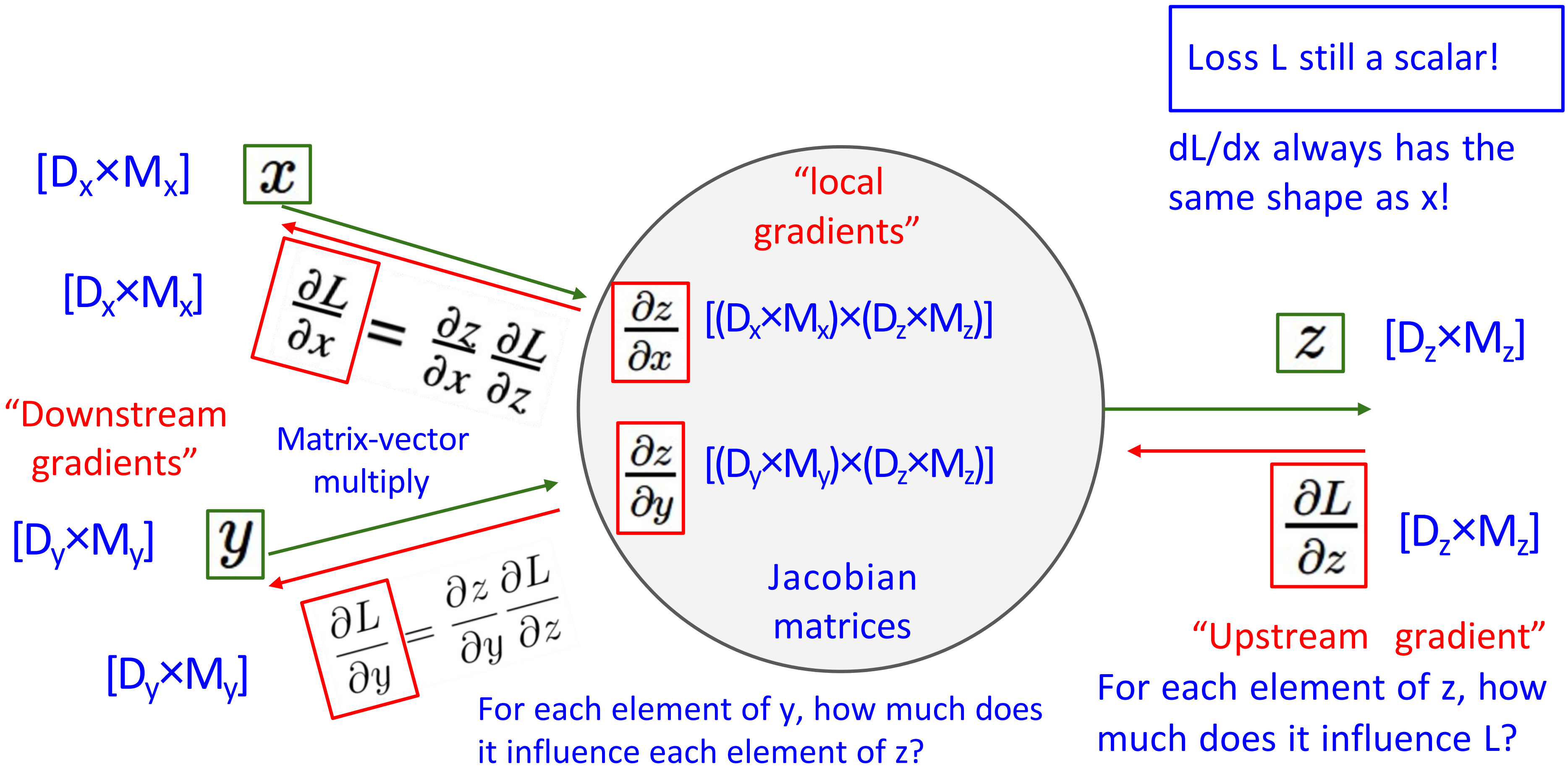


Backprop with Matrices (or Tensors):



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:

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

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

dL/dx:

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

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

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dL/dx:

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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]

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

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]

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

dL/dy: [N×M]

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

dL/dx:

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

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]

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

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]

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

dL/dy: [N×M]

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

dL/dx:

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

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:

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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

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

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

[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:

[? ? ?]
[? ? ?]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

[3 ? ? ?]
[? ? ? ?]

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

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

Example: Matrix Multiplication

x: [N×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:

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

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]

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

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:

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

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:

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

$dL/dx_{1,1}$

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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

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

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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

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]

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

dL/dy: [N×M]

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

dL/dx:

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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

$dL/dx_{1,1}$

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

Example: Matrix Multiplication

x: [N×D]

[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:

[? ? ?]
[? ? ?]

Local Gradient Slice:

$dy/dx_{1,1}$

[3 2 1 -1]
[0 ? ? ?]

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

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

$dL/dx_{1,1}$

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

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:

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

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]

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

Matrix Multiply *y = xw*

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

y: [N×M]

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

dL/dy: [N×M]

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

dL/dx:

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

$dL/dx_{1,1}$

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

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

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

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:

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

Local Gradient Slice:

$dy/dx_{2,3}$

[0 0 0 0]
[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]

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

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:

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

Local Gradient Slice:

$dy/dx_{2,3}$

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

$dL/dx_{2,3}$

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

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

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

Example: Matrix Multiplication

x: [N×D]

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

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:

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

$dL/dx_{i,j}$

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

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

Example: Matrix Multiplication

x: [N×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:

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

$$\underbrace{dL/dx}_{[N \times D]} = \underbrace{(dL/dy)}_{[N \times M]}\ \underbrace{w^T}_{[M \times D]}$$

$dL/dx_{i,j}$

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

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

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

Example: Matrix Multiplication

x: [N×D]

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

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:

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

$$\underbrace{dL/dx}_{[N \times D]} = \underbrace{(dL/dy)}_{[N \times M]}\ \underbrace{w^T}_{[M \times D]}$$

$$\underbrace{dL/dw}_{[D \times M]} = \underbrace{x^T}_{[D \times N]}\ \underbrace{(dL/dy)}_{[N \times M]}$$

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

Backpropagation: Another View

$$
\begin{tikzcd}
x_0 \arrow[r, "f_1"] & x_1 \arrow[r, "f_2"] & x_2 \arrow[r, "f_3"] & x_3 \arrow[r, "f_4"] & L \\
D_0 & D_1 & D_2 & D_3 & \text{scalar}
\end{tikzcd}
$$

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

Backprop: Higher-Order Derivatives

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

D_0 $\quad$ D_1 $\quad$ 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

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

Hessian matrix
H of second derivatives.

$D_0 \times D_0$

Hessian / vector multiply

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

$D_0 \times D_0$ 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

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

Hessian matrix
H of second derivatives.

D_0 x D_0

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

(if v doesn't depend on x_0)

D_0 x D_0 D_0

Backprop: Higher-Order Derivatives

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

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

Hessian matrix
H of second derivatives.

Hessian / vector multiply

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

(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!

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

Hessian matrix H of second derivatives.

Hessian / vector multiply

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

(if v doesn't depend on x_0)

Backprop: Higher-Order Derivatives

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

D_0 | D_1 | scalar | D_1 | D_0 | scalar

Backprop!

This is implemented in PyTorch / Tensorflow!

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

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)

$D_0 \times D_0$ $\quad D_0$

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

Backprop!

This is implemented in PyTorch / Tensorflow!

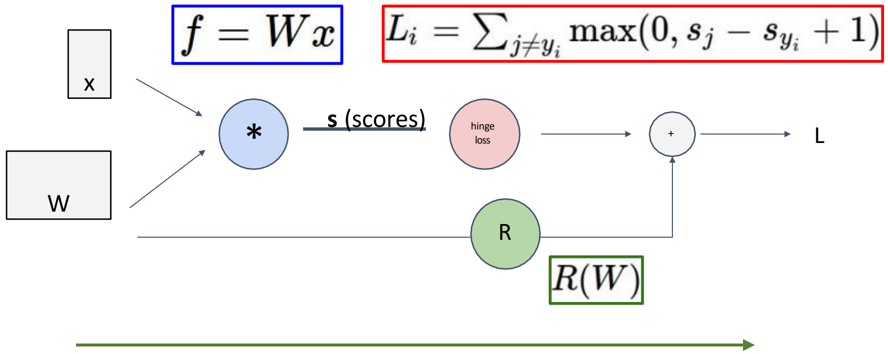
Example: Regularization to penalize the norm of the gradient

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

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

Summary

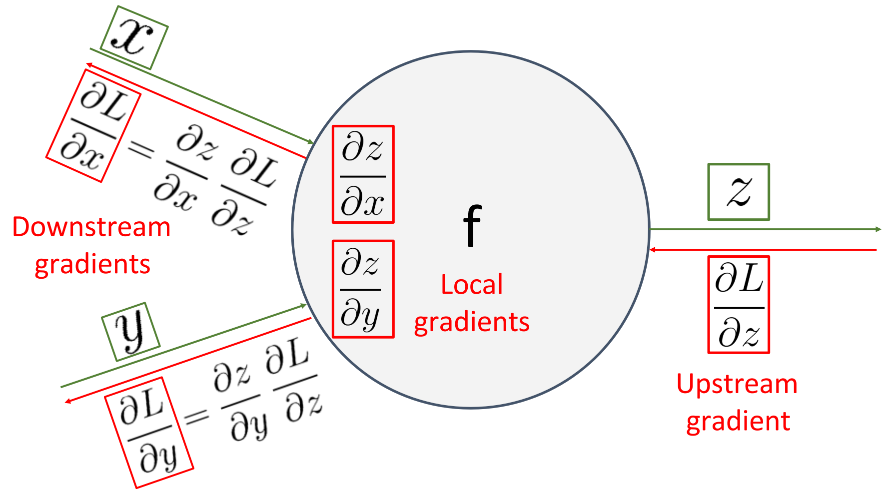
Represent complex expressions as **computational graphs**



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.

```
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
```