ROB 498/599: Deep Learning for Robot Perception (DeepRob)

Lecture 6: Backpropagation

01/29/2025

https://deeprob.org/w25/

ROBOTICS

Today

- Feedback and Recap (5min)
- Backpropagation
  - P1 - Linear Classifier gradients (20min)
  - Computational Graph: Examples of calculating backprop (30min)
  - Backprop with vectors (20min)
- Summary and Takeaways (5min)

P1 Hints

- `.view` vs. `.reshape`
  - `.view` more memory efficient, but only works with contiguous memory tensor. Preferred in our P1.
  - `.reshape` works with both contiguous and non-contiguous memory tensor. May return a view or a copy.
- `torch.chunk(tensor, NumChucks, dim)`: split a tensor in chunks - useful in cross validation
- `Compute_distances_no_loops` - good place to debug (see https://piazza.com/class/m4pgejar4ua2qf/post/49)
  - Hint: Euclidean distance $dist = \sqrt{(p-q)^2} = p^2 + q^2 - 2p \cdot q$

https://mmuratarat.github.io/2019-01-27/derivation-of-softmax-function

P1 Hints

- Deriving Derivatives `dW` for Linear Classifiers

- We have some dataset of (x, y)
- We have a **score function:**
- We have a **loss function:**

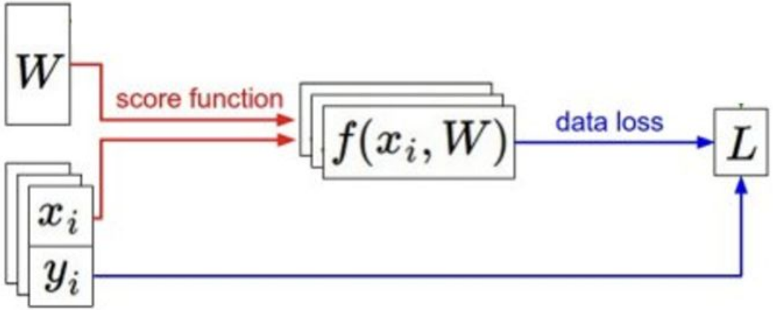
$$s = f(x; W, b) = Wx + b$$

Linear classifier

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda \sum_i w_i^2$$

Softmax: $L_i = -\log\left(\frac{\exp(s_{y_i})}{\sum_j \exp(s_j)}\right)$

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

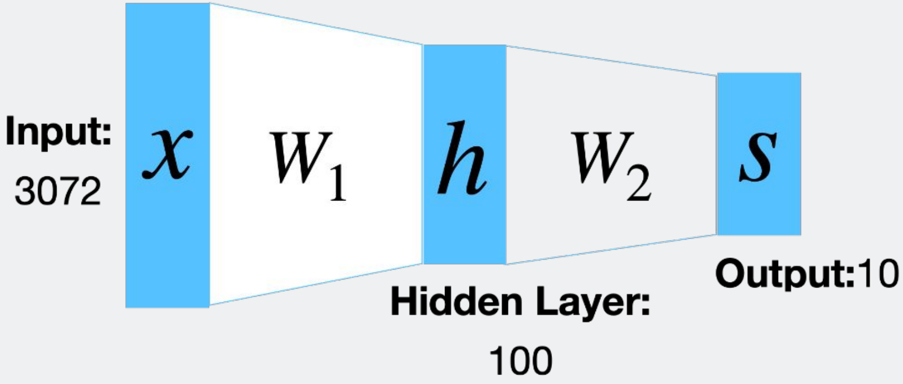


Recap

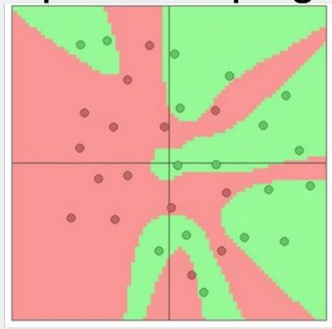
P1 Deadline: Feb. 2, 2025

From linear classifiers to fully-connected networks

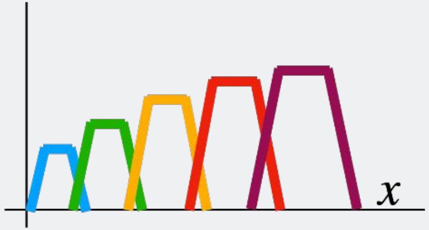
$$f(x) = W_2 \max(0, W_1 x + b_1) + b_2$$



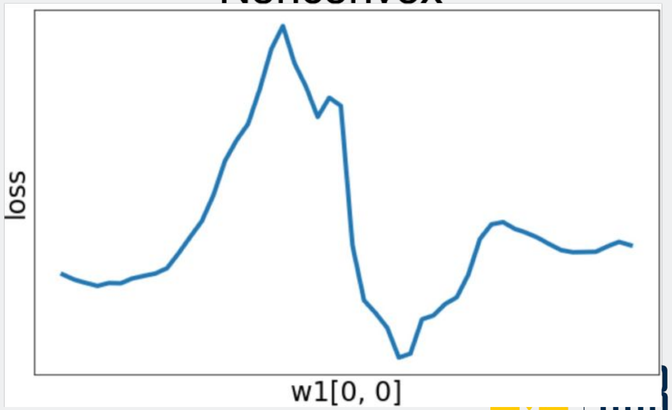
Space Warping



Universal approximation



Nonconvex



How to Compute Gradients?

$$s = W_2 \underbrace{\boxed{\max(0, W_1 x + b_1)}}_{\text{ReLU activation}} + b_2$$ Nonlinear score function

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

$$R(W) = \sum_k W_k^2$$ L2 regularization

$$L(W_1, W_2, b_1, b_2) = \underbrace{\boxed{\frac{1}{N} \sum_{i=1}^{N} L_i}}_{\text{Data loss}} + \underbrace{\boxed{\lambda R(W_1) + \lambda R(W_2)}}_{\text{Regularization term}}$$ Total loss

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

Bad Idea: Derive $\nabla_W L$ on paper

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

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

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

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

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

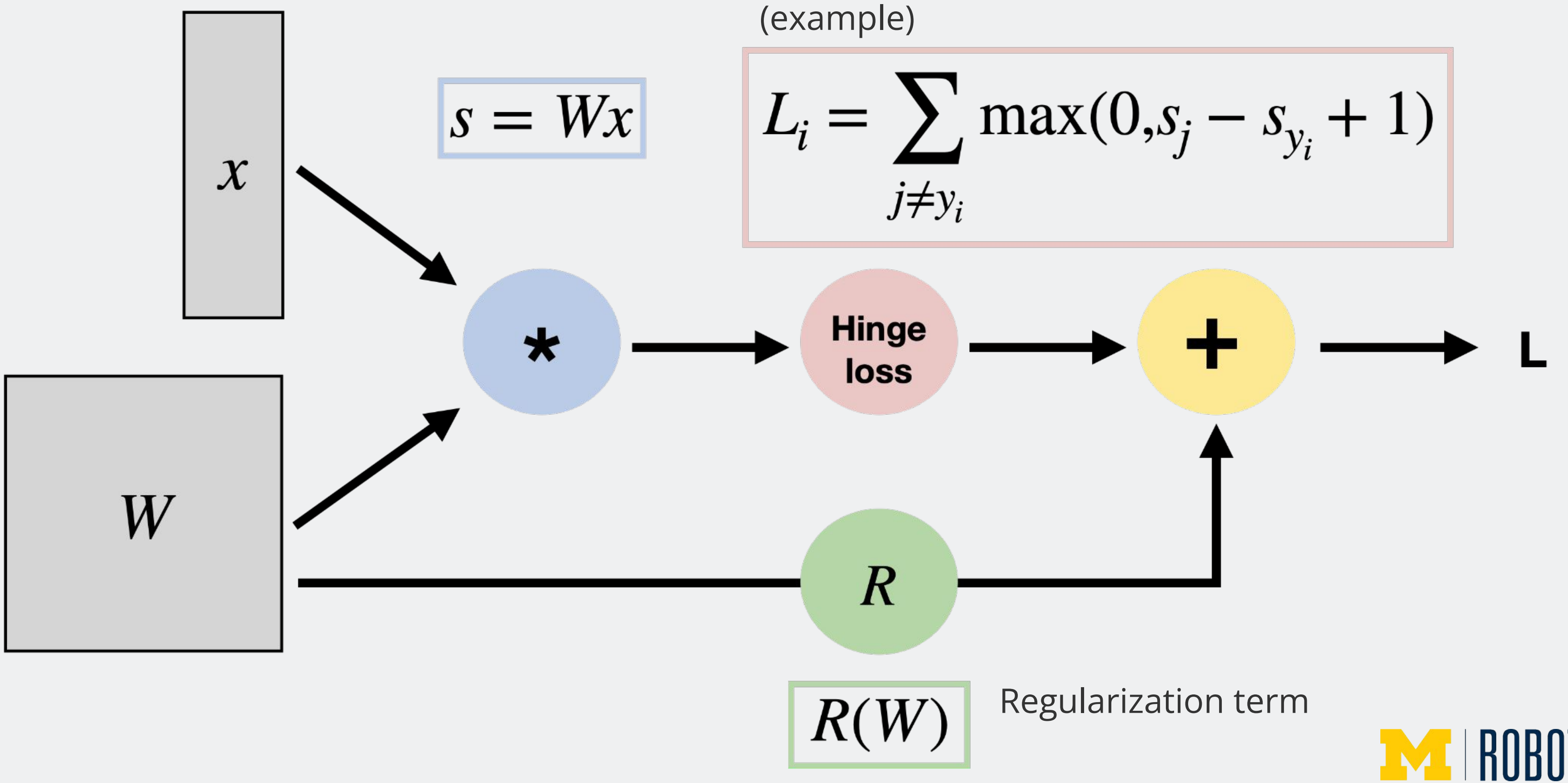
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x - W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

Problem: Very tedious with lots of matrix calculus

Problem: What if we want to change the 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

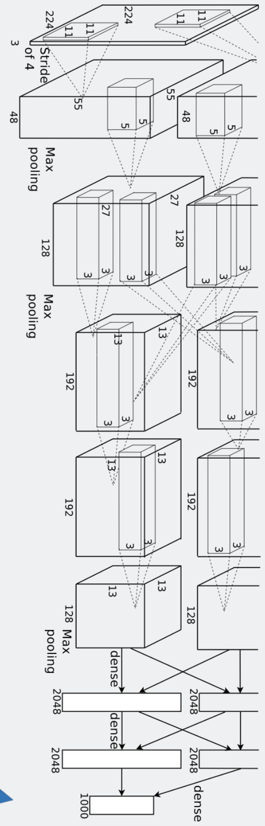


Deep Network (AlexNet)

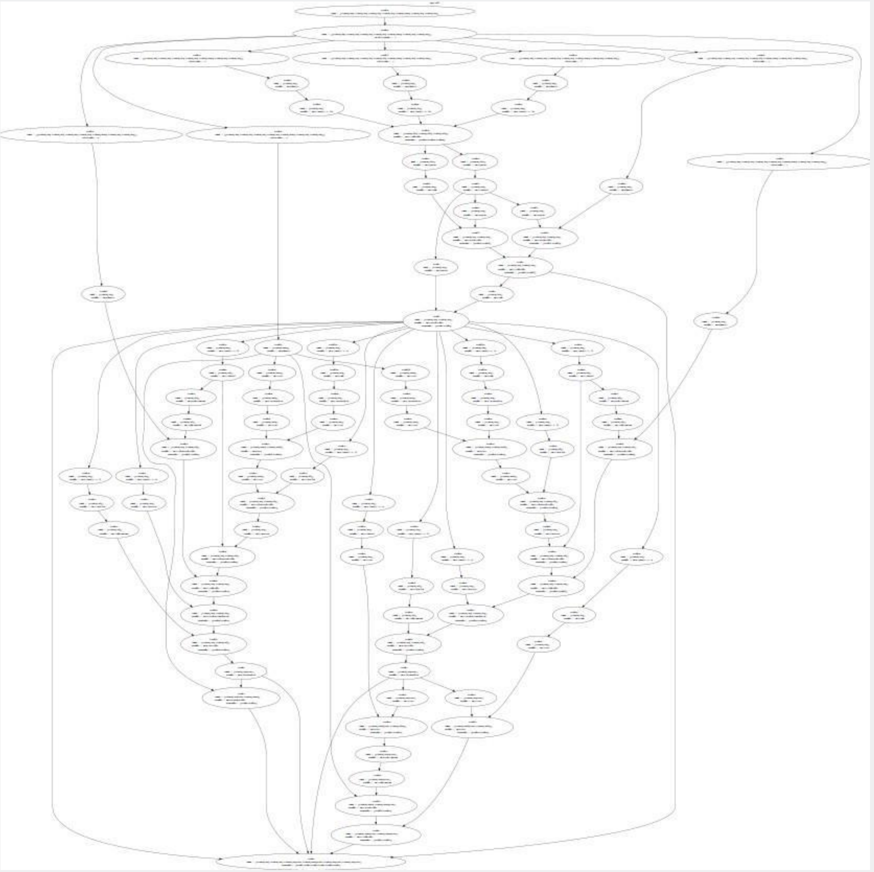
Input image

Weights

Loss



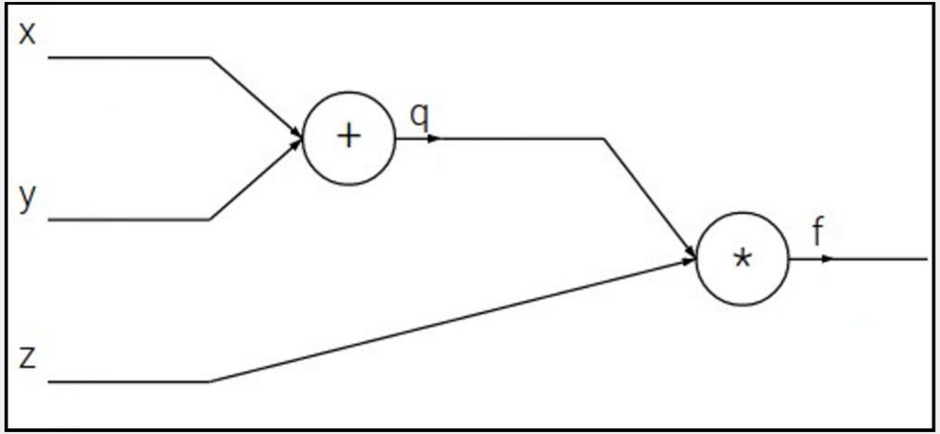
Deep Network (Neural Turing Machine)



https://arxiv.org/abs/1410.5401
andrej karpathy (graph)

Backpropagation: A simple example

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



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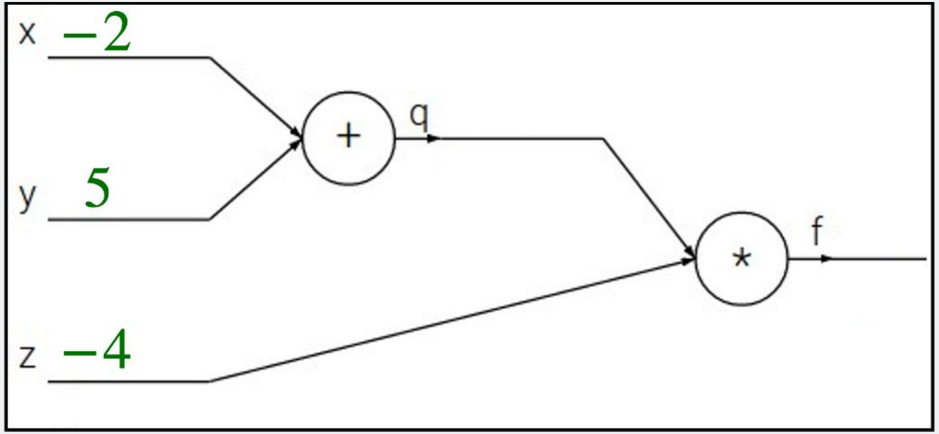
Backpropagation: A simple example

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

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



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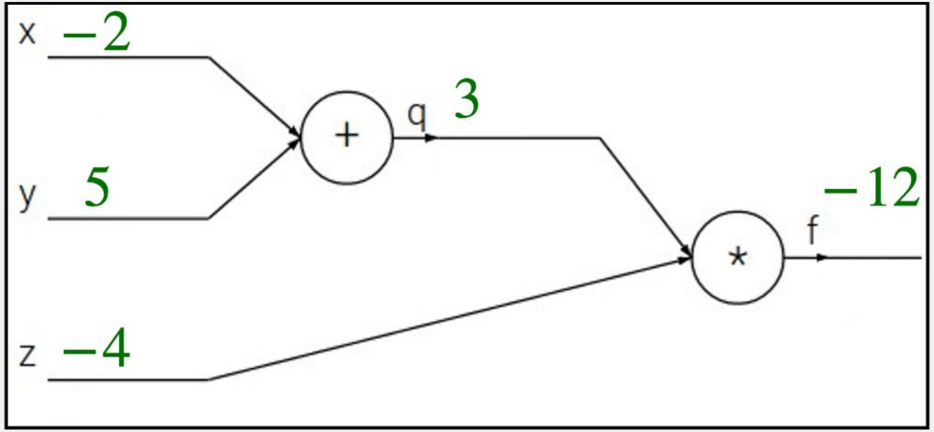

1. Forward pass: Compute outputs

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

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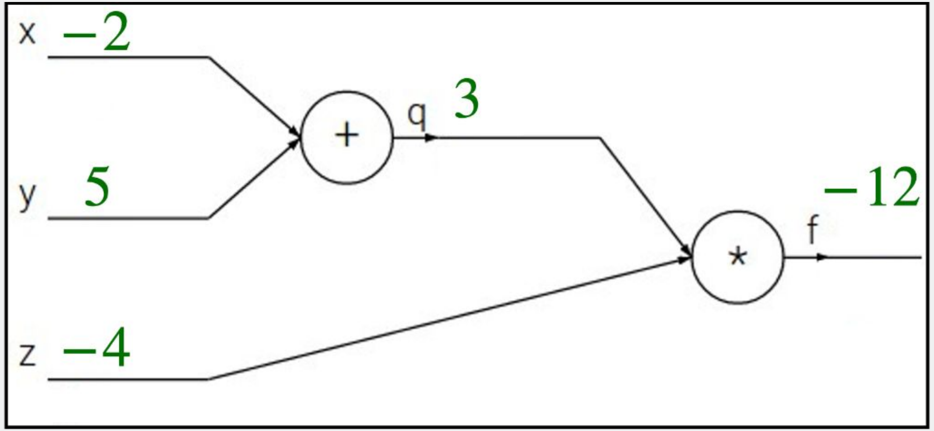

1. Forward pass: Compute outputs

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

2. Backward pass: Compute derivatives

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

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Backpropagation: A simple example

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

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

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

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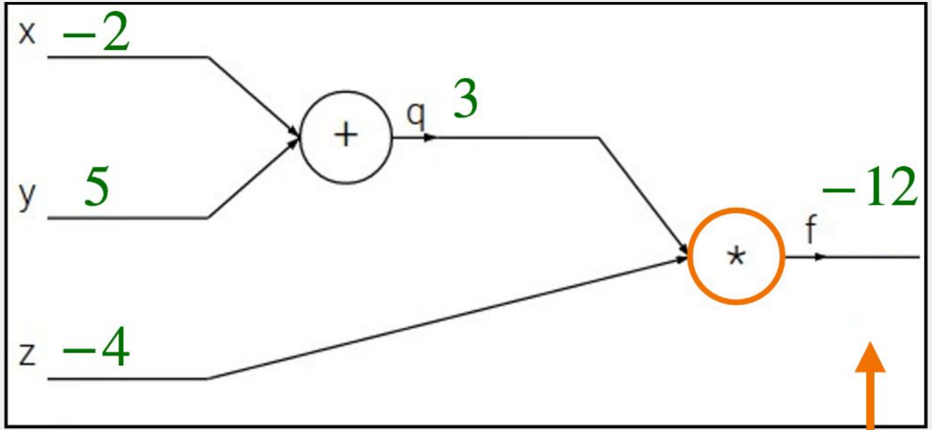
Want: $\dfrac{\partial f}{\partial x}, \dfrac{\partial f}{\partial y}, \dfrac{\partial f}{\partial z}$



$\boxed{\dfrac{\partial f}{\partial f}}$

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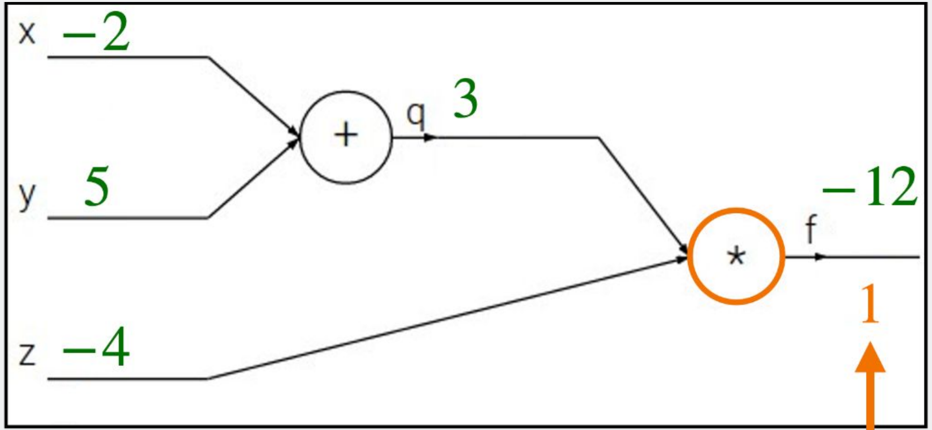

$$\boxed{\frac{\partial f}{\partial f}}$$

Backpropagation: A simple example

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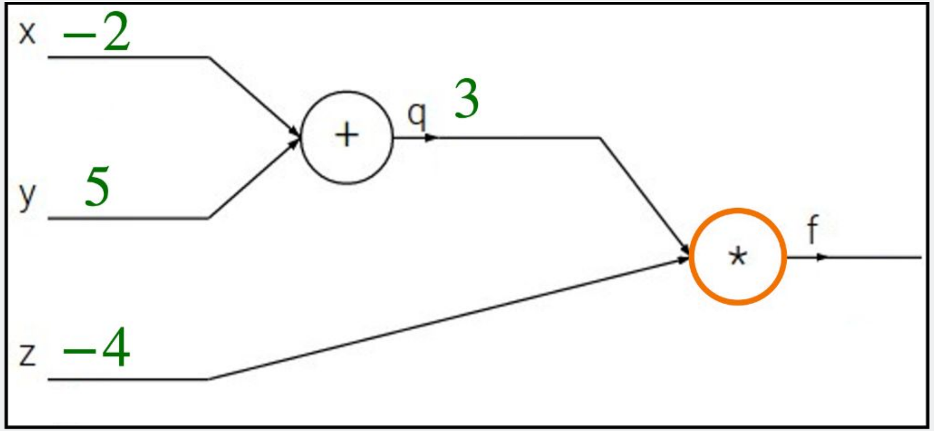

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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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

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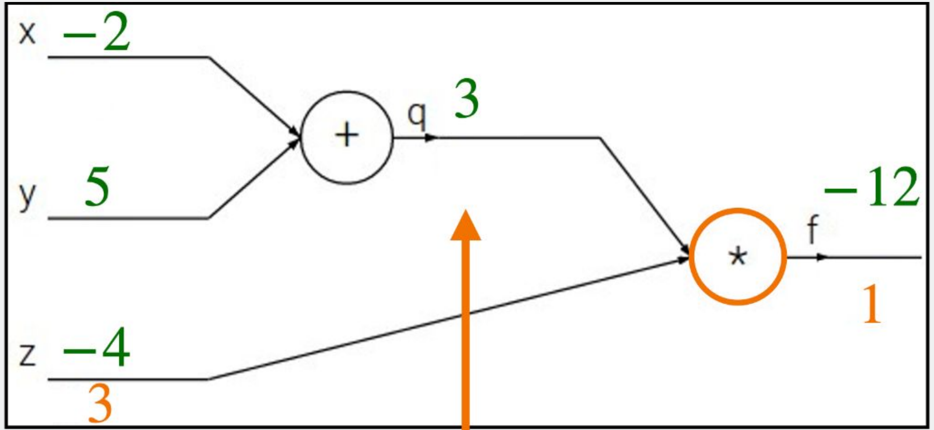

$\boxed{\dfrac{\partial f}{\partial q}}$ =???

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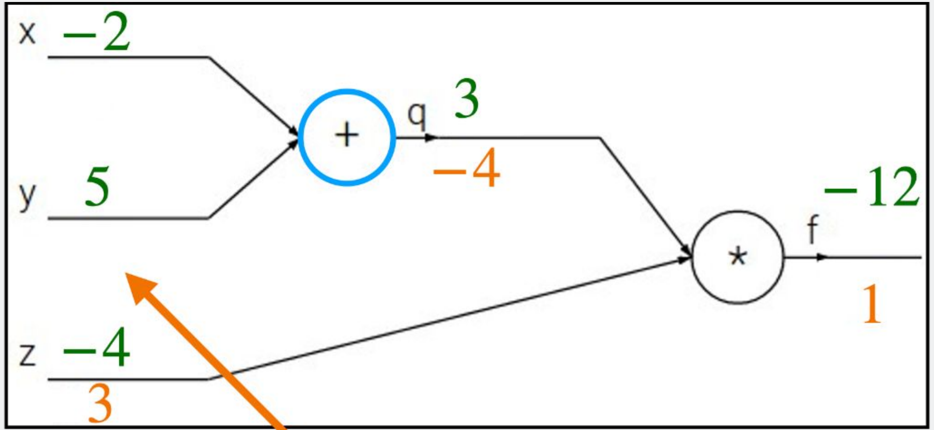
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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

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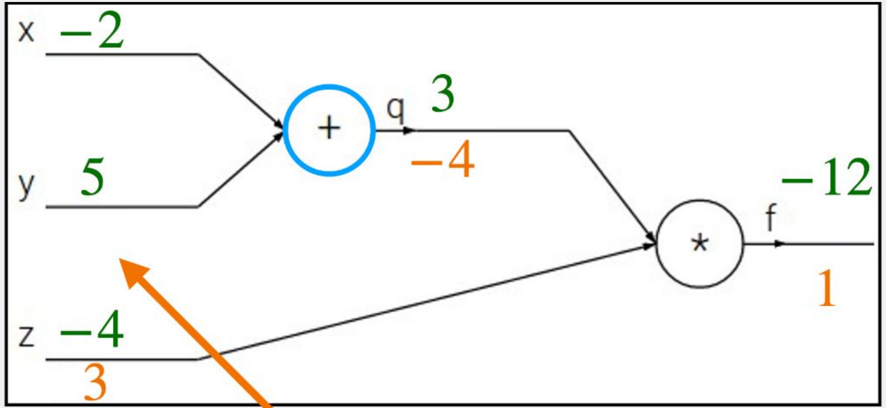

$$\boxed{\frac{\partial f}{\partial y} = \frac{\partial q}{\partial y} \frac{\partial f}{\partial q}} = ???$$

Downstream Gradient

Local Gradient

Upstream Gradient

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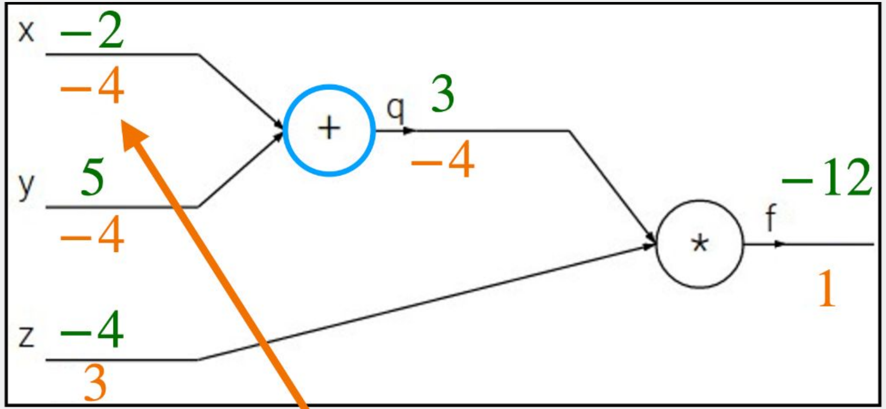
Backpropagation: A simple example

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

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



1. **Forward pass**: Compute outputs

$\boxed{q = x + y}$ $\quad f = q \cdot z$

2. **Backward pass**: Compute derivatives

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

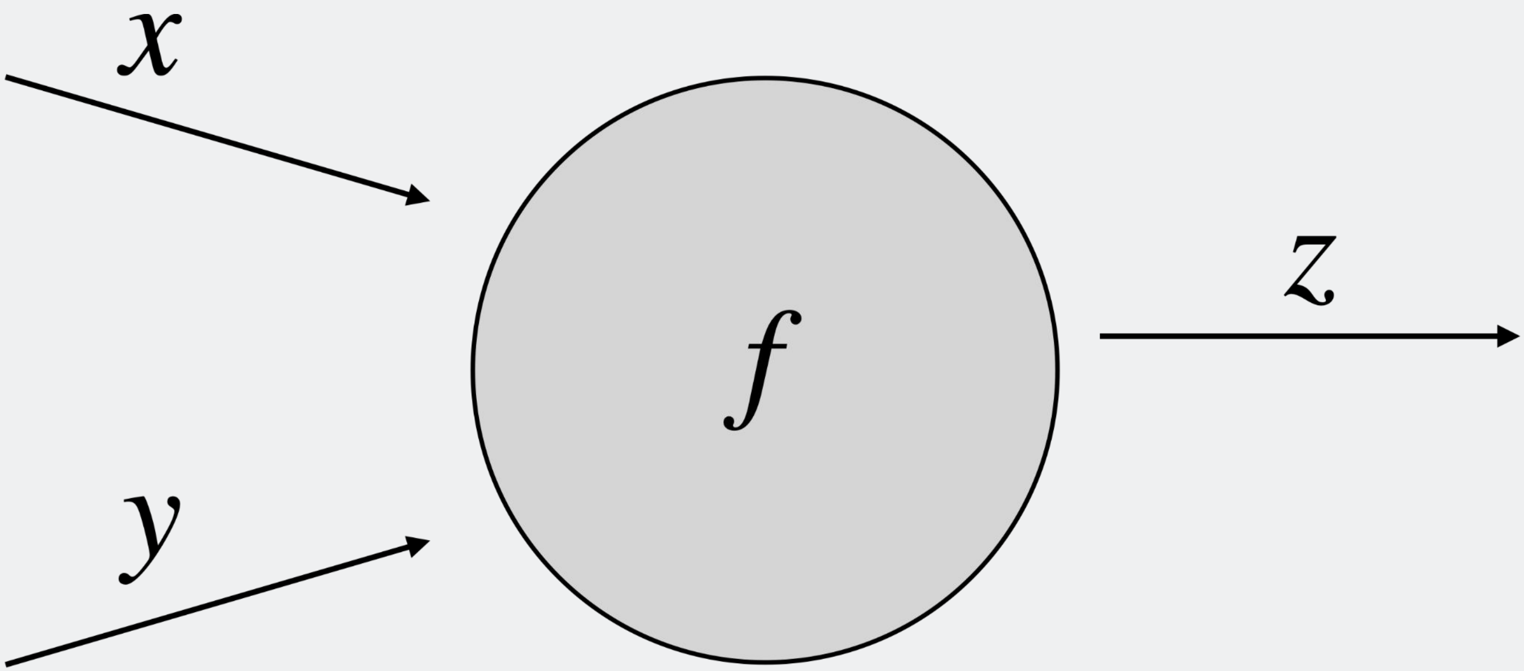
$$\boxed{\frac{\partial f}{\partial x} = \frac{\partial q}{\partial x}\frac{\partial f}{\partial q}} \qquad \boxed{\frac{\partial q}{\partial x} = 1}$$

Downstream Gradient

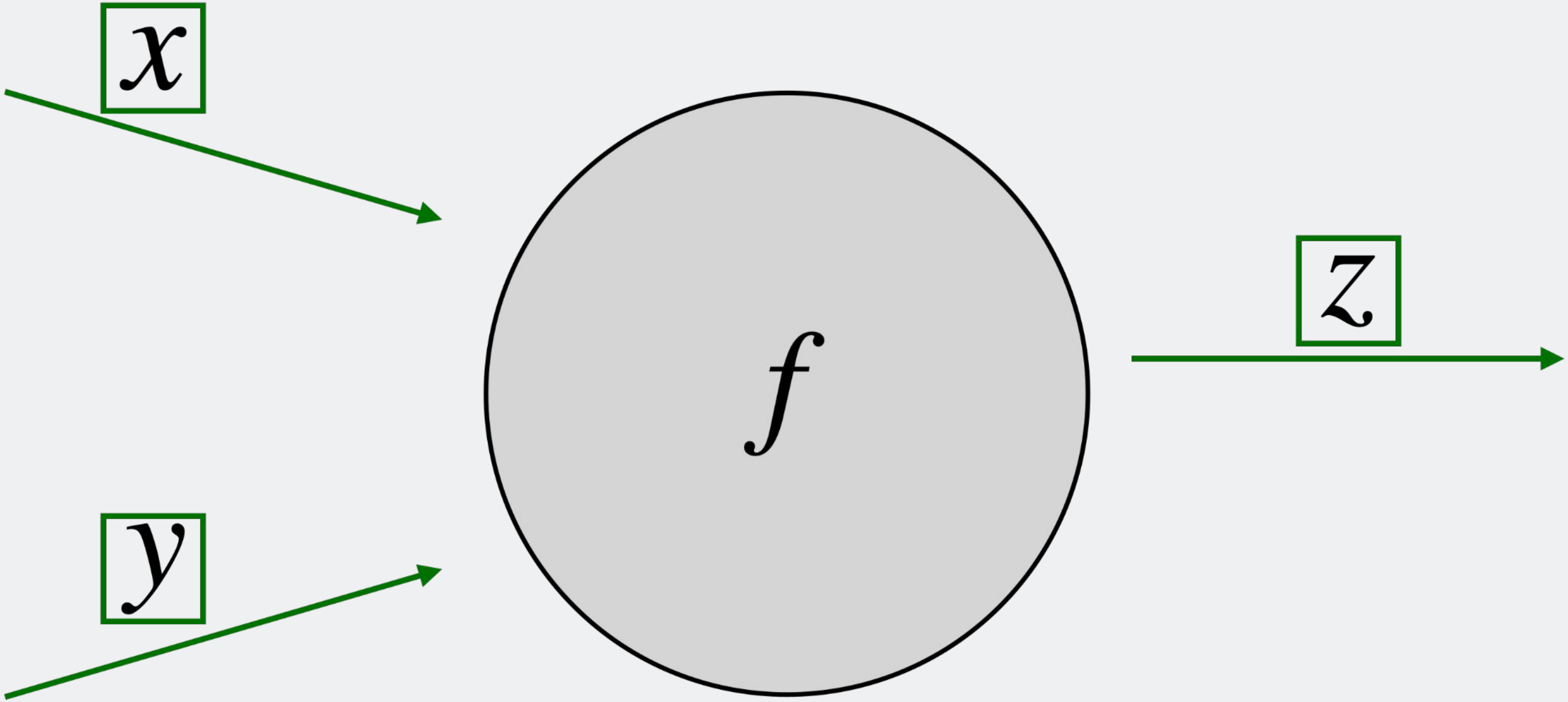
Local Gradient

Upstream Gradient

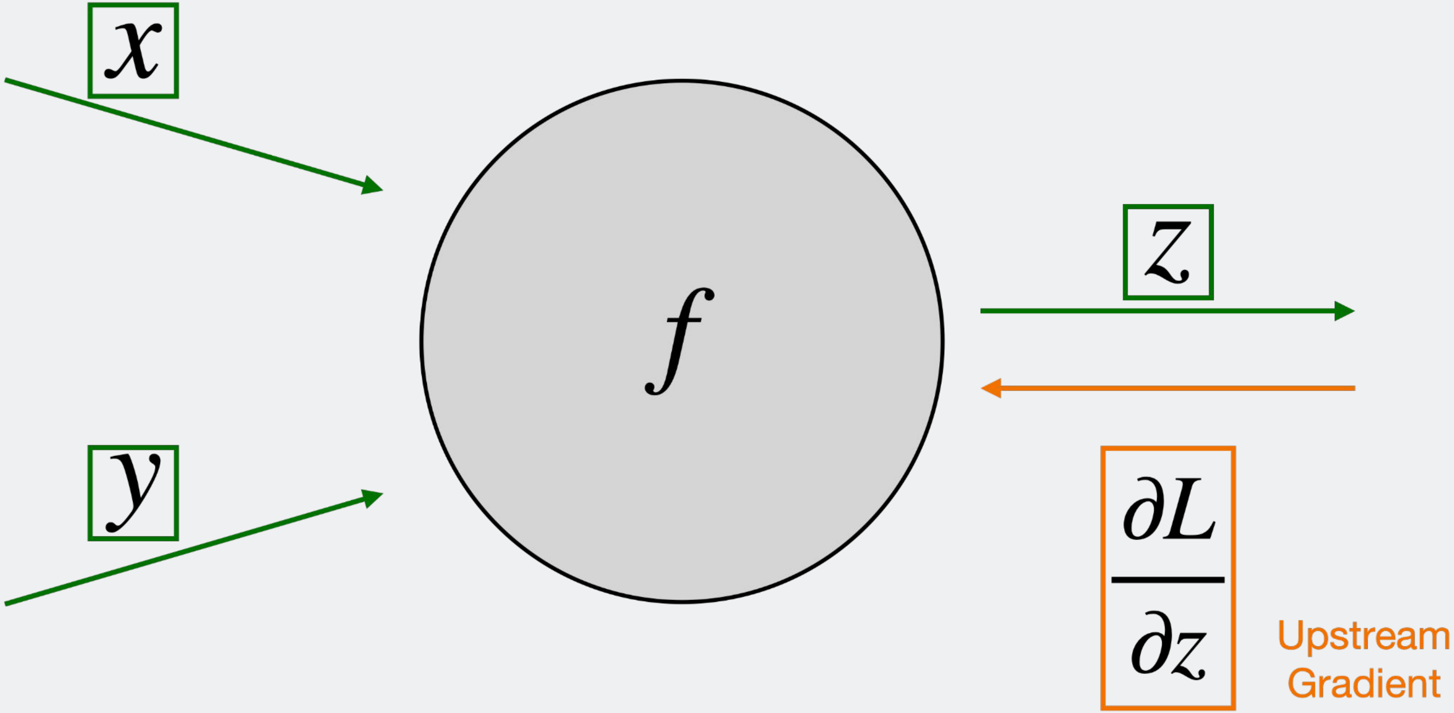
Local Properties of Backpropagation



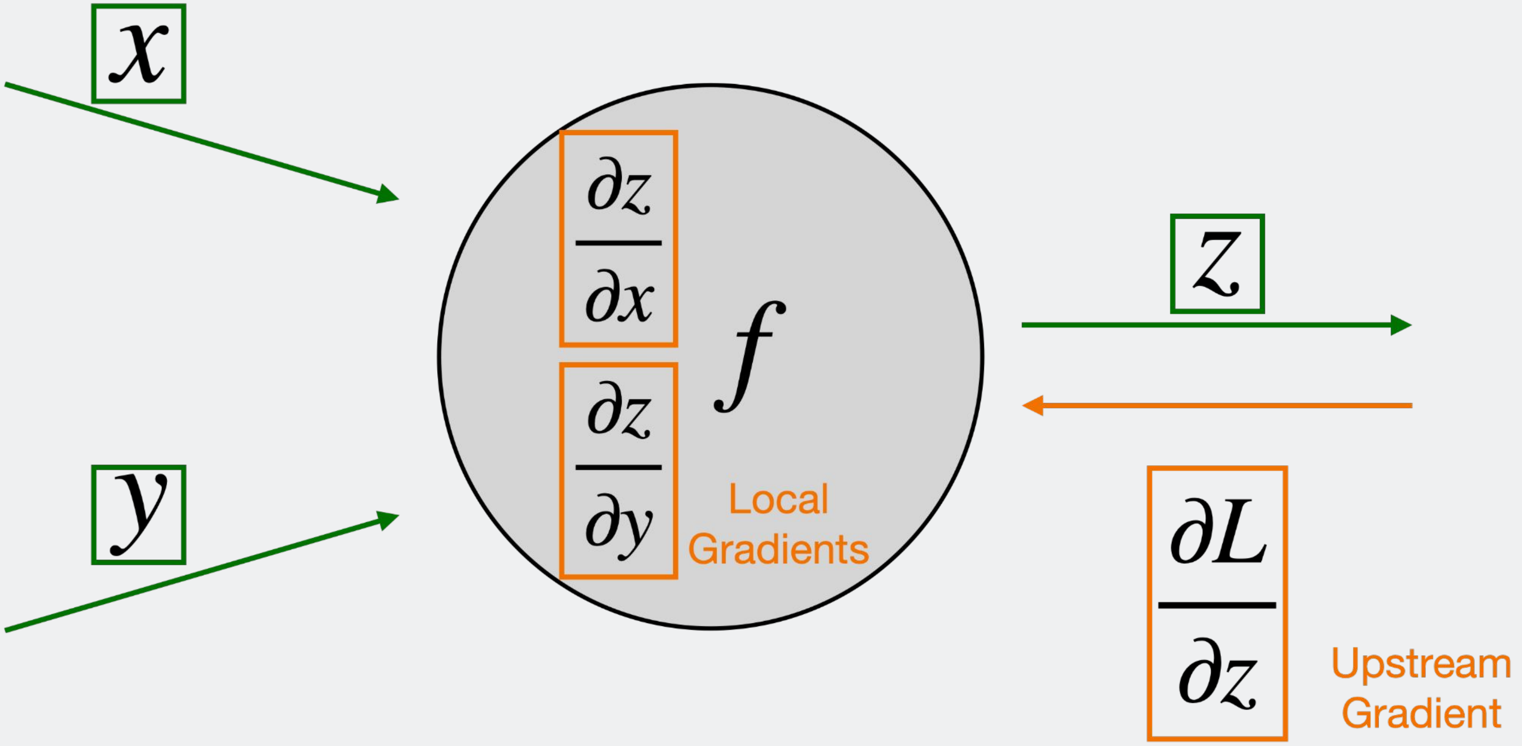
Local Properties of Backpropagation



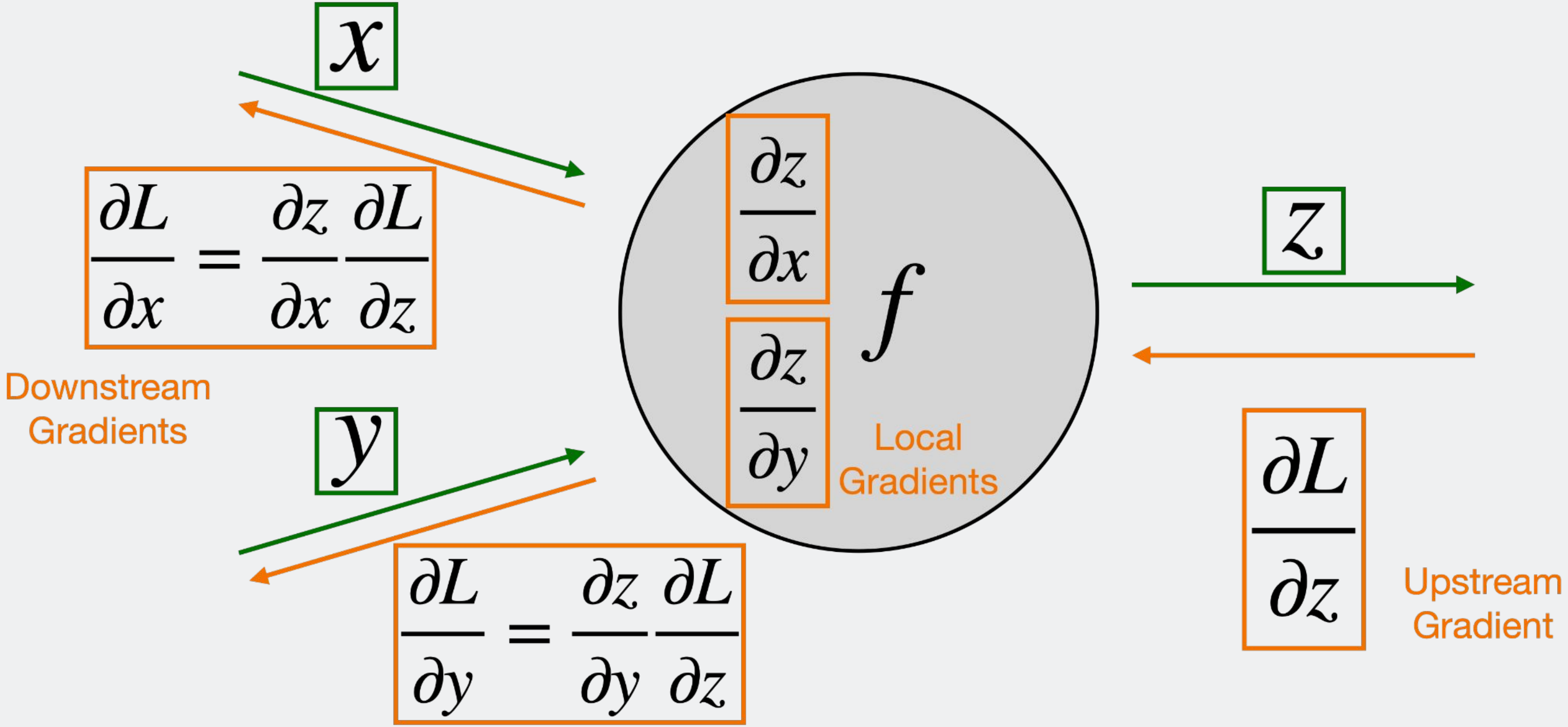
Local Properties of Backpropagation



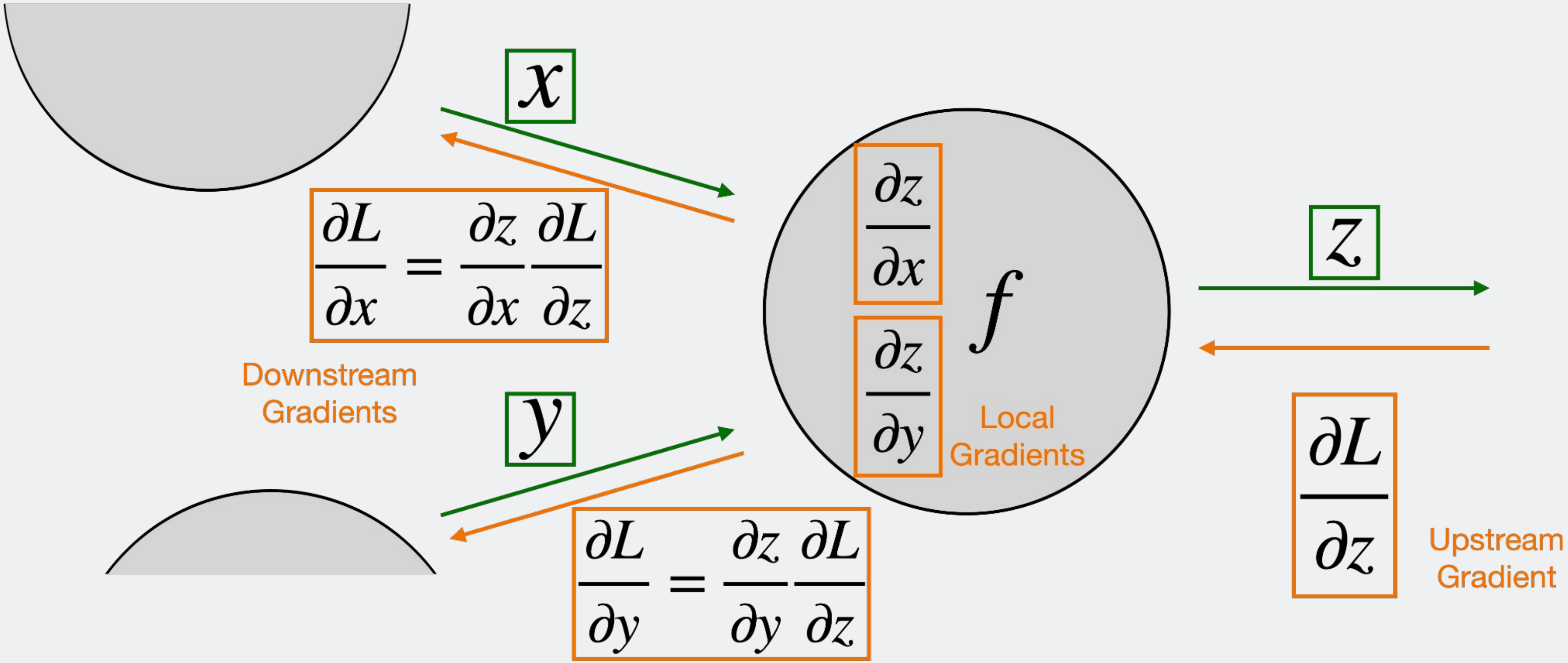
Local Properties of Backpropagation



Local Properties of Backpropagation



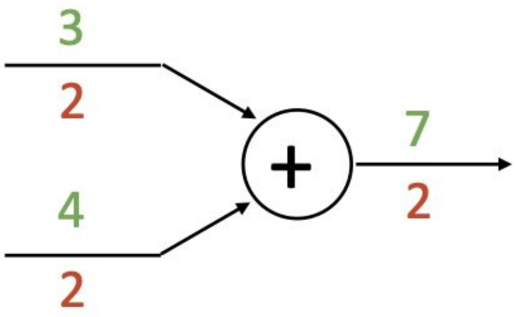
Local Properties of Backpropagation



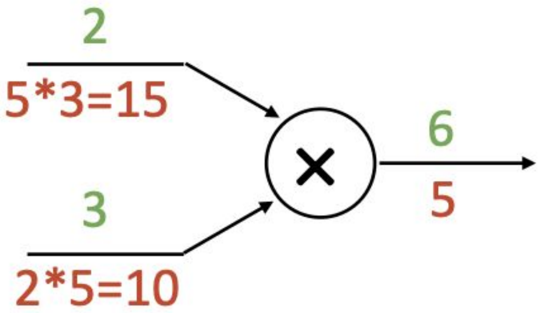
Patterns in Gradient Flow

important!

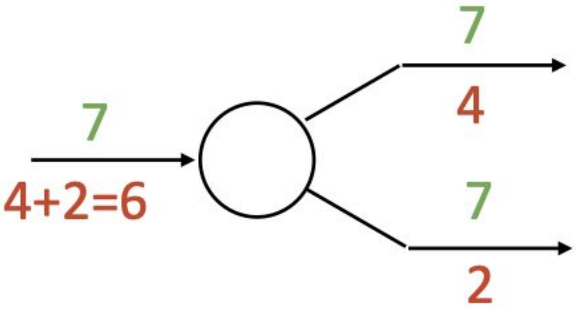
add gate: gradient distributor



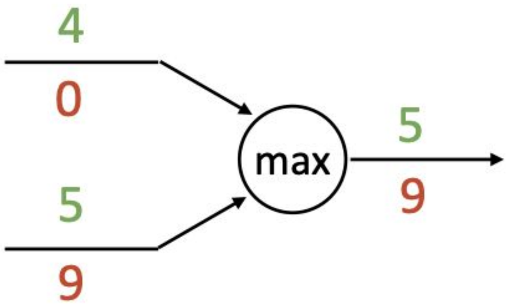
mul gate: "swap multiplier"



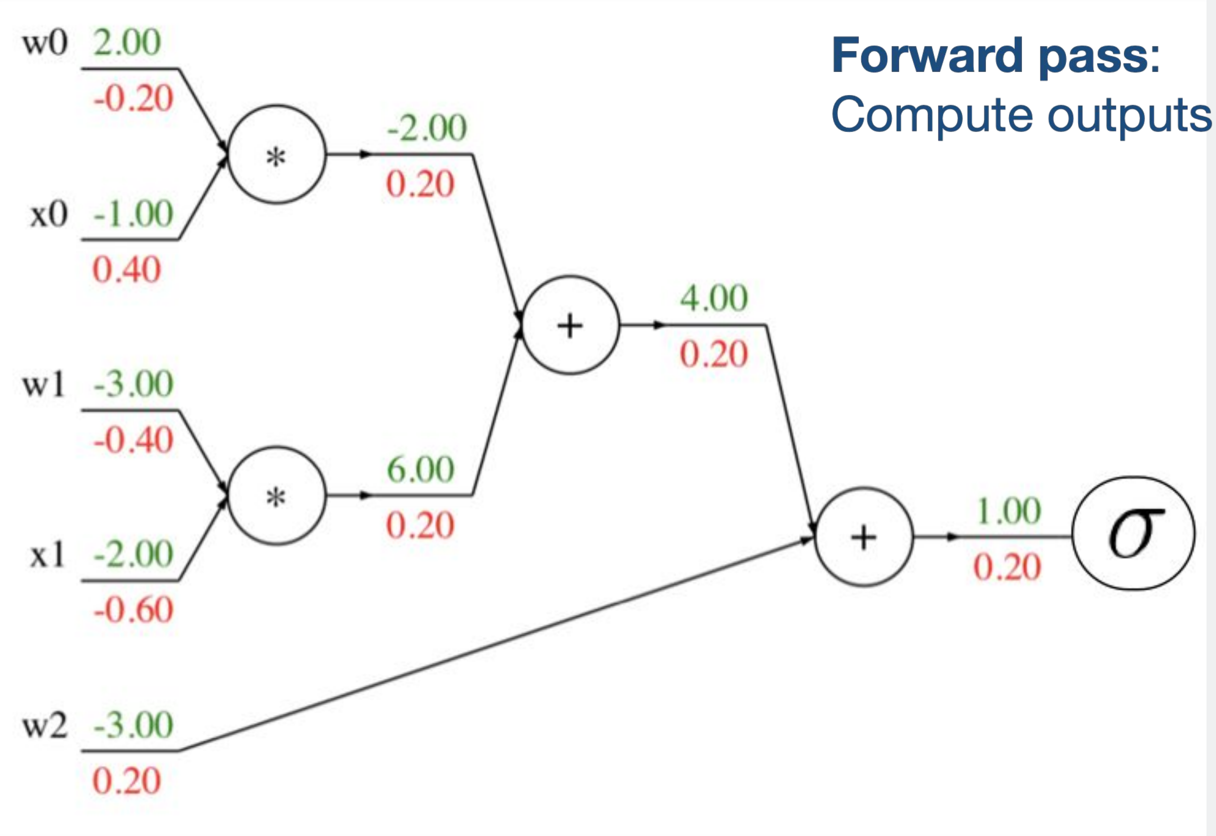
copy gate: gradient adder



max gate: gradient router



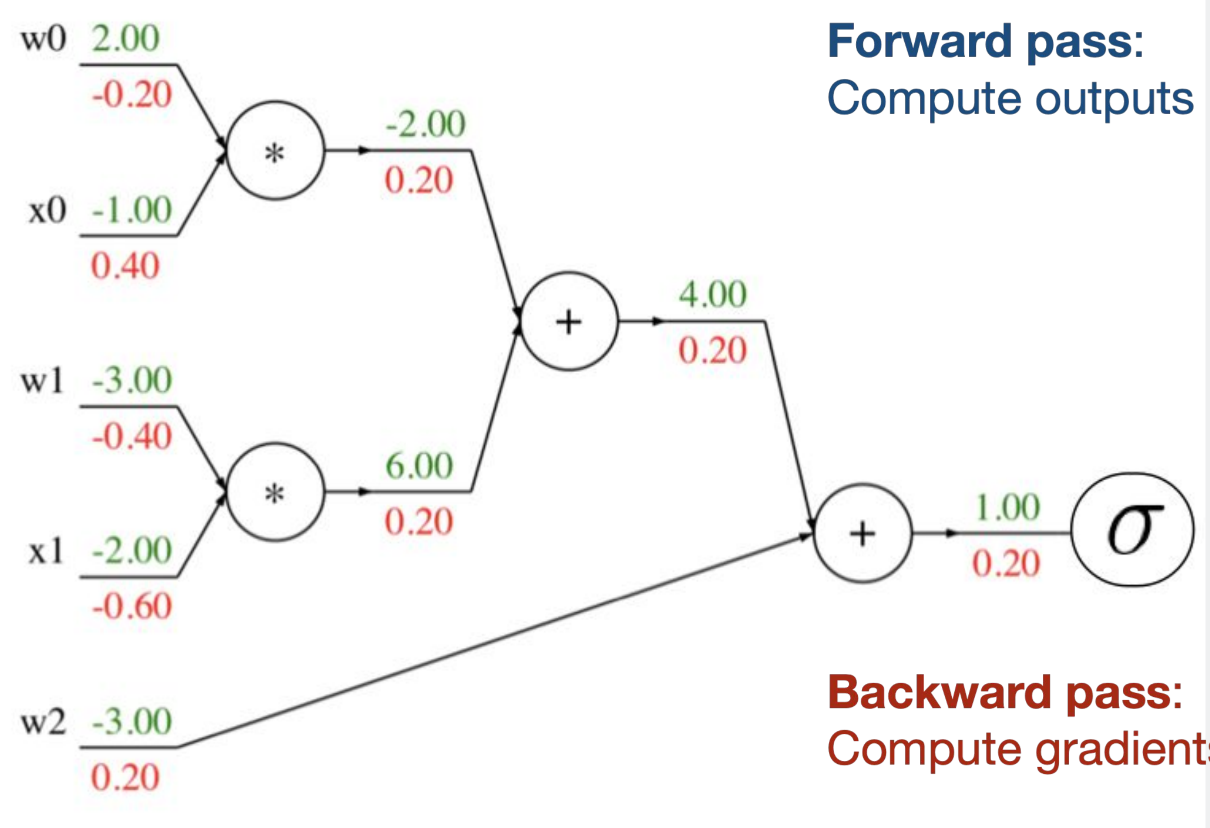
Backprop Implementation: "Flat" gradient code



Forward pass: Compute outputs

```
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 outputs

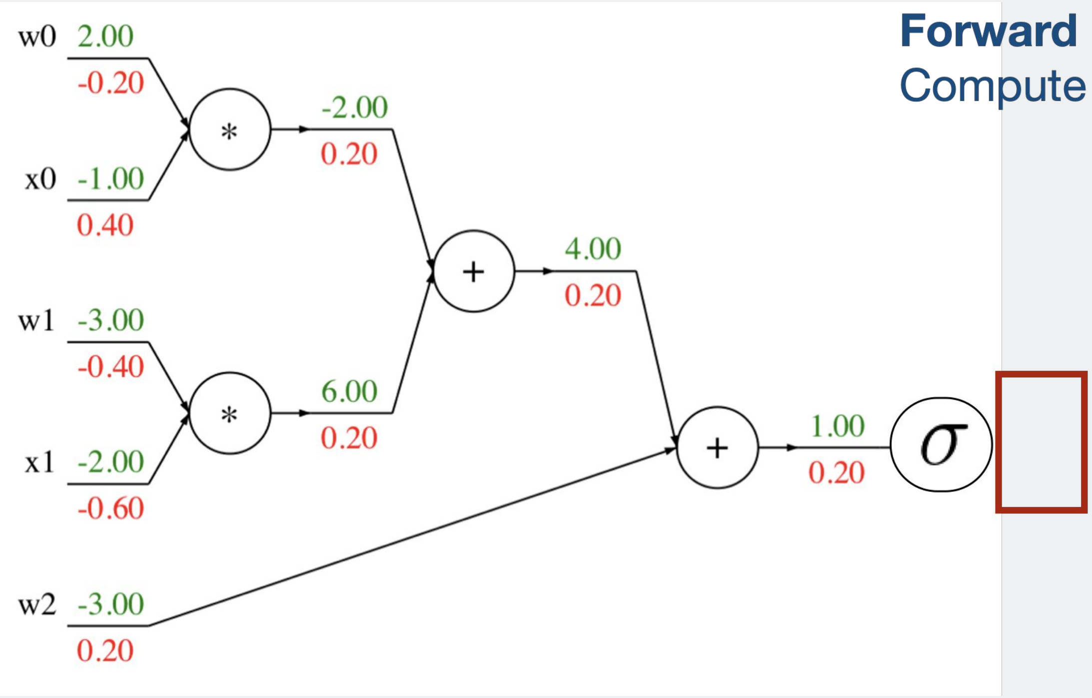
Backward pass:
Compute gradients

```
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 outputs

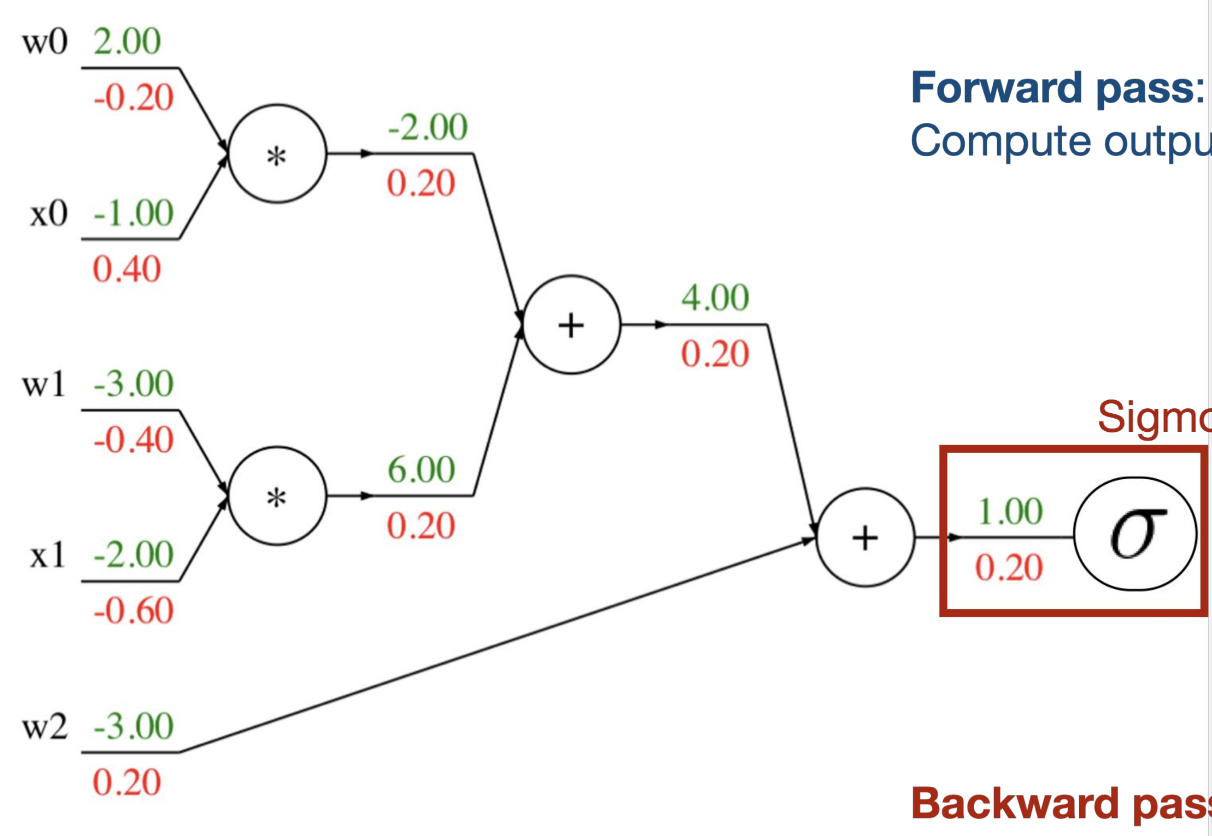
```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

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
```

Backward pass:
Compute gradients

Backprop Implementation: "Flat" gradient code



Forward pass:
Compute outputs

Sigmoid

Backward pass:
Compute gradients

```
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
```

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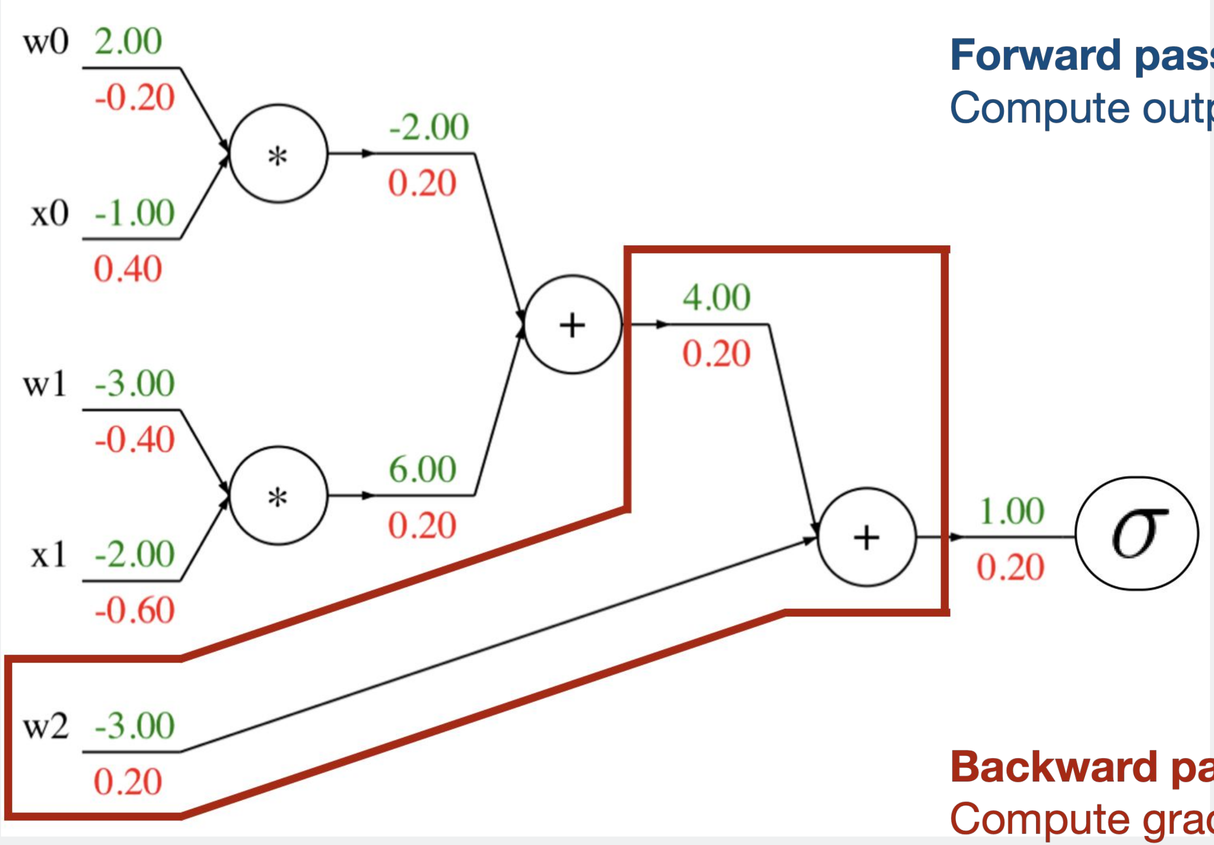
Backprop Implementation: “Flat” gradient code



Forward pass:
Compute outputs

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

Add

```
  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
```

Backward pass:
Compute gradients

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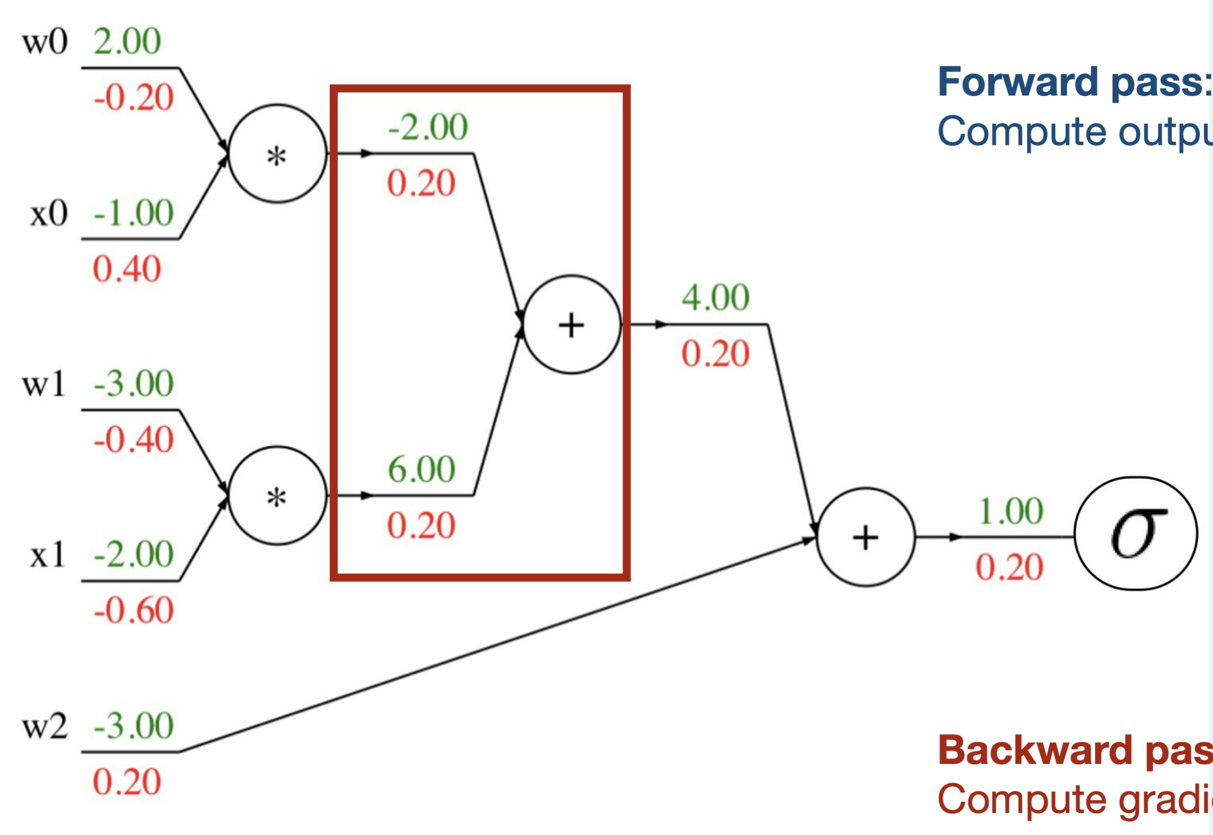
Backprop Implementation: “Flat” gradient code



Forward pass:
Compute outputs

```
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    s2 = s0 + s1
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Add

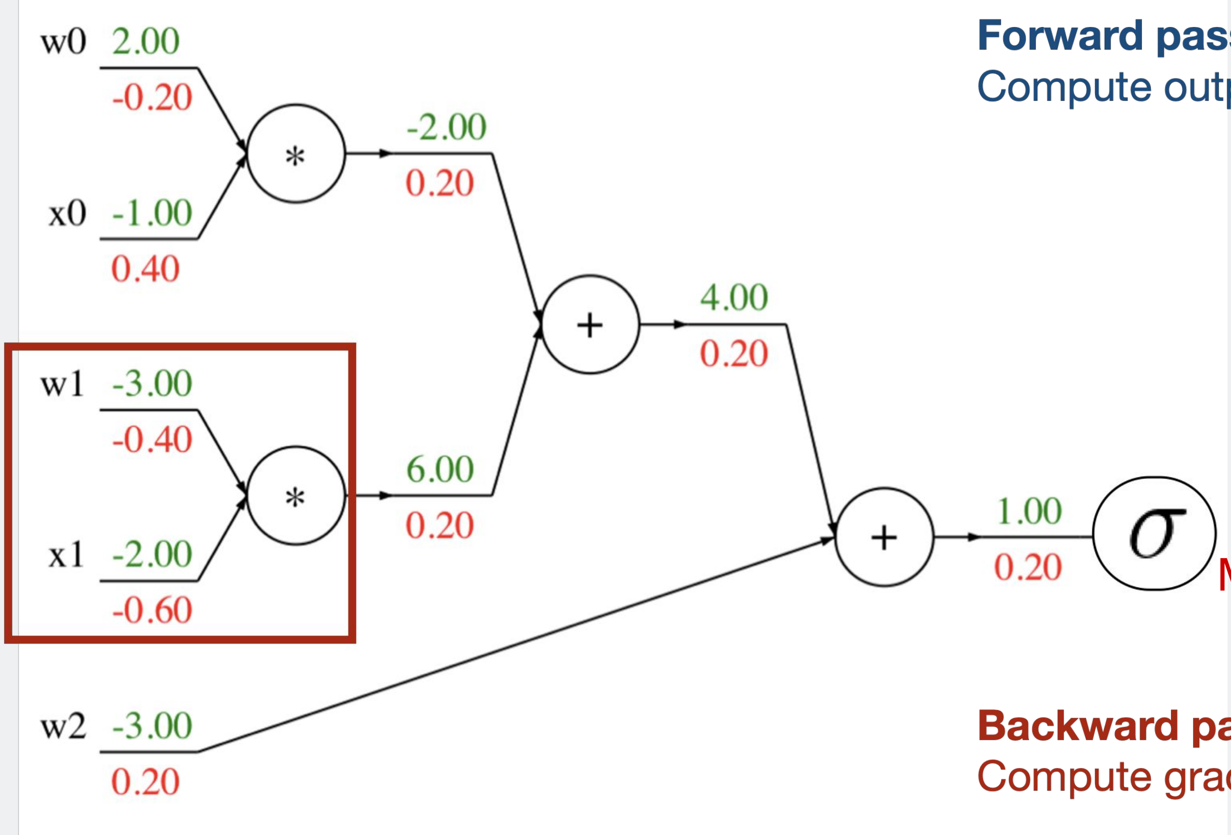
```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Backward pass:
Compute gradients

ROBOTICS

x

Backprop Implementation: "Flat" gradient code



Forward pass:
Compute outputs

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

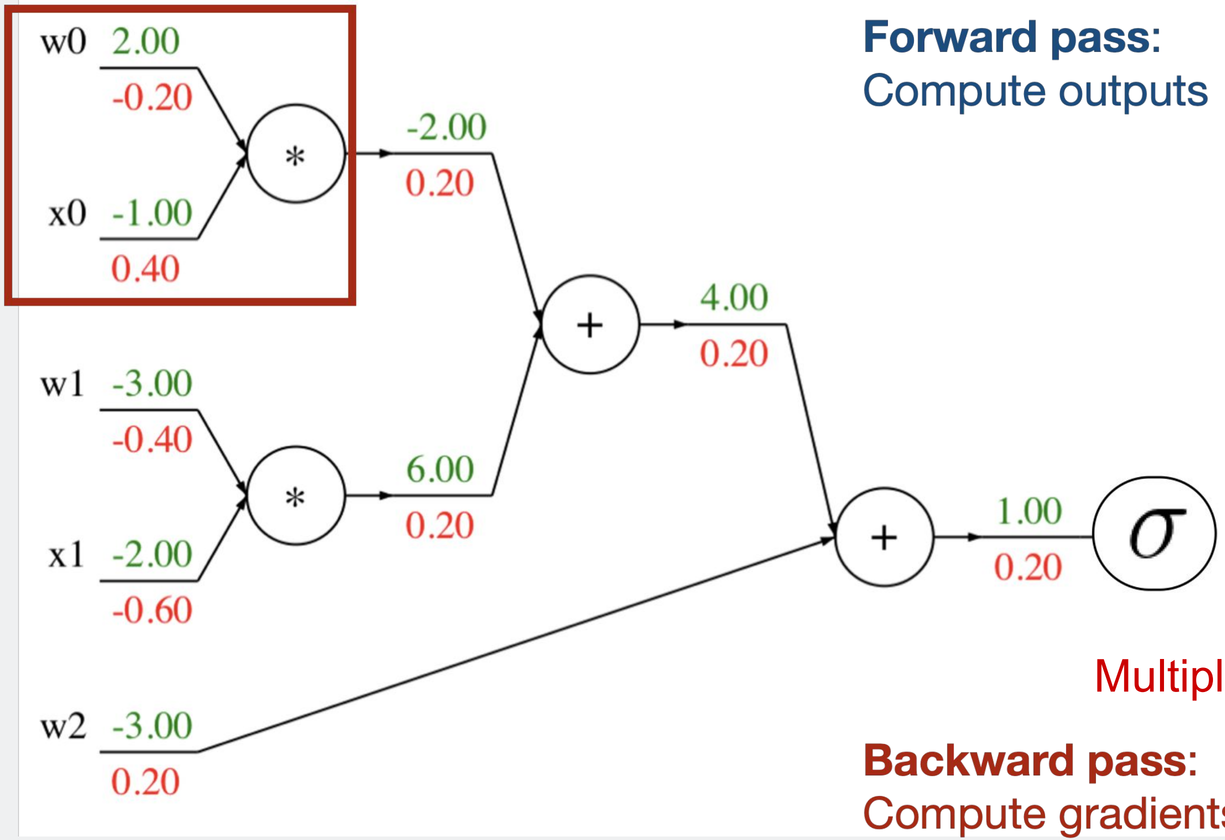
Multiply

```
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
```

Backward pass:
Compute gradients

ROBOTICS

Backprop Implementation: “Flat” gradient code



Forward pass:
Compute outputs

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

Multiply

```
    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
```

Backward pass:
Compute gradients

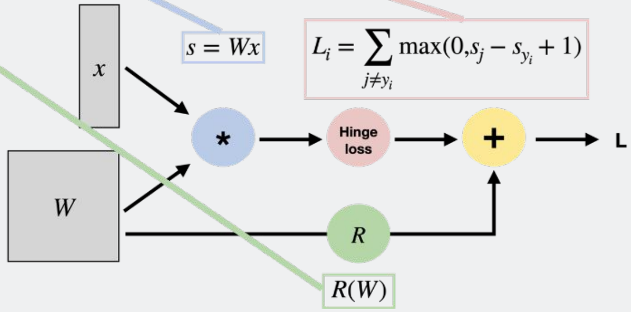
“Flat” backprop: Do this for Project 2

Forward pass:
Compute outputs

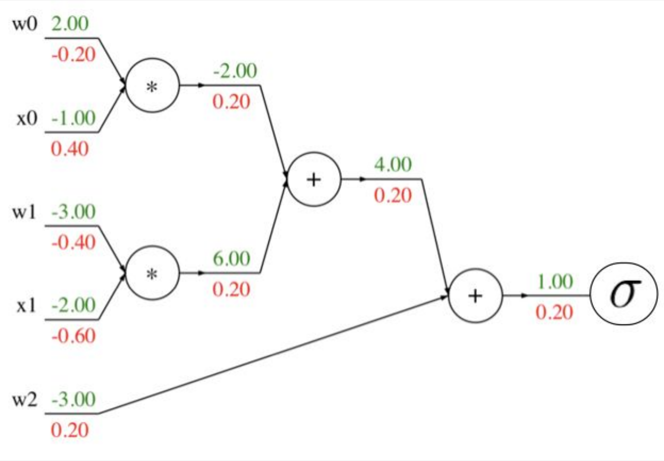
```
###############################################################################
# TODO:                                                                       #
# Implement a vectorized version of the structured SVM loss, storing the      #
# result in loss.                                                             #
###############################################################################
# Replace "pass" statement with your code
num_classes = W.shape[1]
num_train = X.shape[0]
score = # ...
correct_class_score = # ...
margin = # ...
data_loss = # ...
reg_loss = # ...
loss += data_loss + reg_loss
###############################################################################
#                              END OF YOUR CODE                               #
###############################################################################
```

Backward pass:
Compute gradients

```
###############################################################################
# TODO:                                                                       #
# Implement a vectorized version of the gradient for the structured SVM      #
# loss, storing the result in dW.                                             #
#                                                                             #
# Hint: Instead of computing the gradient from scratch, it may be easier      #
# to reuse some of the intermediate values that you used to compute the      #
# loss.                                                                       #
###############################################################################
# Replace "pass" statement with your code
dmargins = # ...
dscores = # ...
dW = # ...
###############################################################################
#                              END OF YOUR CODE                               #
###############################################################################
```



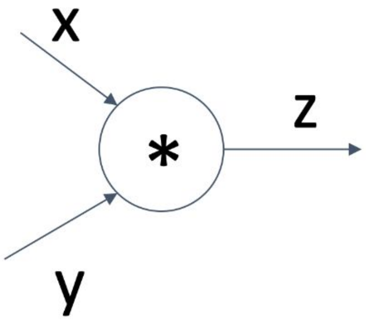
Backprop Implementation: Modular API



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 w/ 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**:

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

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?

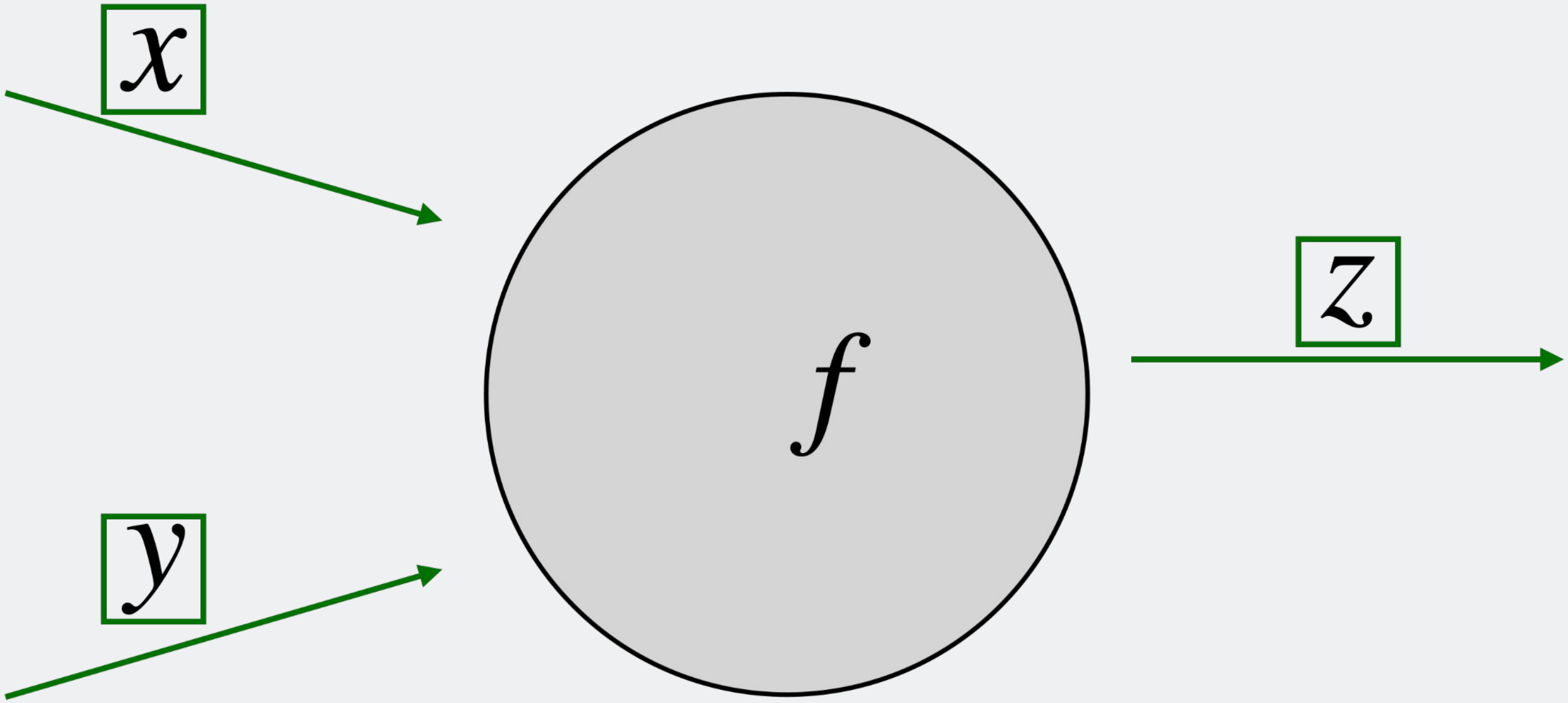
$x \in \mathbb{R}^N, y \in \mathbb{R}^M$

Derivative is **Jacobian**:

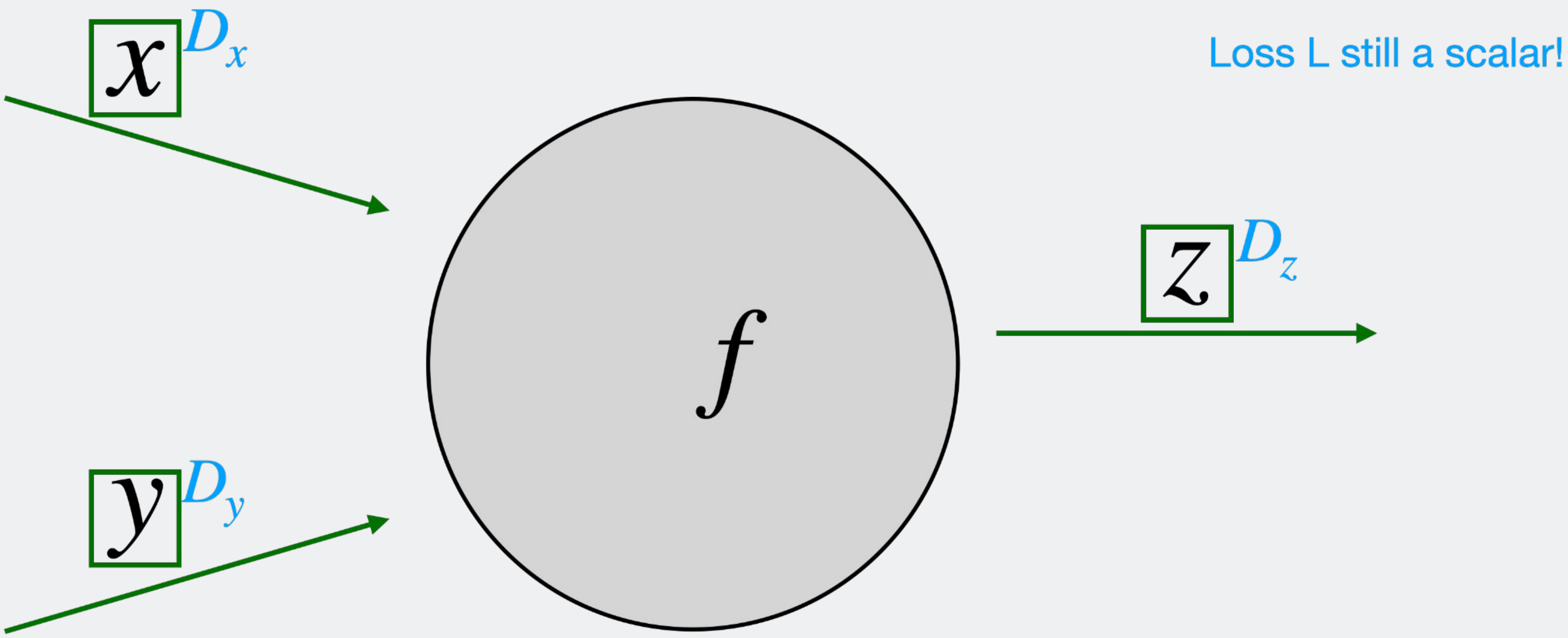
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M}, \quad \left(\frac{\partial y}{\partial x}\right)_{i,j} = \frac{\partial y_j}{\partial x_i}$$

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

Backprop with Vectors

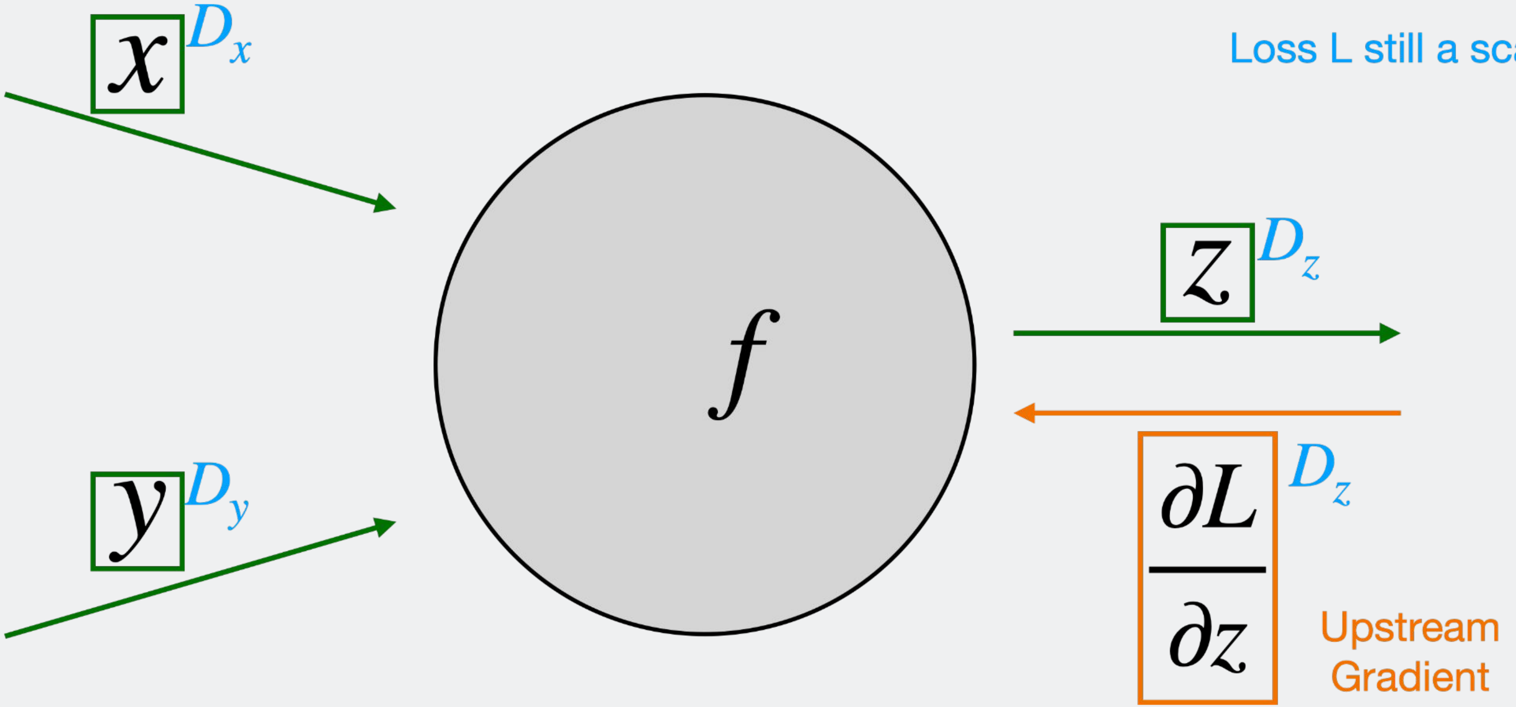


Backprop with Vectors



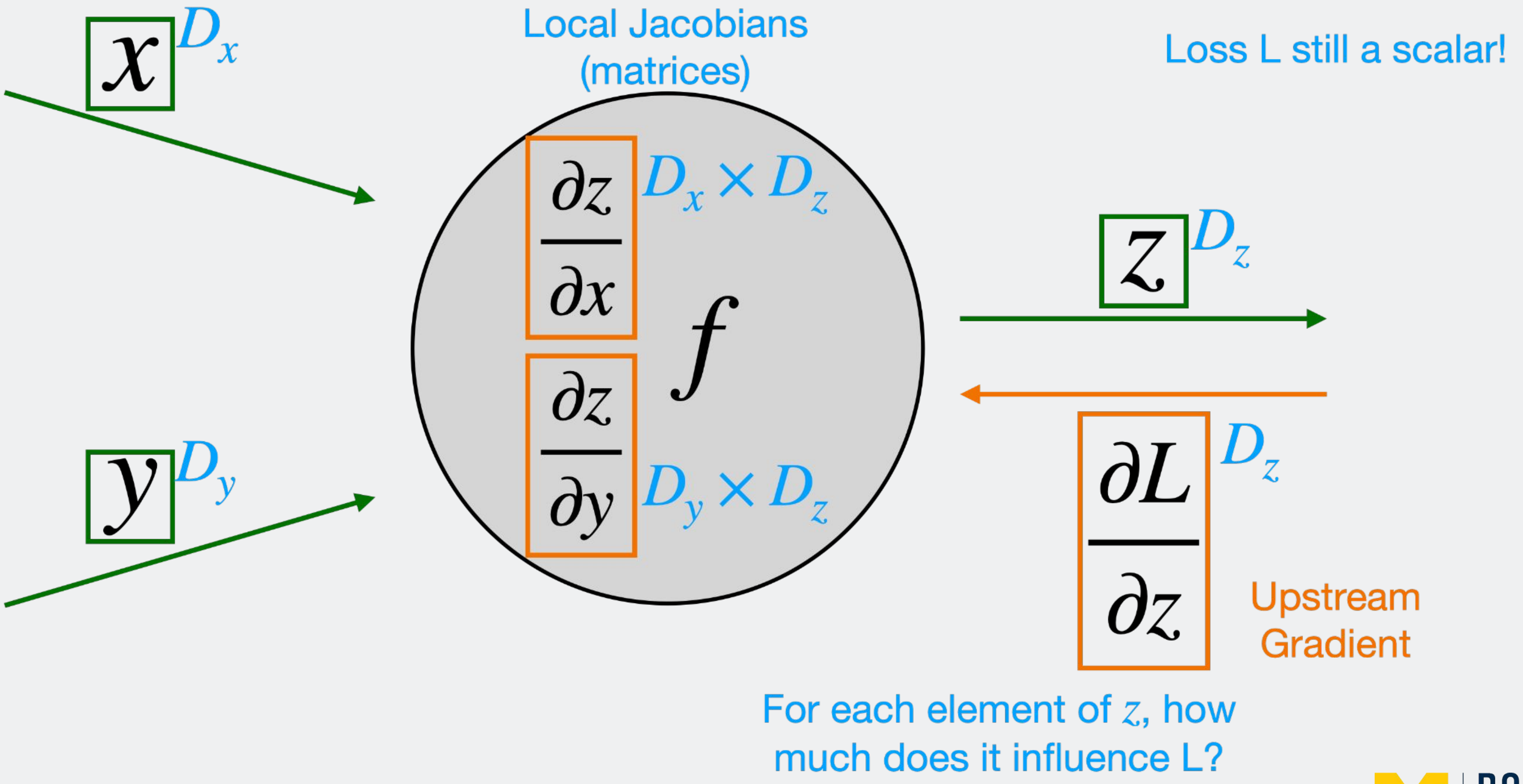
Backprop with Vectors

Loss L still a scalar!



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

Backprop with Vectors



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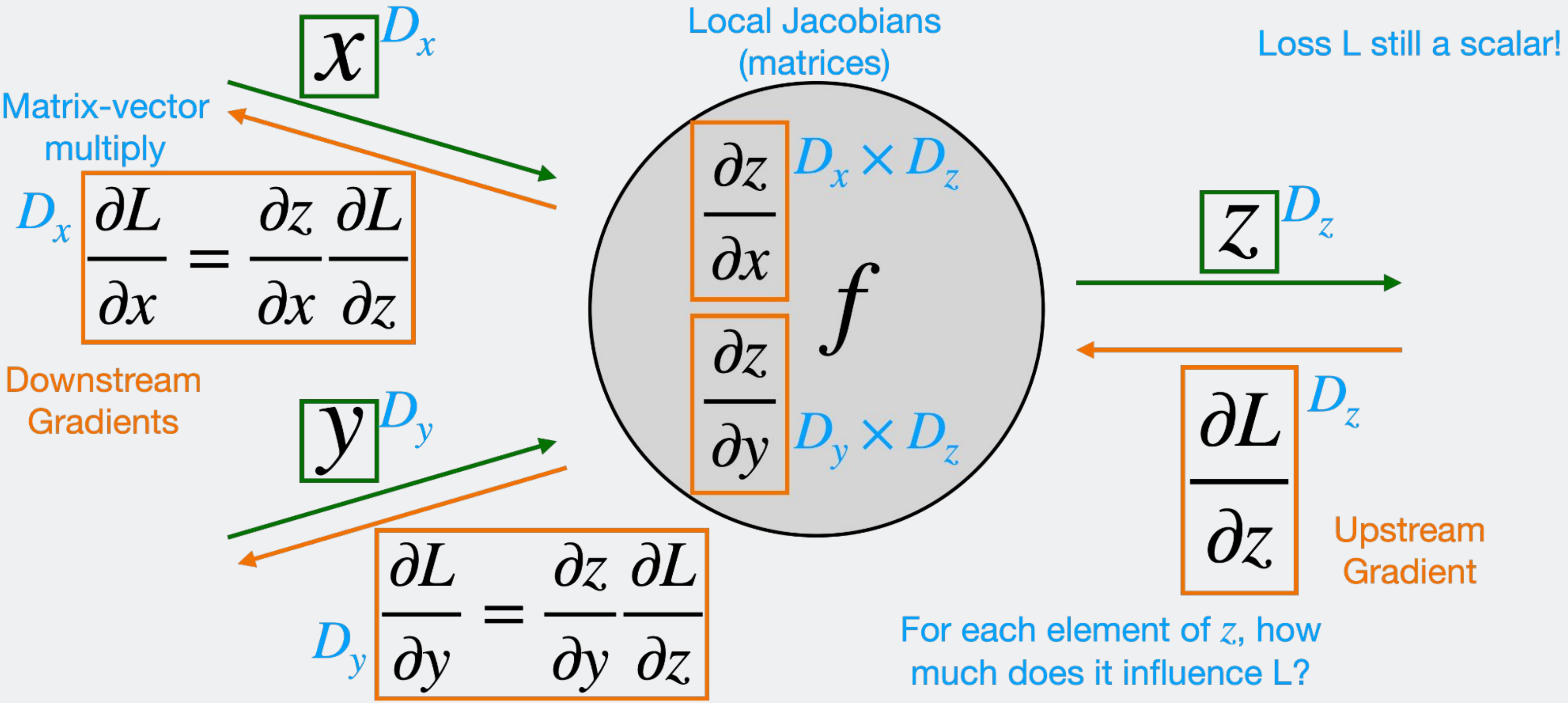

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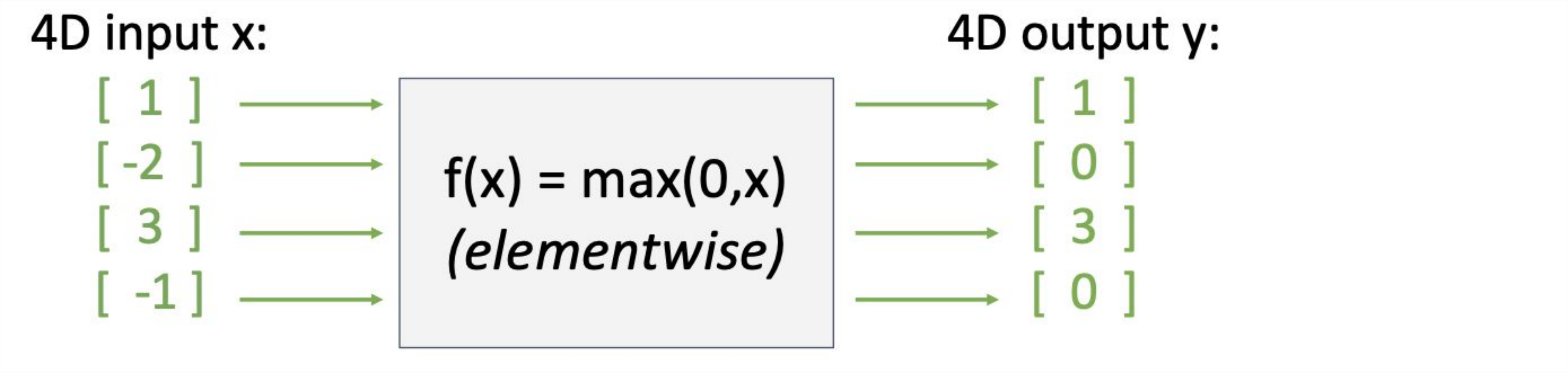

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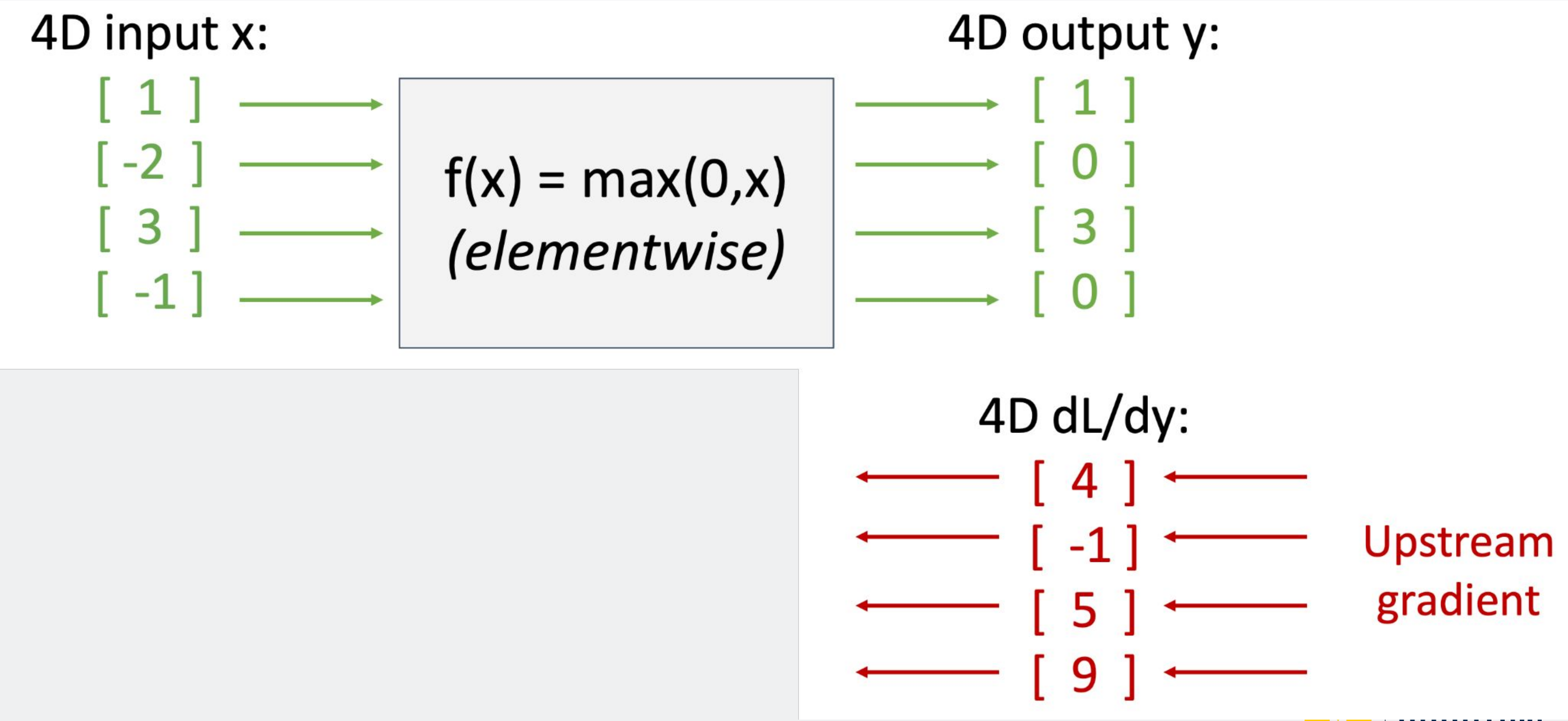

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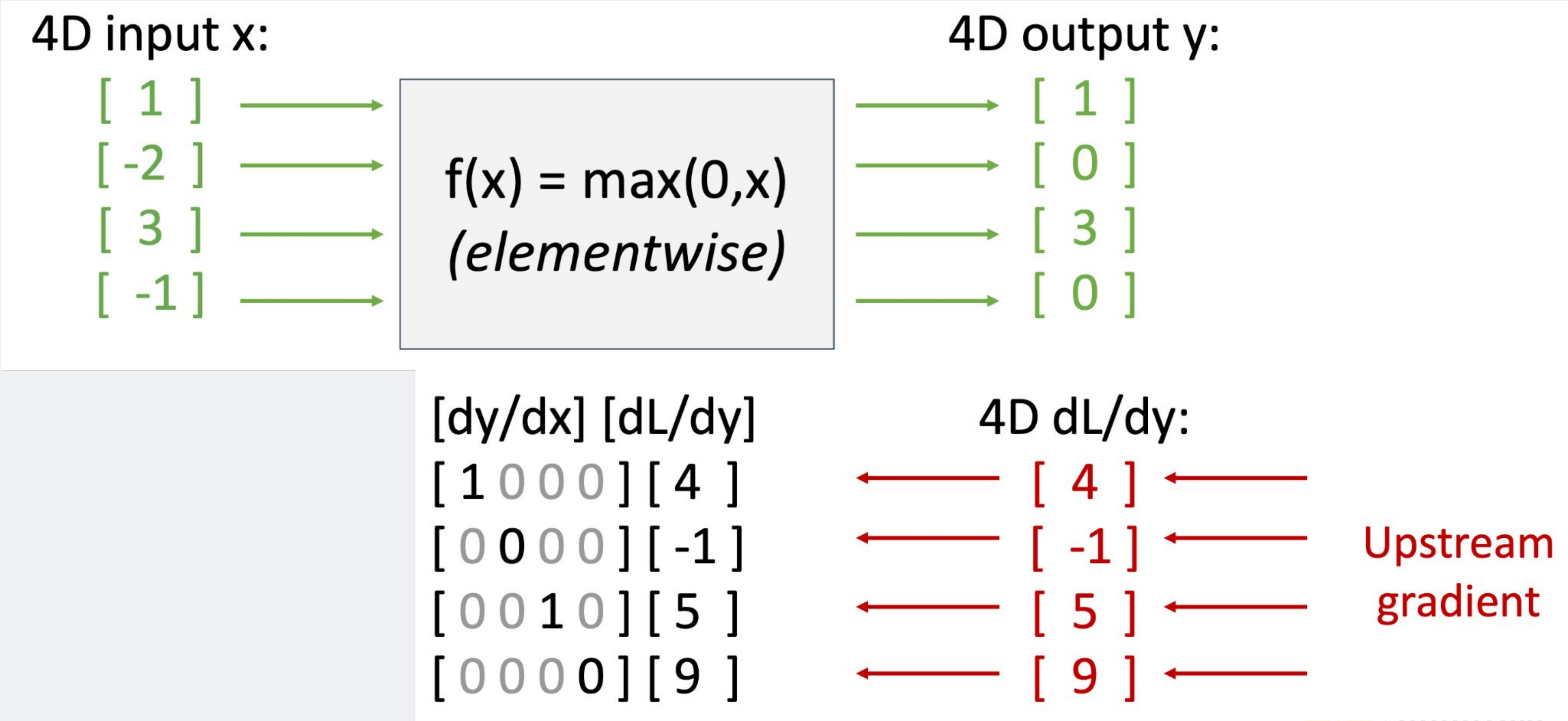
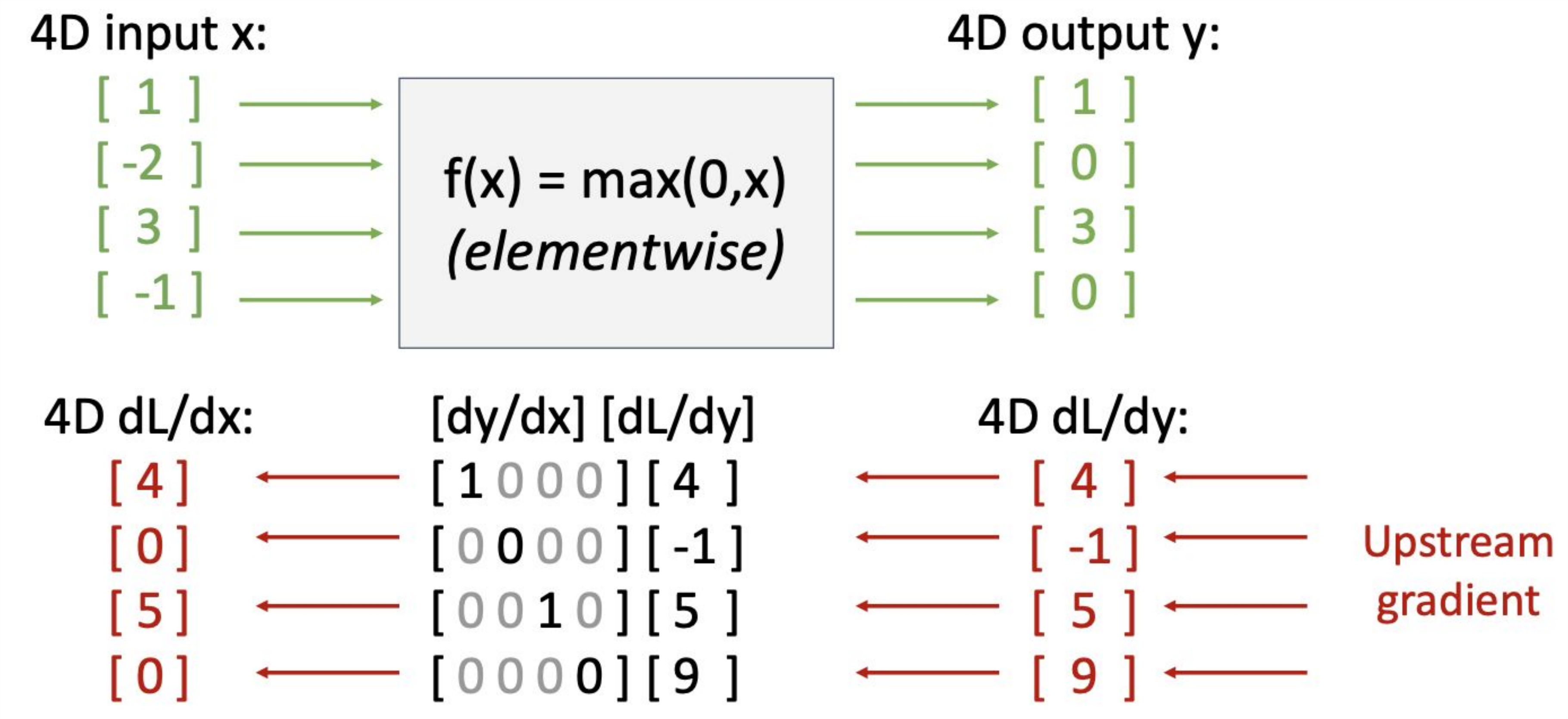
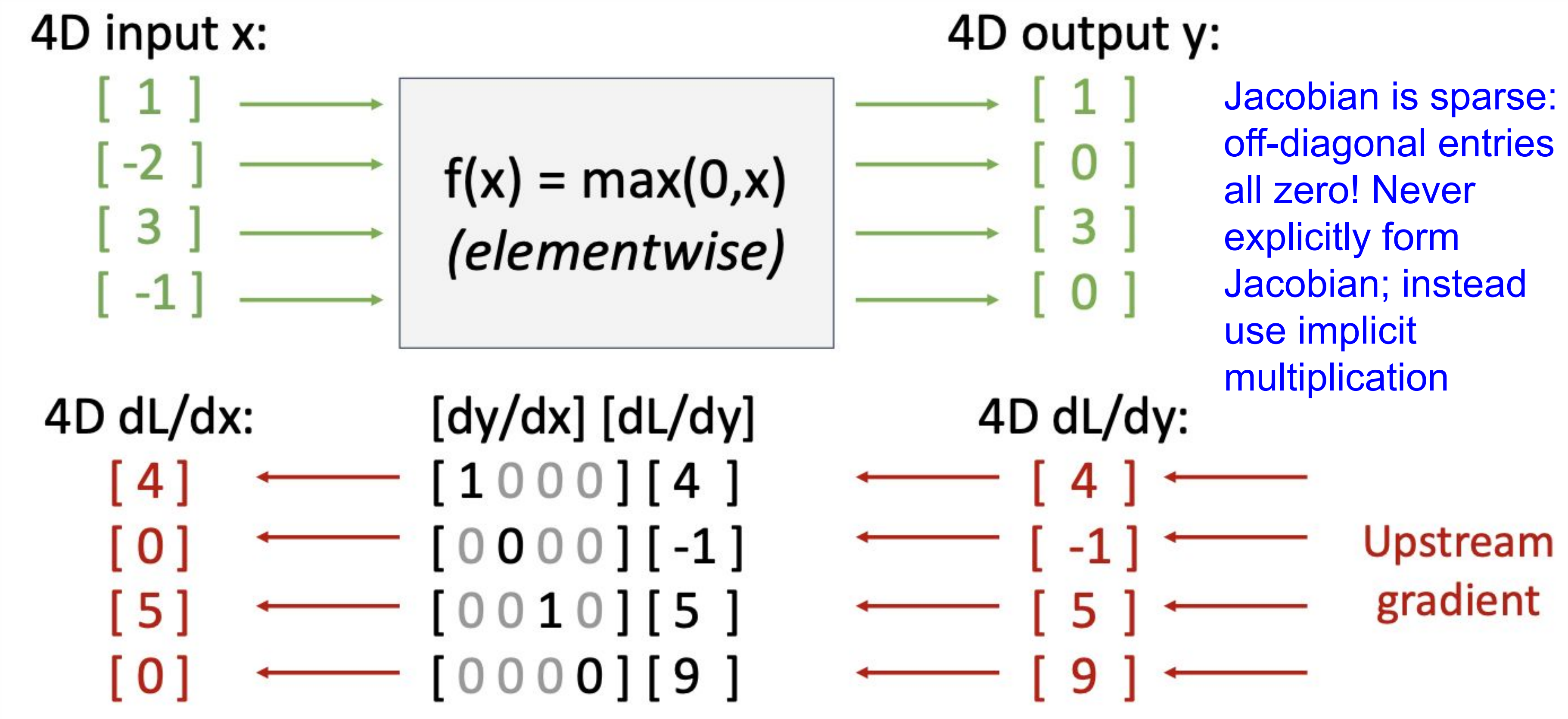


Backprop with Vectors

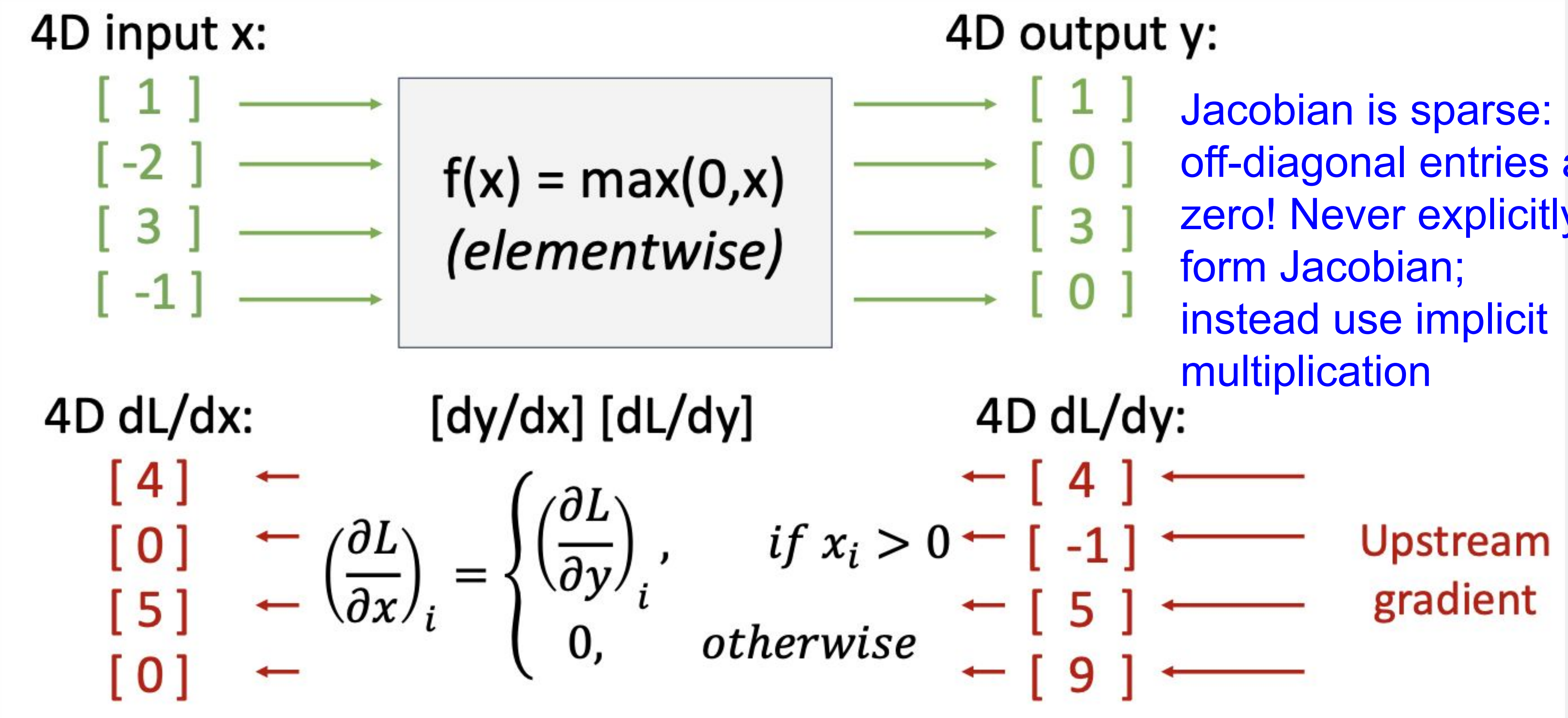


Backprop with Vectors



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

Backprop with Vectors



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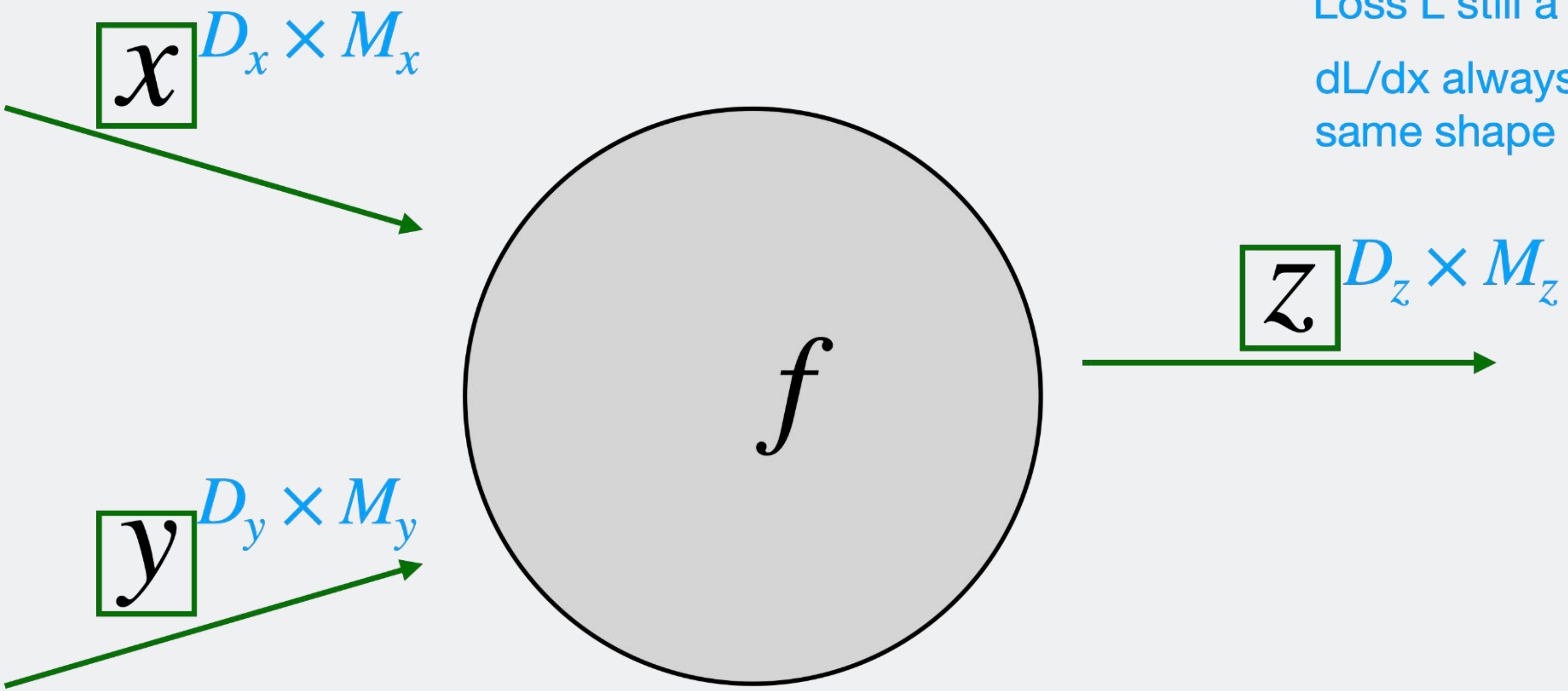
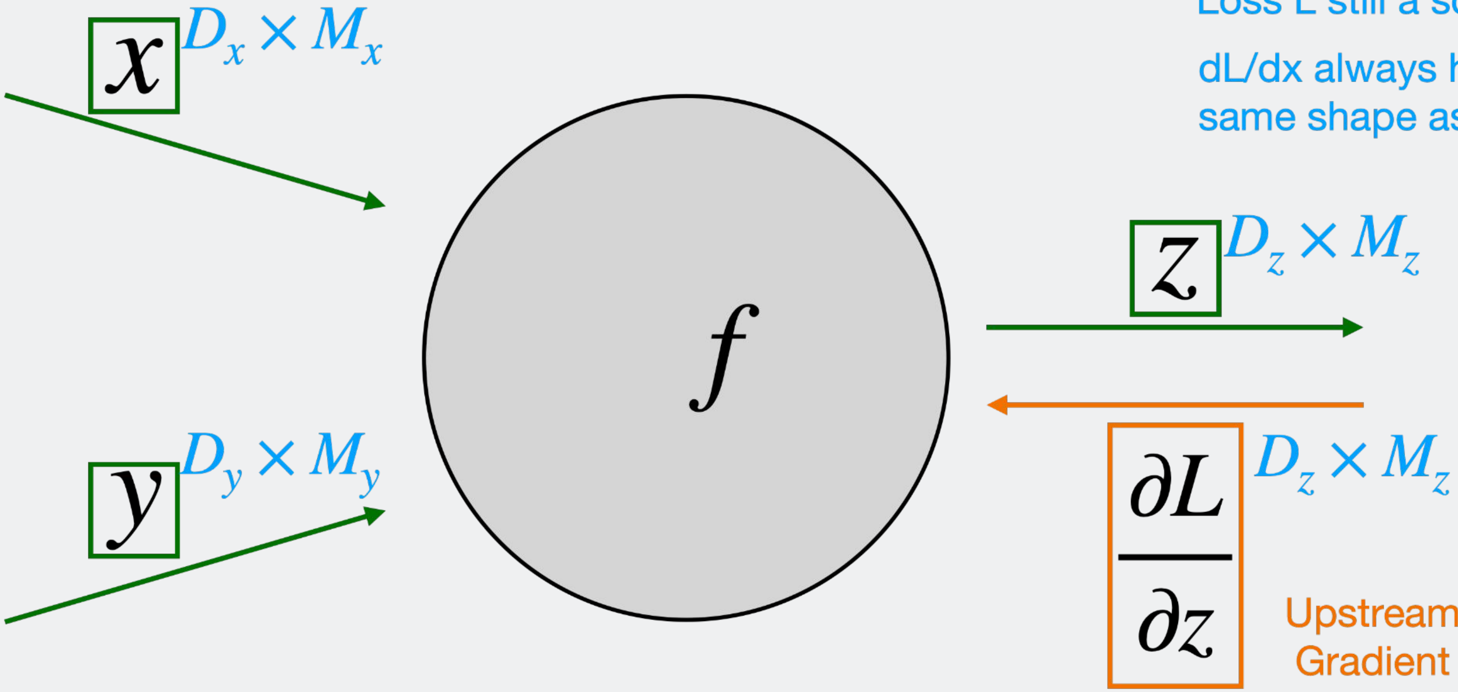
Backprop with Matrices (or Tensors)

Loss L still a scalar!

dL/dx always has the same shape as x!



Backprop with Matrices (or Tensors)



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

Backprop with Matrices (or Tensors)

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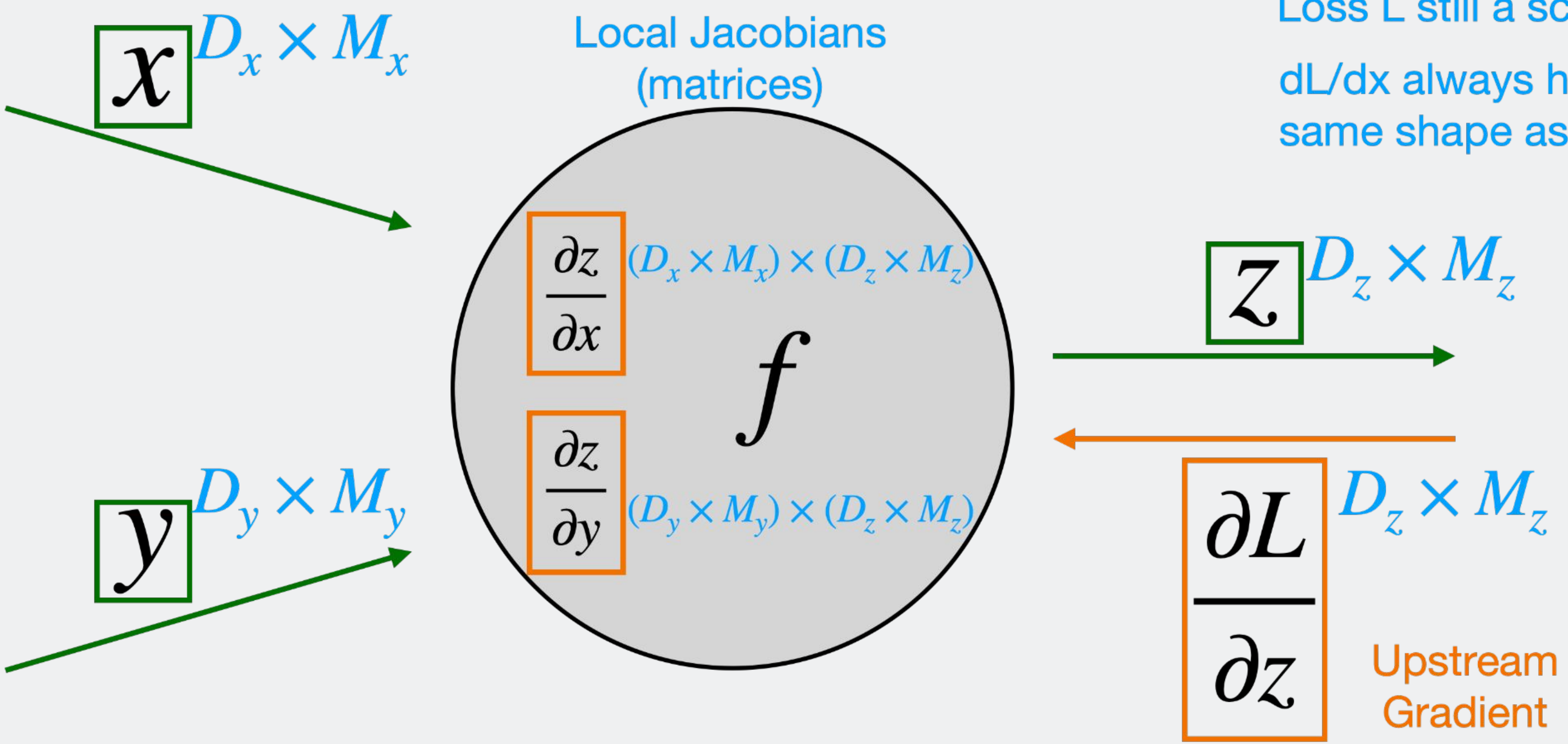

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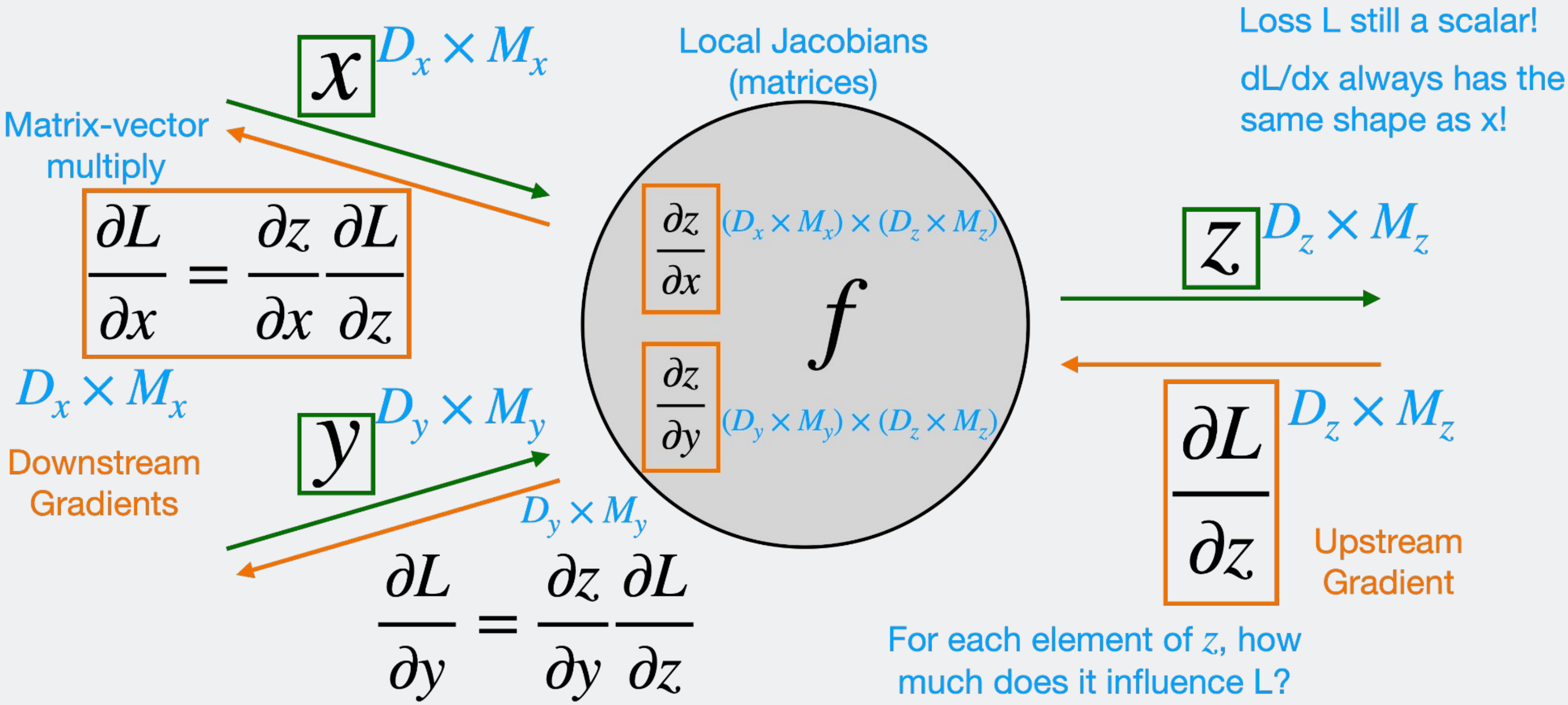
Backprop with Matrices (or Tensors)



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 $y = xw$

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

→

y: [N×M]

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

ROBOTICS

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

M ROBOTICS

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dL/dx: [N×D]

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

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

x: [N×D]

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w: [D×M]

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

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dL/dx: [N×D]

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

Local Gradient Slice:

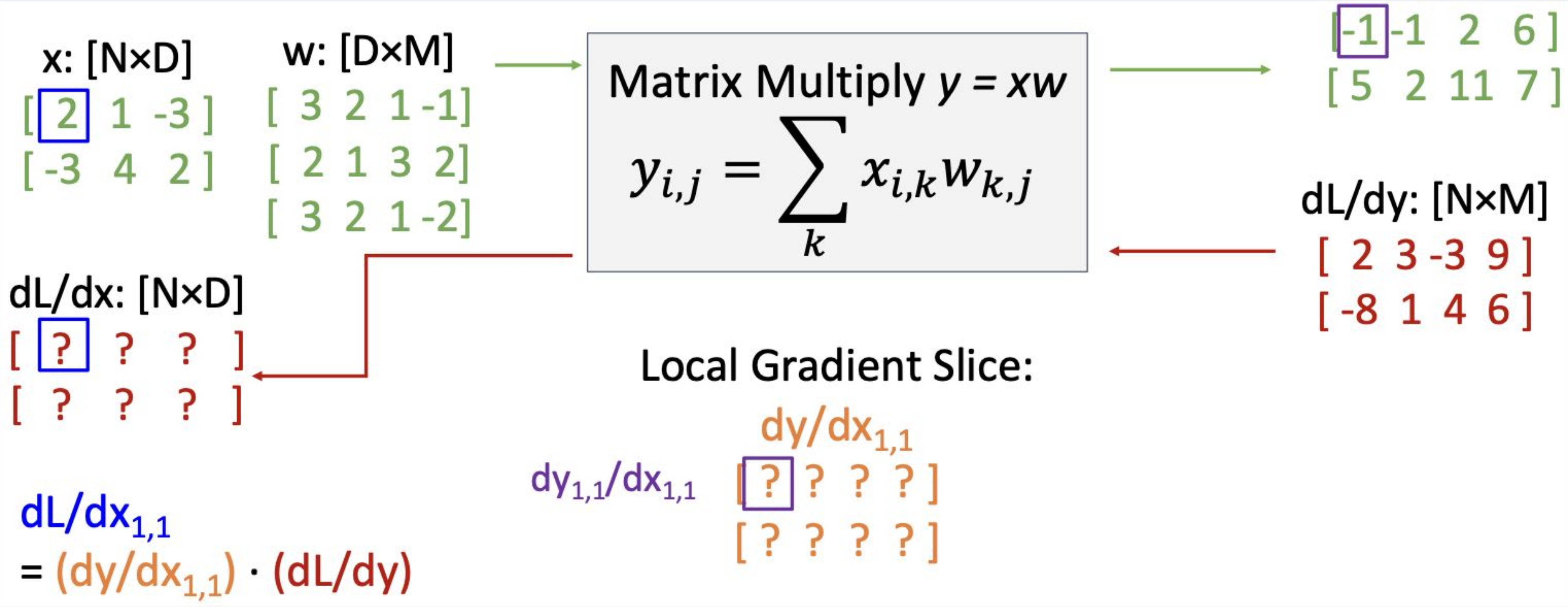
$dy/dx_{1,1}$

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

$dL/dx_{1,1}$

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

Example: Matrix Multiplication



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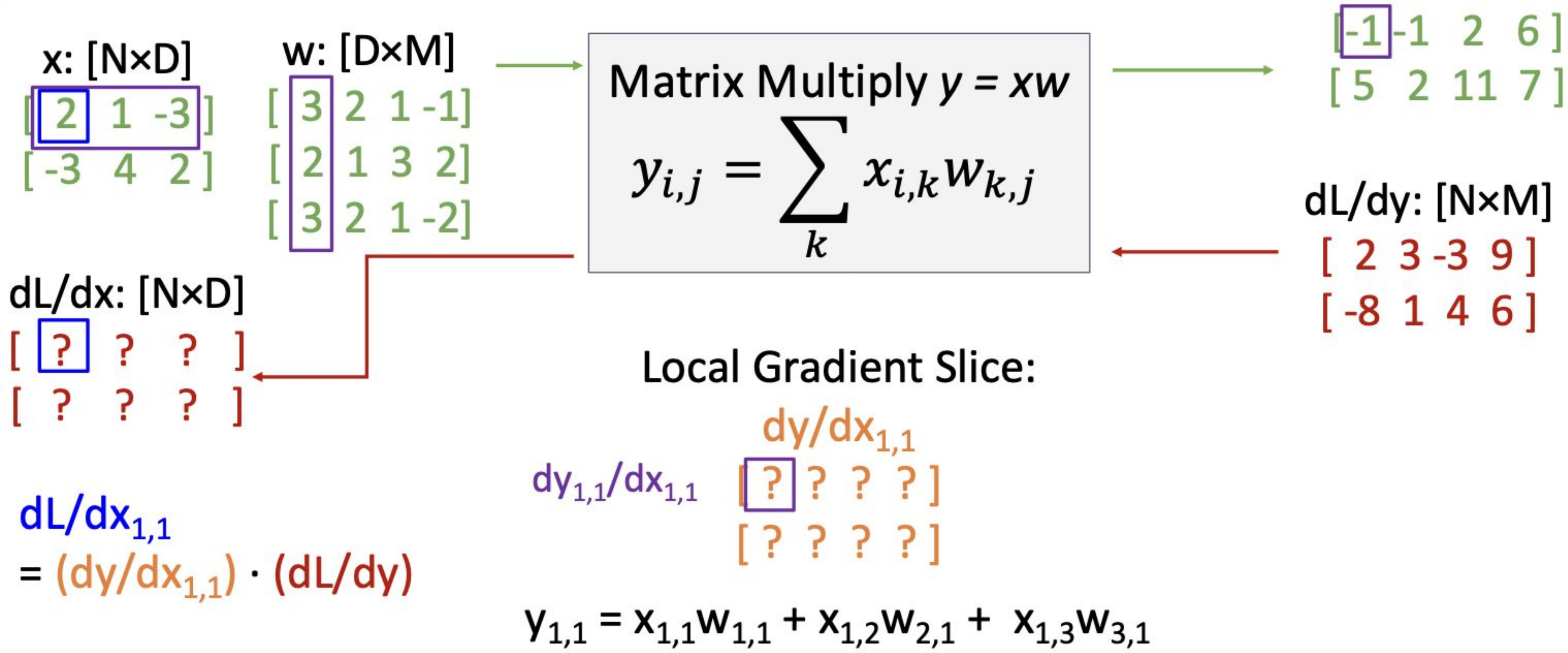

Example: Matrix Multiplication

x: [N×D]

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w: [D×M]

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

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

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

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:

$dy/dx_{1,1}$

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

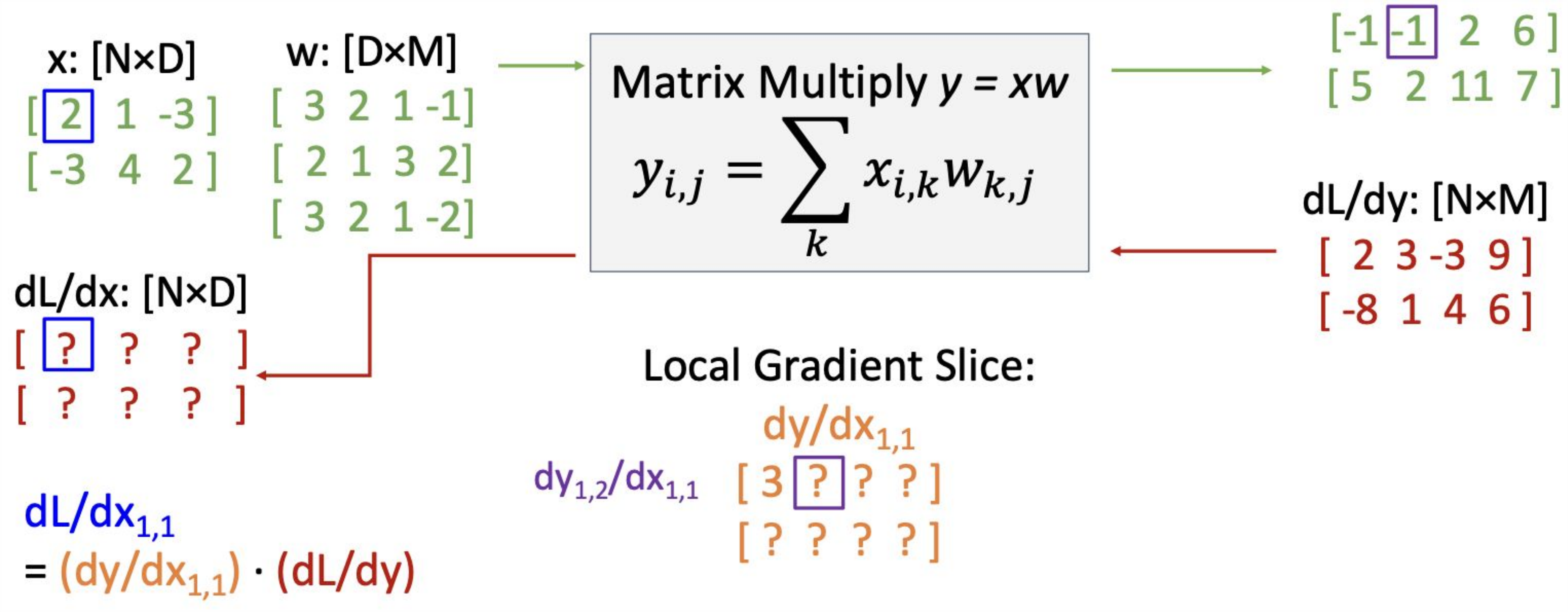
$dL/dx_{1,1}$

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

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

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

Example: Matrix Multiplication



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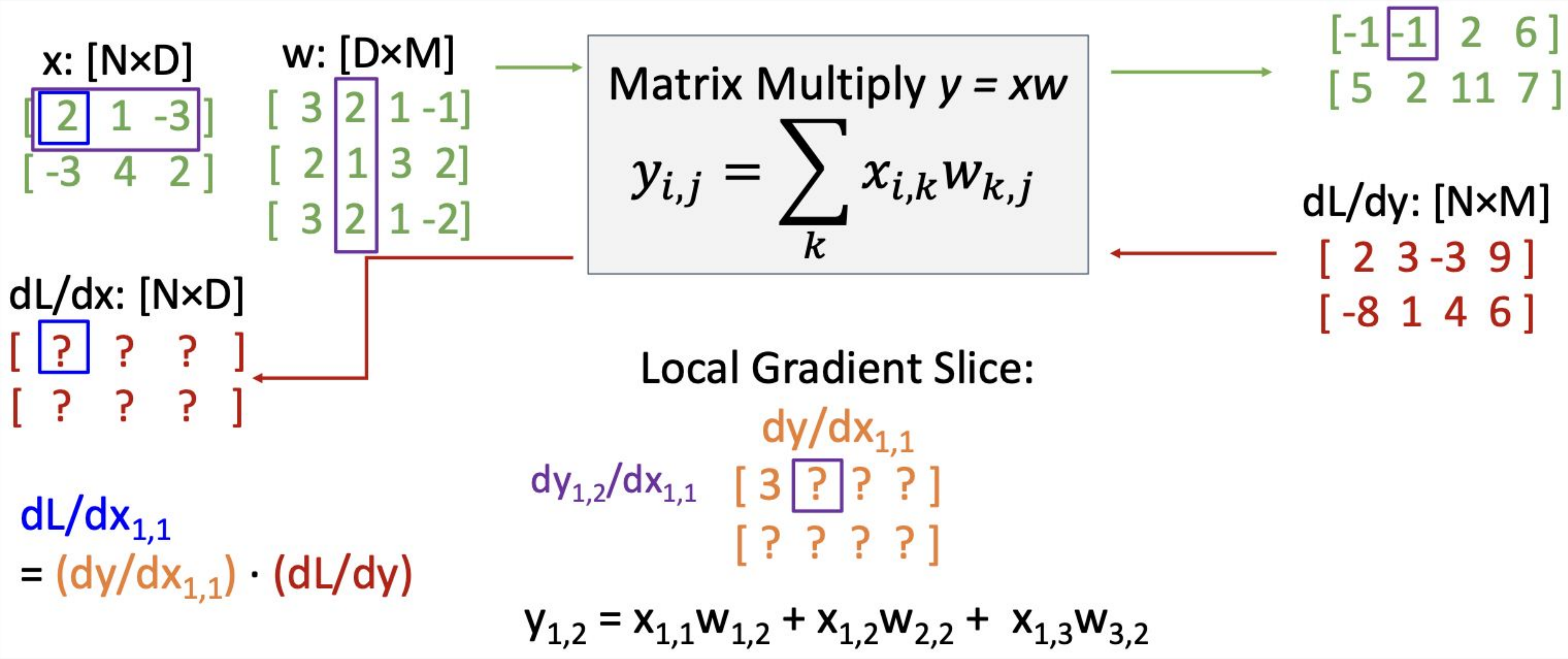

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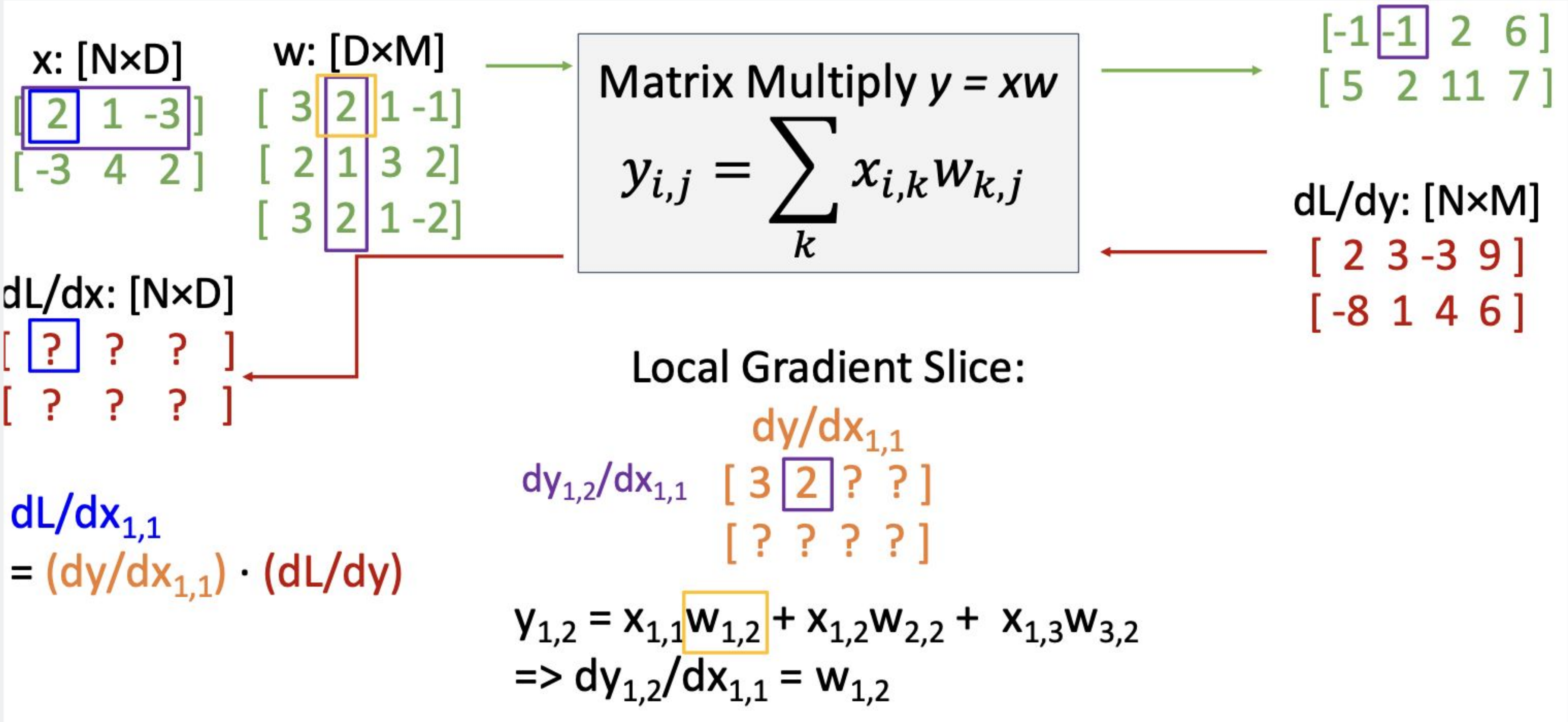

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$$\begin{bmatrix} -1 & -1 & 2 & 6 \\ 5 & 2 & 11 & 7 \end{bmatrix}$$

dL/dy: [N×M]

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dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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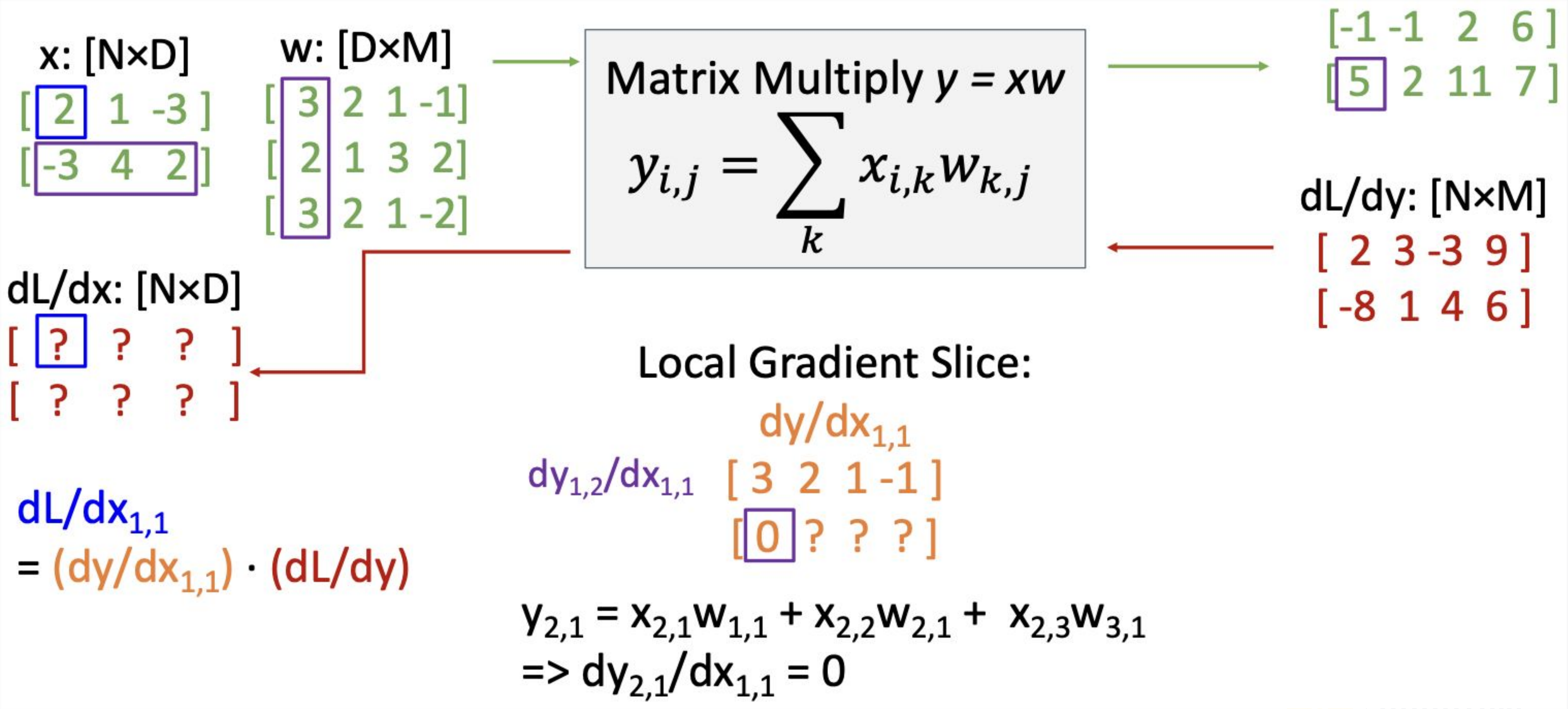
$dL/dx_{1,1}$

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

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

Example: Matrix Multiplication



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

dL/dx: [N×D]

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

Local Gradient Slice:

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

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

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dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{1,1}$

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

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Example: Matrix Multiplication

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w: [D×M]

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Matrix Multiply $y = xw$

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

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

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 $y = xw$

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

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

$dL/dx_{2,3}$

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

ROBOTICS

Example: Matrix Multiplication

x: [N×D]

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

w: [D×M]

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

Matrix Multiply $y = xw$

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

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

Local Gradient Slice:

$dy/dx_{2,3}$

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

$dL/dx_{2,3}$

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

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

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

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 $y = xw$

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

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

$dL/dx_{i,j}$

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

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

Example: Matrix Multiplication

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dL/dx: [N×D]

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

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

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

$dL/dx_{i,j}$

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

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

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 $y = xw$

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

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

dL/dy: [N×M]

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

dL/dx: [N×D]

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

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

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

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

Backpropagation: Another View

$$
\begin{array}{ccccccccc}
x_0 & \xrightarrow{\quad f_1 \quad} & x_1 & \xrightarrow{\quad f_2 \quad} & x_2 & \xrightarrow{\quad f_3 \quad} & x_3 & \xrightarrow{\quad f_4 \quad} & L \\
D_0 & & D_1 & & D_2 & & D_3 & & \text{scalar}
\end{array}
$$

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

$$\begin{array}{ccccccccc} x_0 & \xrightarrow{f_1} & x_1 & \xrightarrow{f_2} & x_2 & \xrightarrow{f_3} & x_3 & \xrightarrow{f_4} & L \\ D_0 & & D_1 & & D_2 & & D_3 & & \text{scalar} \end{array}$$

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

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

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

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

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

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>

Reverse-Mode Automatic Differentiation

$$\begin{array}{ccccccccc} x_0 & \xrightarrow{f_1} & x_1 & \xrightarrow{f_2} & x_2 & \xrightarrow{f_3} & x_3 & \xrightarrow{f_4} & L \\ D_0 & & D_1 & & D_2 & & D_3 & & \text{scalar} \end{array}$$

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

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

Forward-Mode Automatic Differentiation

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

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

Chain rule

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

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

Beta implementation in PyTorch! https://pytorch.org/tutorials/intermediate/forward_ad_usage.html

Chain rule

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

You can also implement forward-mode AD using two calls to reverse-mode AD! (Inefficient but elegant)

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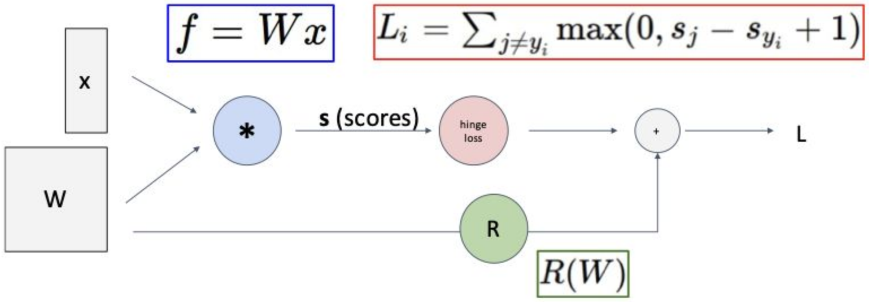
Summary

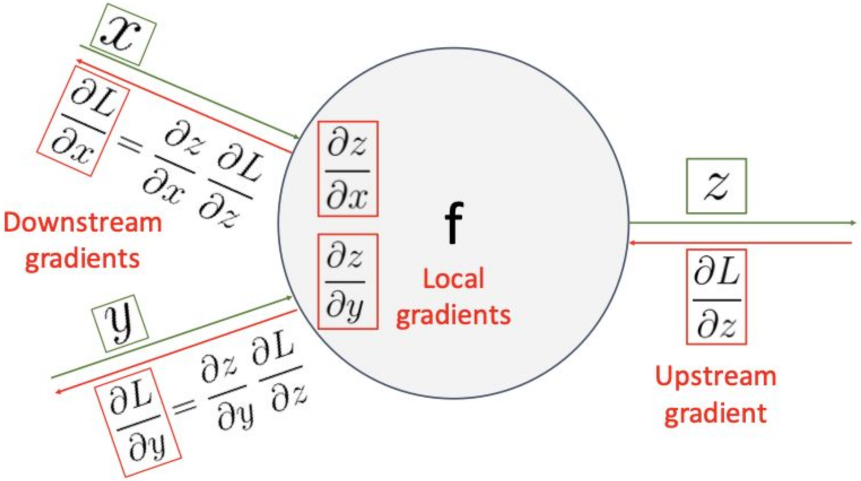
Represent complex expressions as **computational graphs**



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

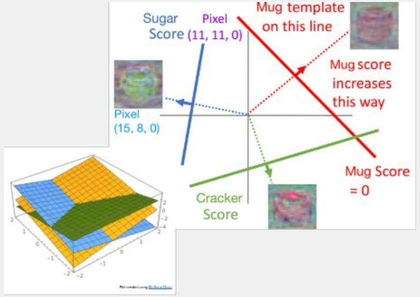
```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)

  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

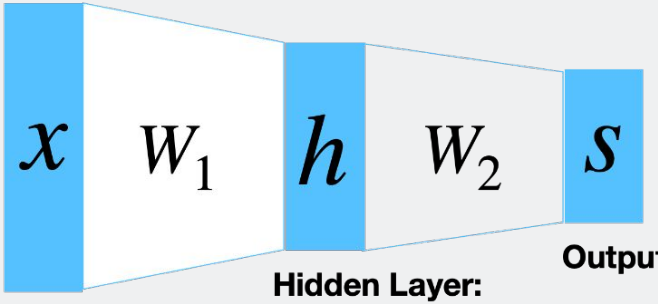
```
class Multiply(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x, y):
    ctx.save_for_backward(x, y)
    z = x * y
    return z
  @staticmethod
  def backward(ctx, grad_z):
    x, y = ctx.saved_tensors
    grad_x = y * grad_z   # dz/dx * dL/dz
    grad_y = x * grad_z   # dz/dy * dL/dz
    return grad_x, grad_y
```

Summary



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

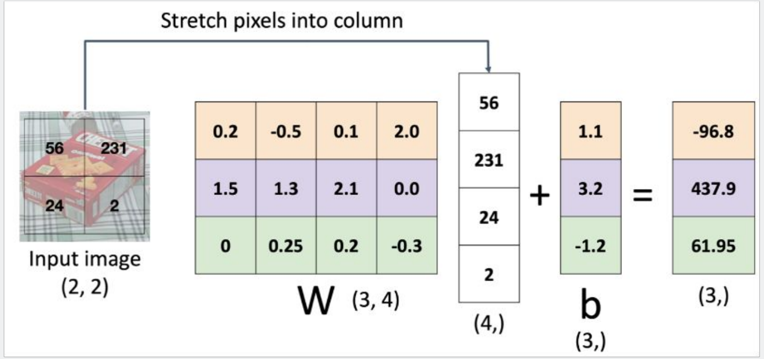
Input: 3072



Output:10

Hidden Layer: 100

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



Next up: Convolutional Neural Networks

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