# CS 4644 / 7643-A: LECTURE 5
# DANFEI XU

Topics:

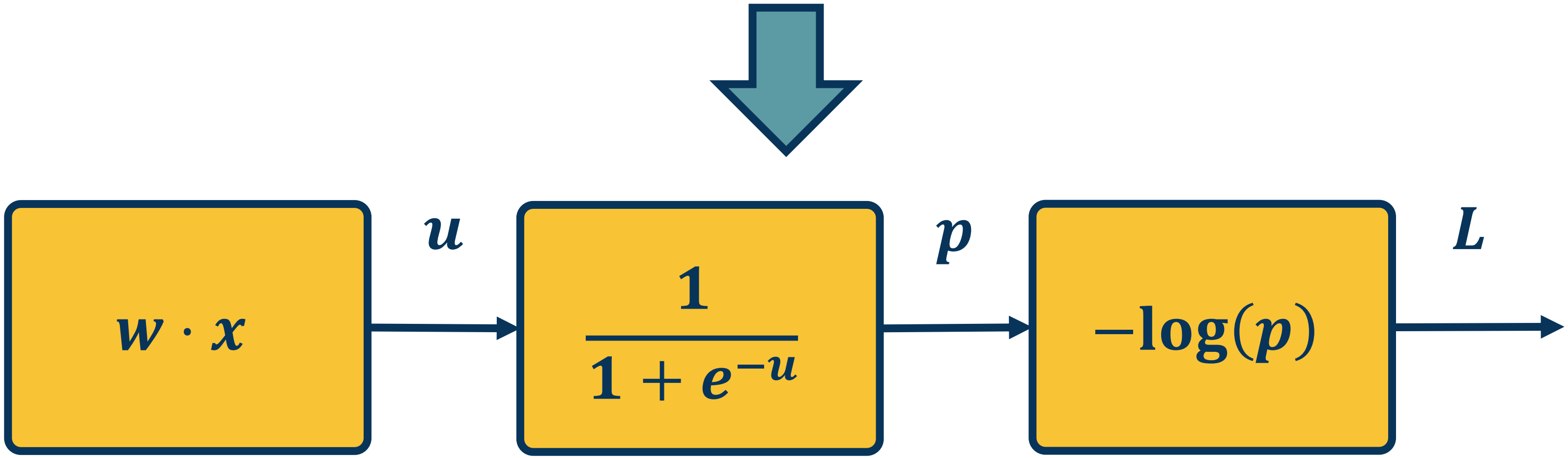
- Backpropagation
- Neural Networks
- Jacobians

- **PS1/HW1 are out! Due Sep 19th**

- **Project:**
  - Teaming thread on piazza
  - Proposal due Sep 26th
  - Will send out instruction soon

- Next lecture will be on how to pick a project

$$-\log\left(\frac{1}{1+e^{-w\cdot x}}\right)$$




*Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun*

# Machine Learning Example


$$\frac{\partial L}{\partial w} = \frac{\partial L}{\partial p}\frac{\partial p}{\partial u}\frac{\partial u}{\partial w}$$

Chain rule and Backpropagation!

*Adapted from slides by: Marc'Aurelio Ranzato, Yann LeCun*

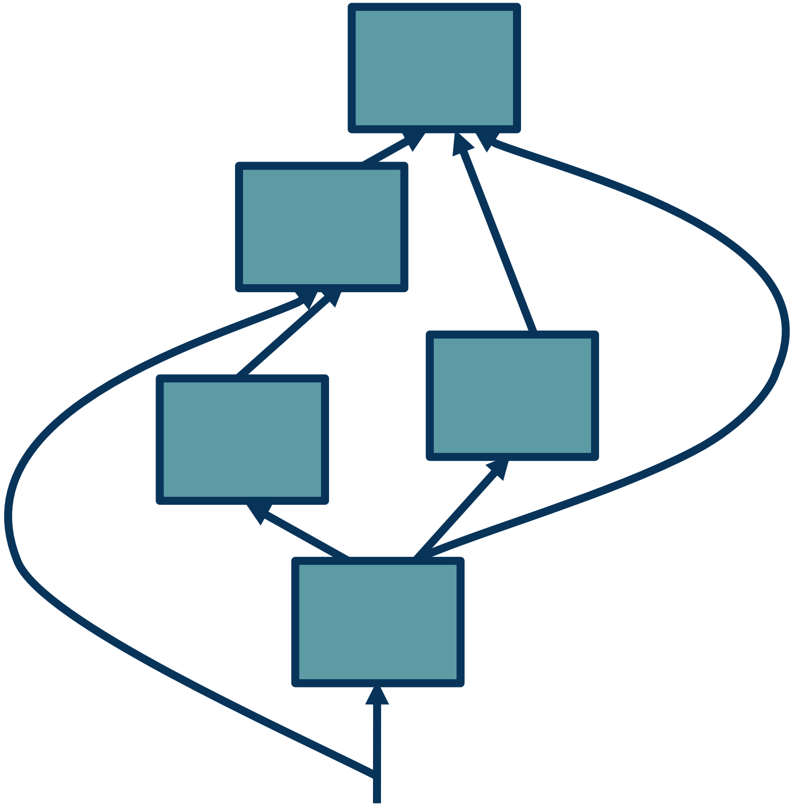
# Recap: Computation Graph

We will view the function / model as a **computation graph**

**Key idea**: break a complex model into atomic computation nodes that can be computed efficiently.

Graph can be any **directed acyclic graph (DAG)**

- Modules must be differentiable to support gradient computations for gradient descent



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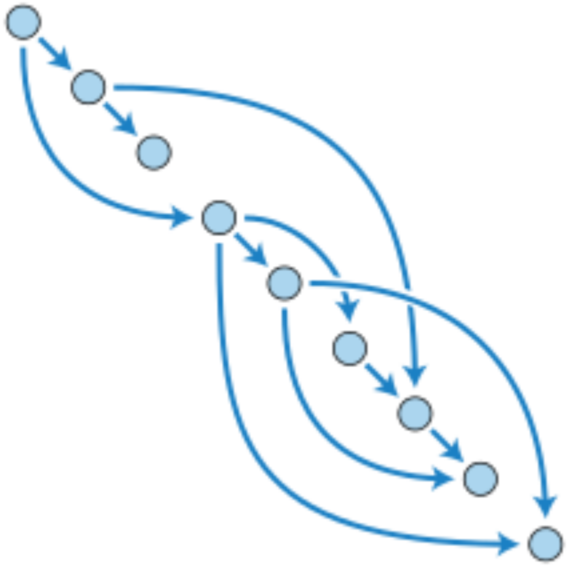
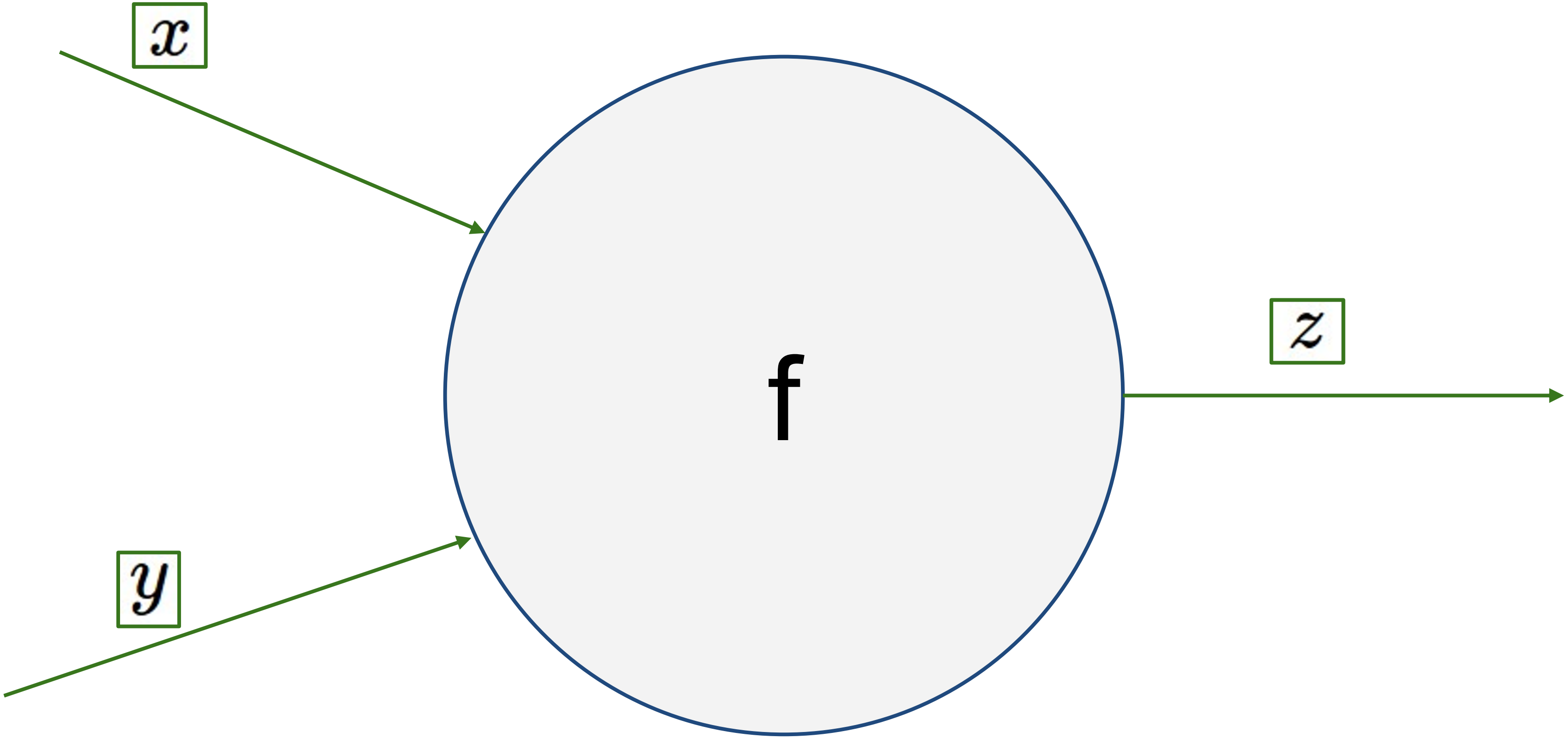
# Directed Acyclic Graphs (DAGs)



# A computation node

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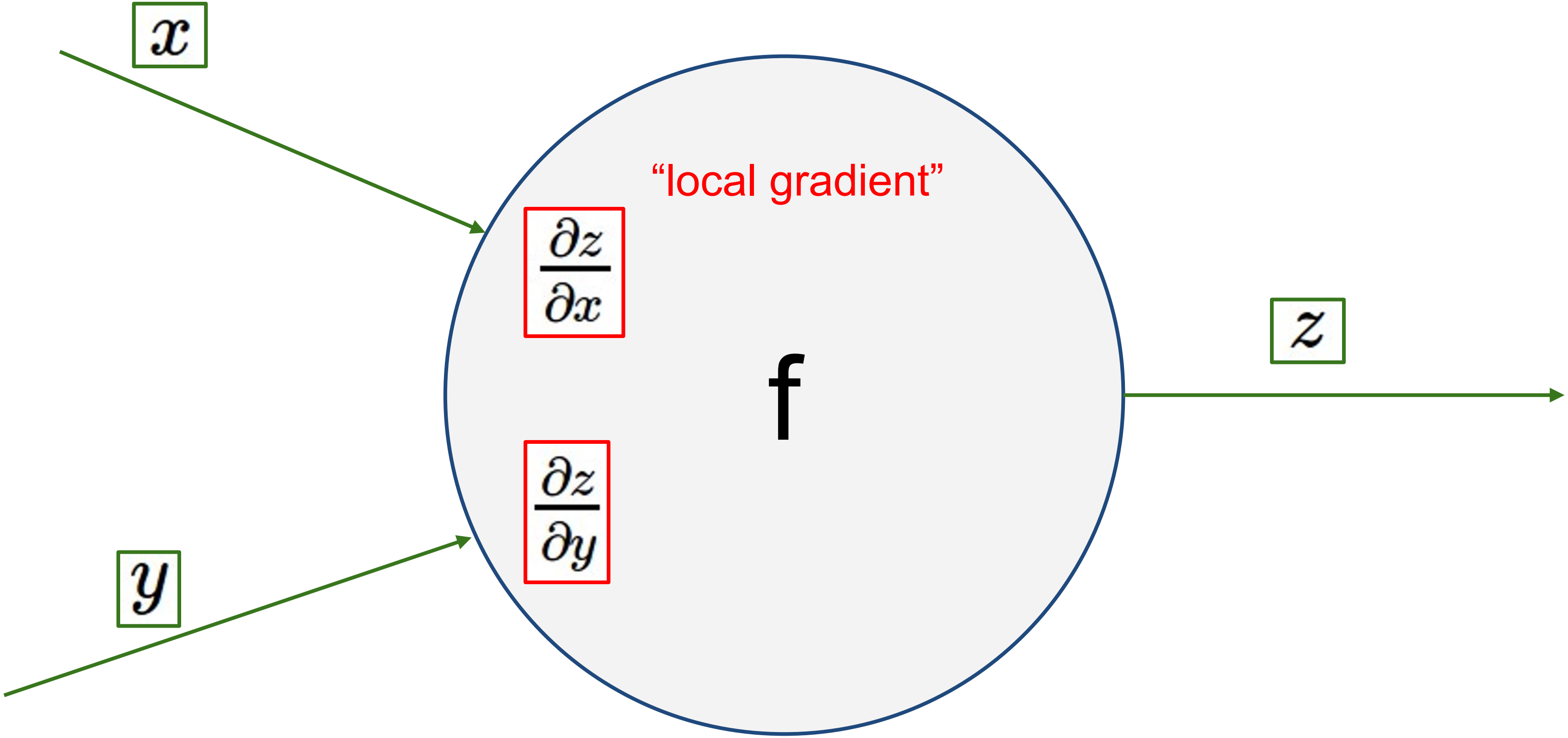
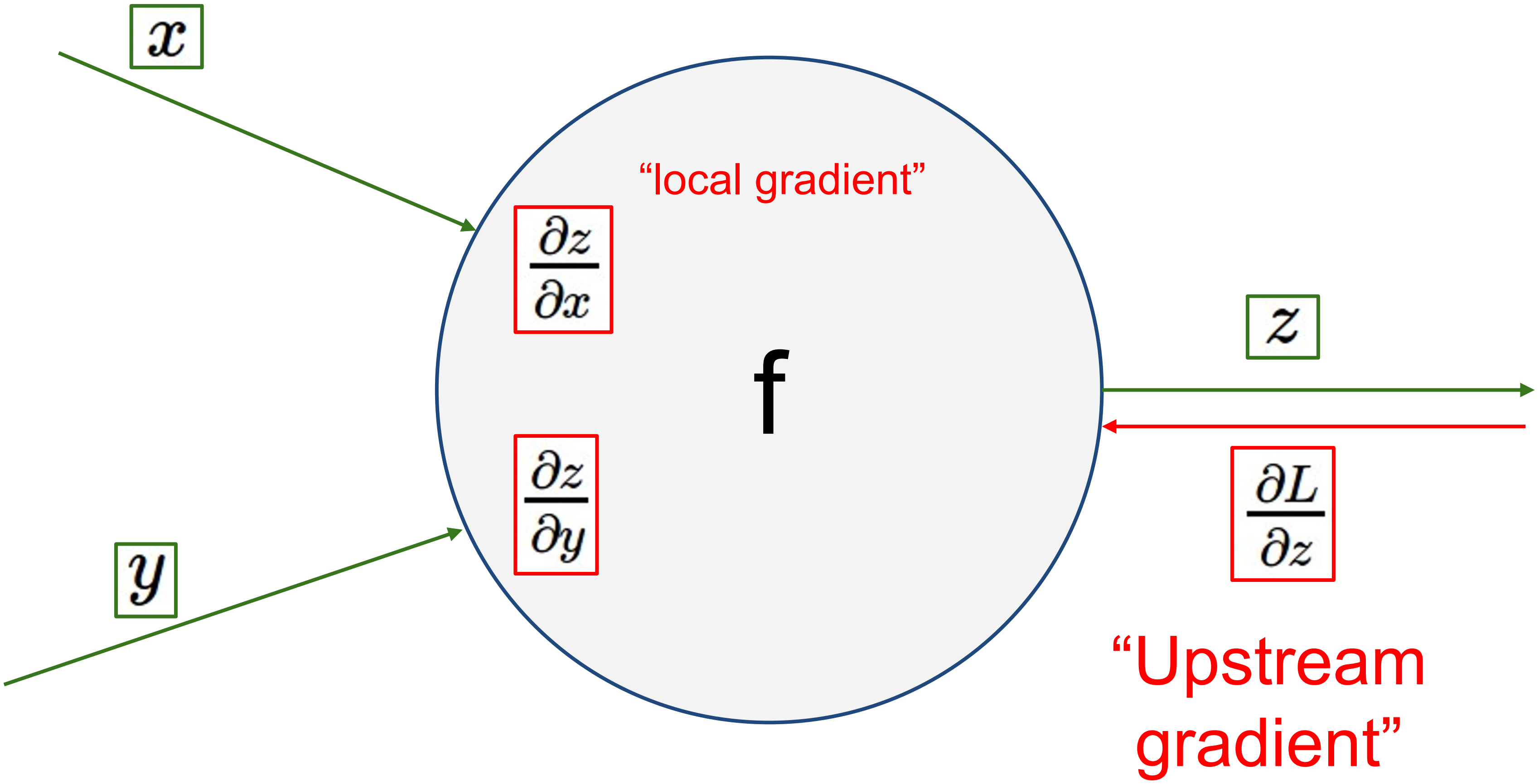

x
"local gradient"
∂z/∂x
f
z
∂z/∂y
y

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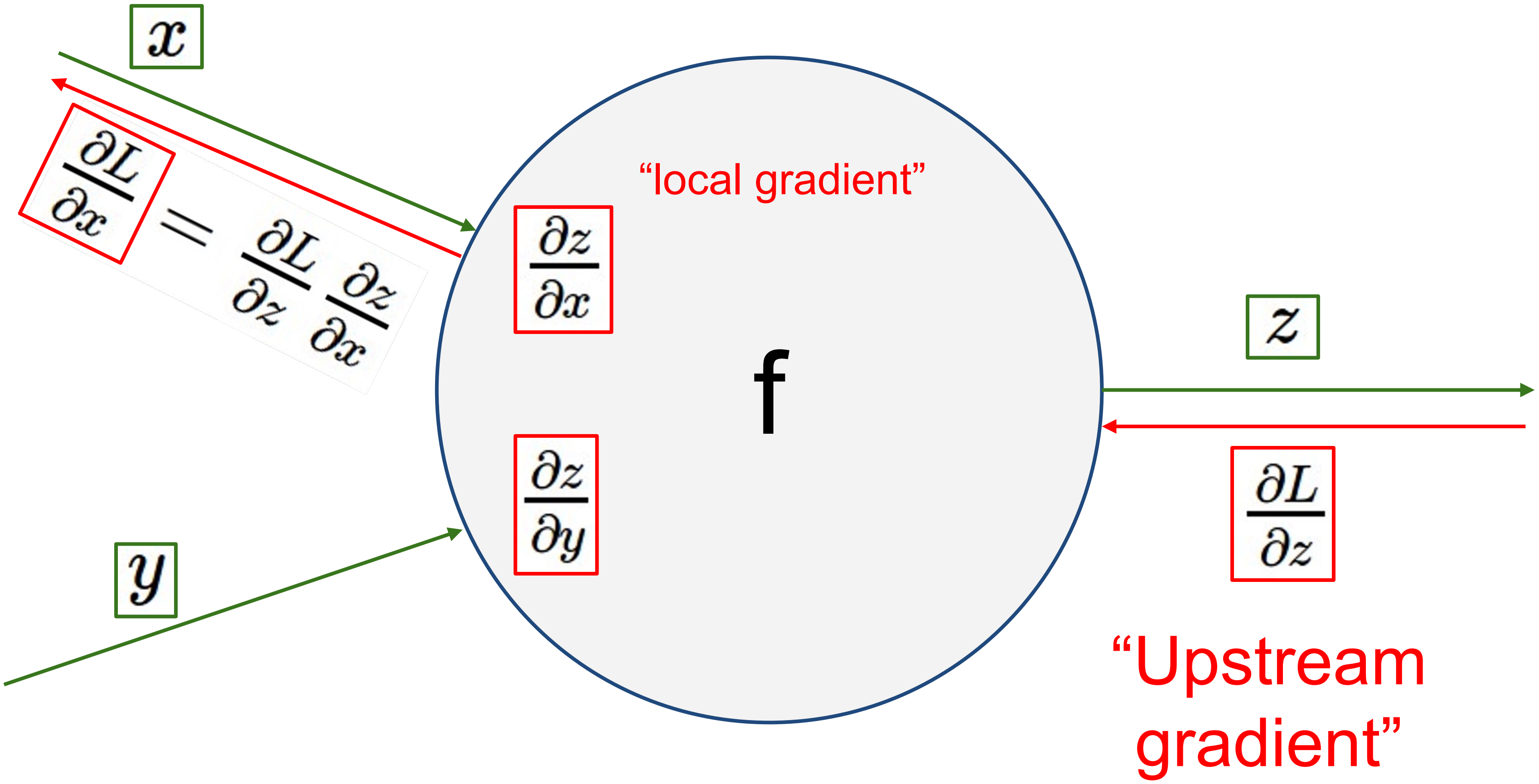


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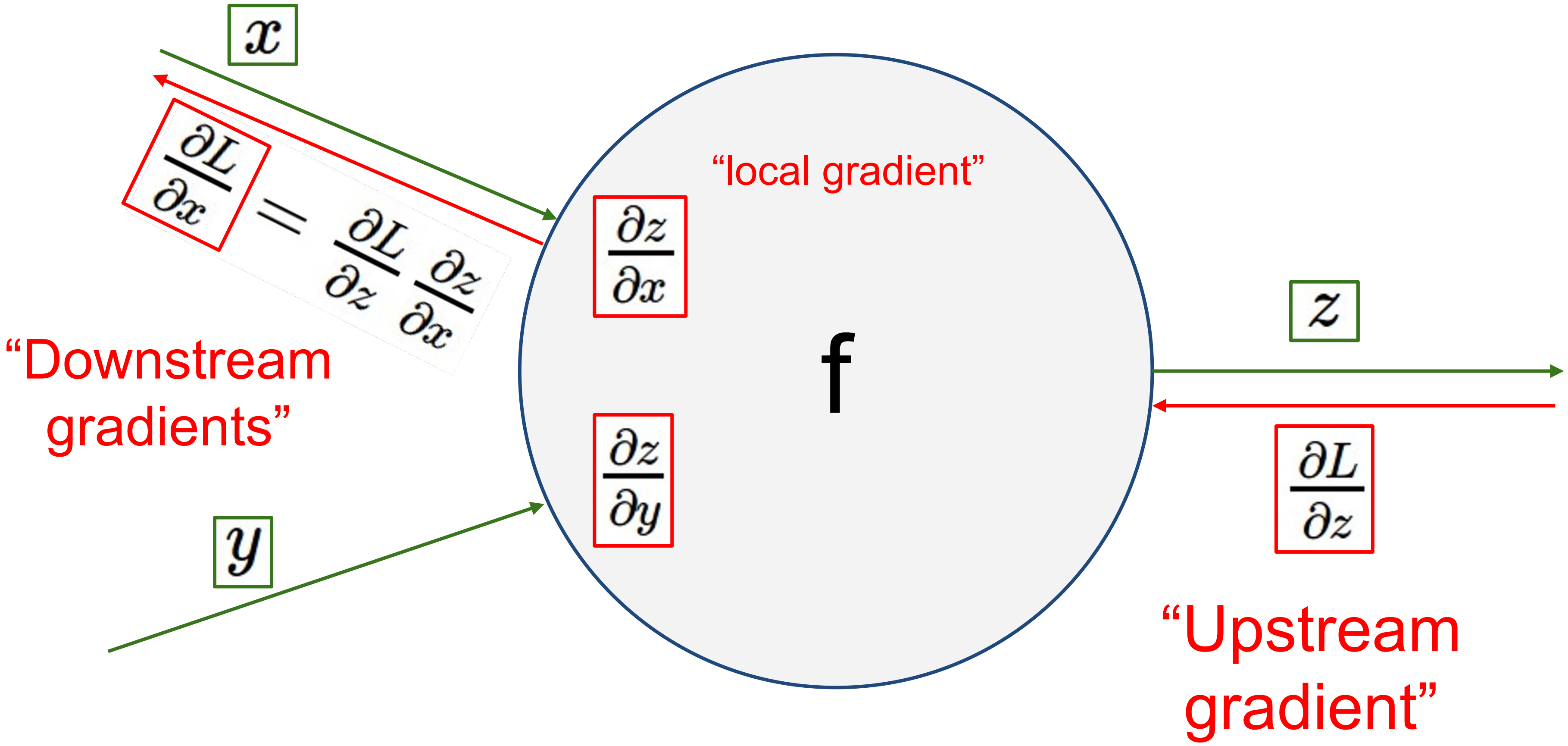


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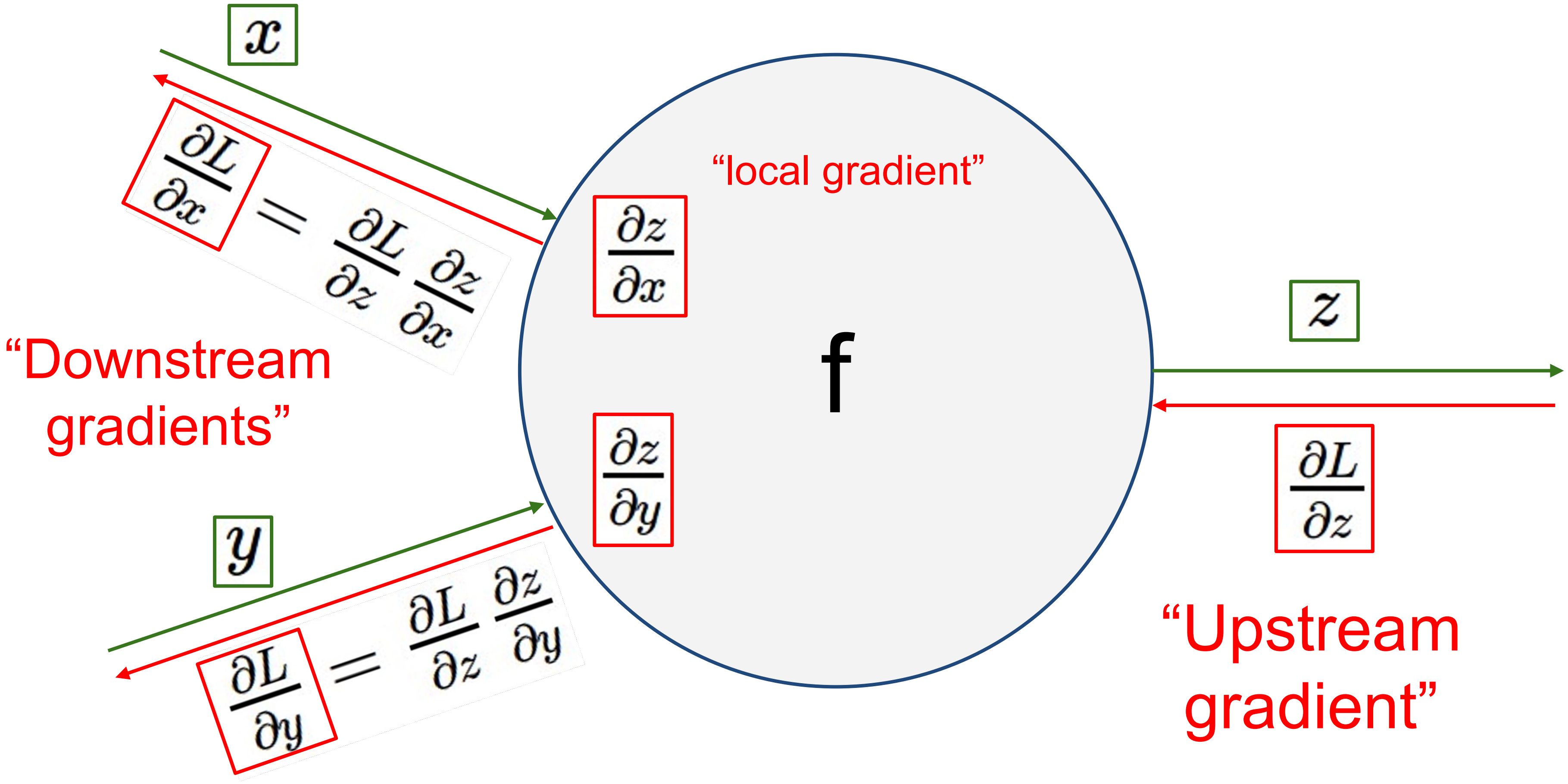


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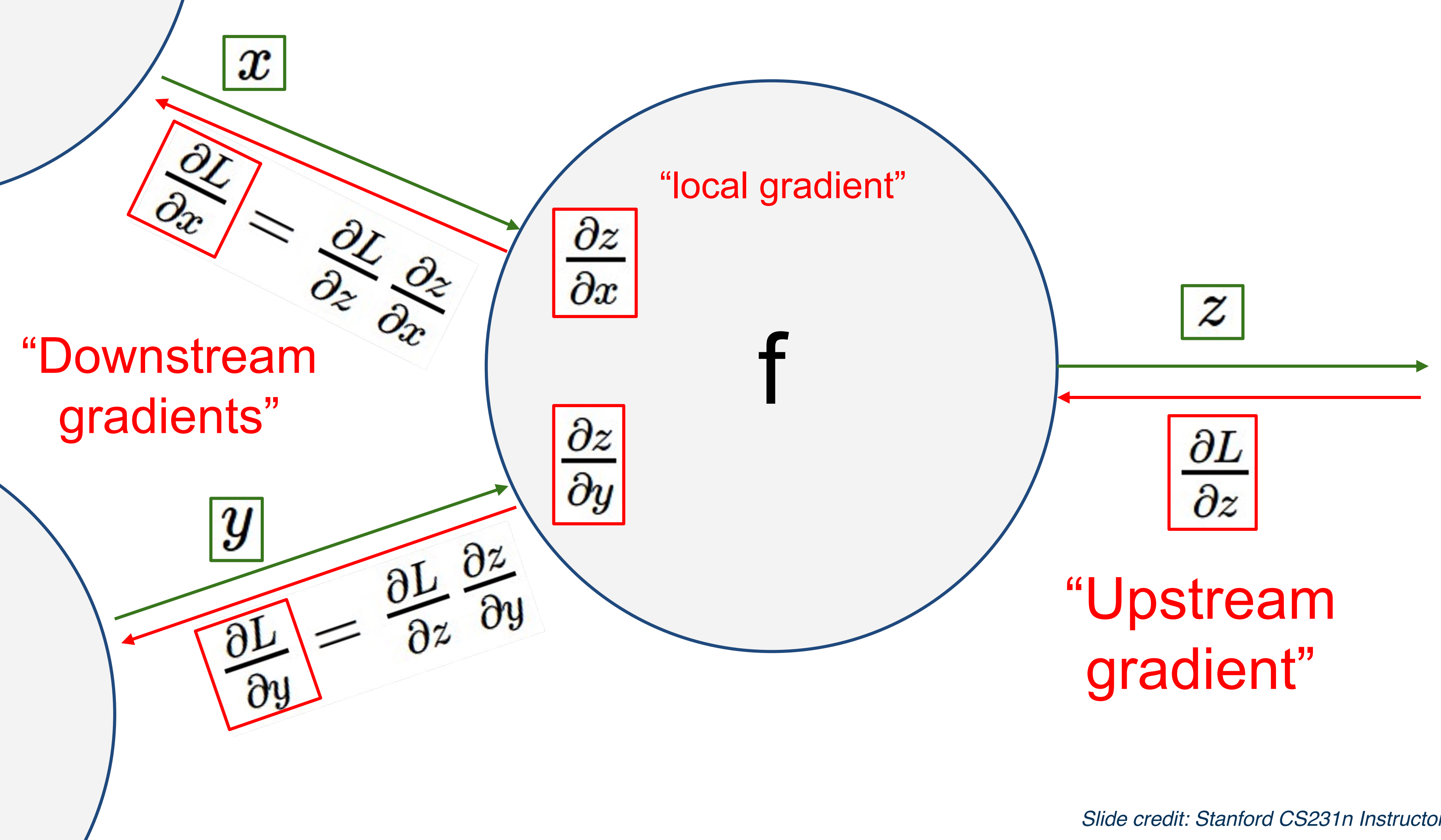


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# Backpropagation: a simple example

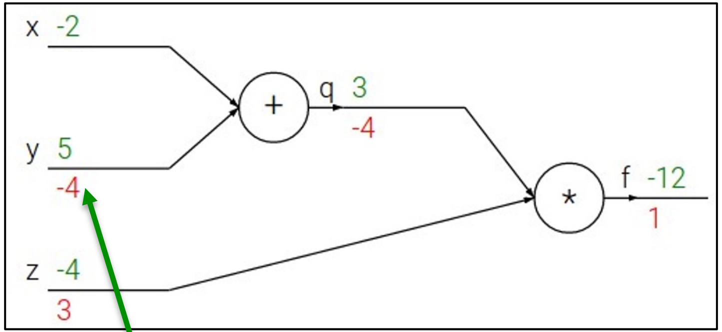
$$f(x,y,z) = (x+y)z$$

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

$$\boxed{q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1}$$

$$\boxed{f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q}$$

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




Chain rule:

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

Upstream gradient

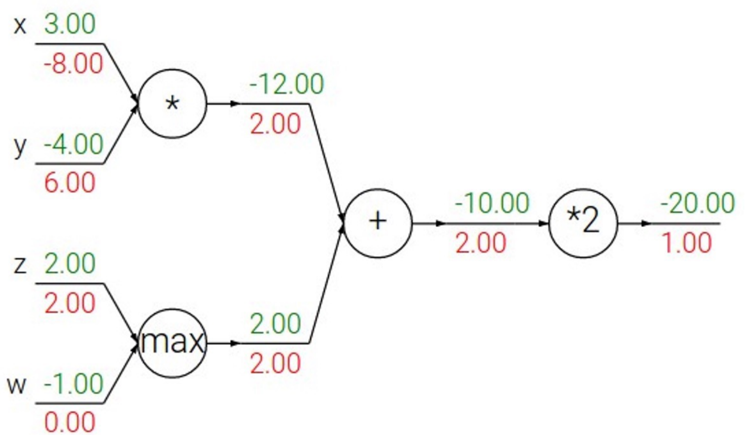
Local gradient

# Patterns in backward flow

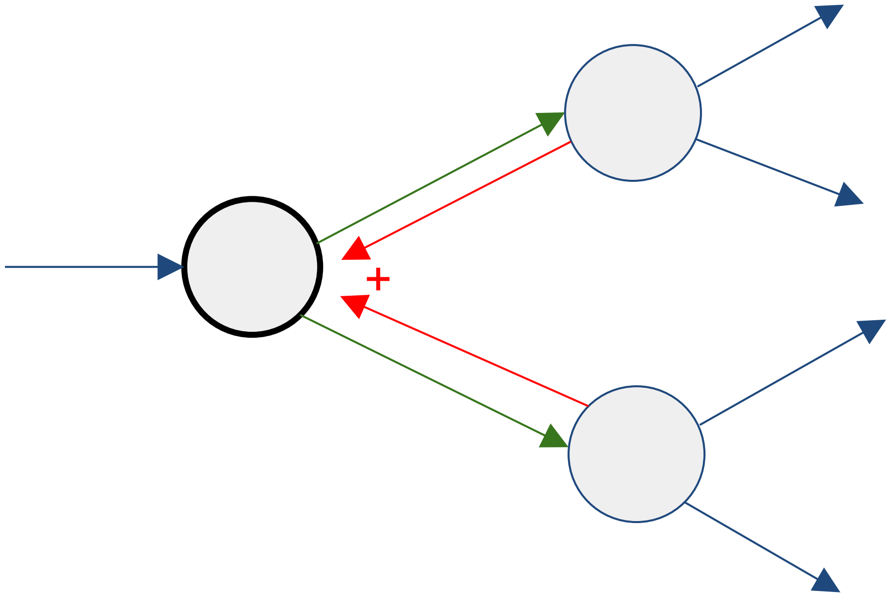
**add** gate: gradient distributor

**max** gate: gradient router

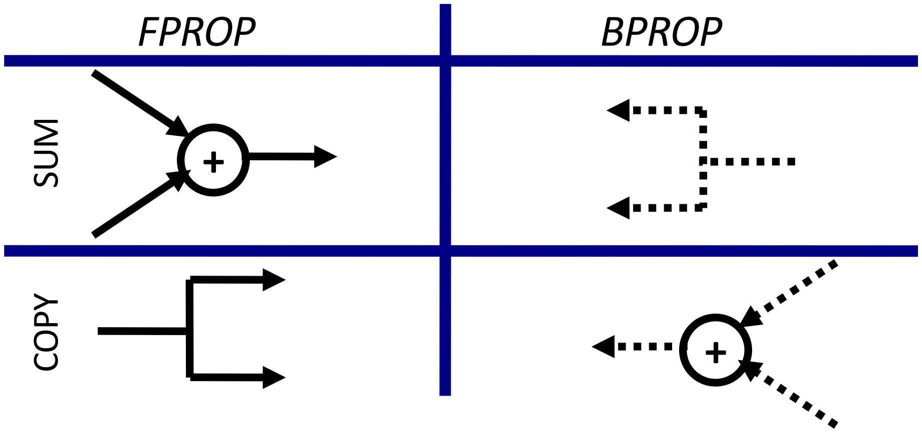
**mul** gate: gradient switcher



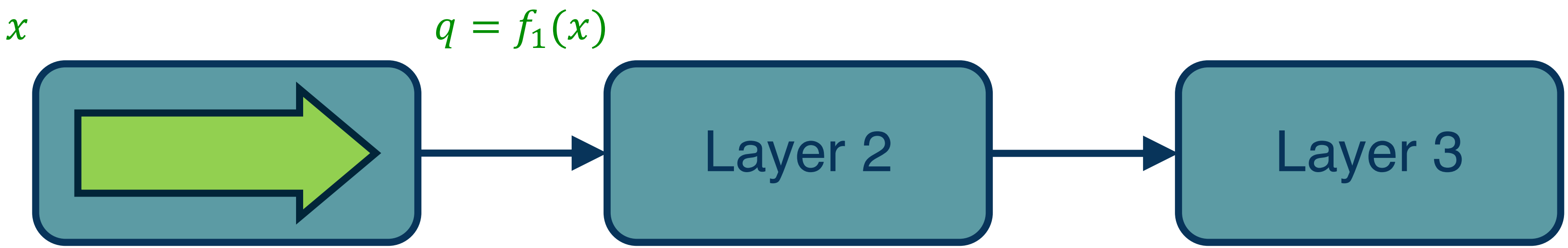
# Gradients add at branches



# Duality in Fprop and Bprop



## **Step 1:** Compute Loss on Mini-Batch: **Forward Pass**

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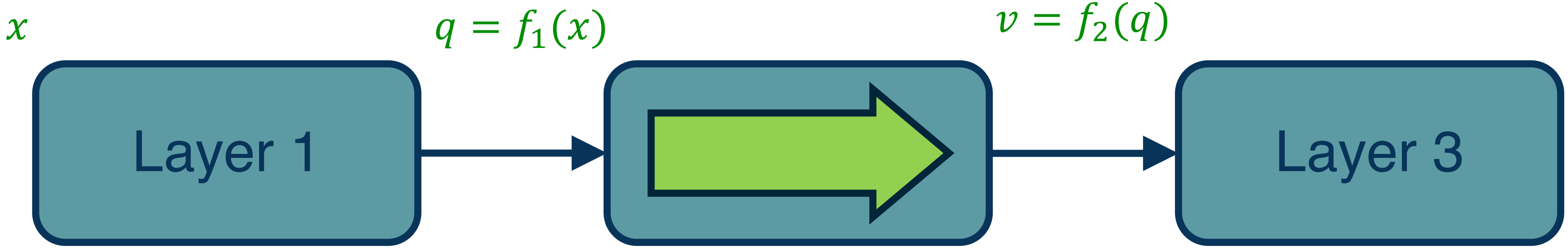
# **Step 1:** Compute Loss on Mini-Batch: **Forward Pass**

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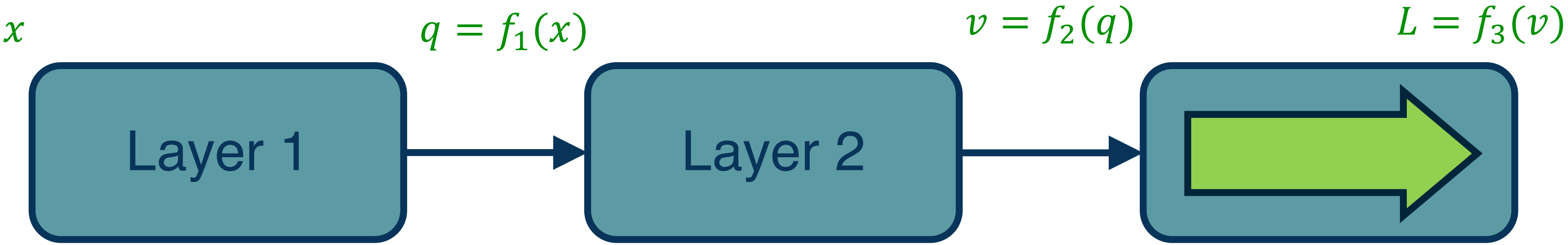
## **Step 1:** Compute Loss on Mini-Batch: **Forward Pass**



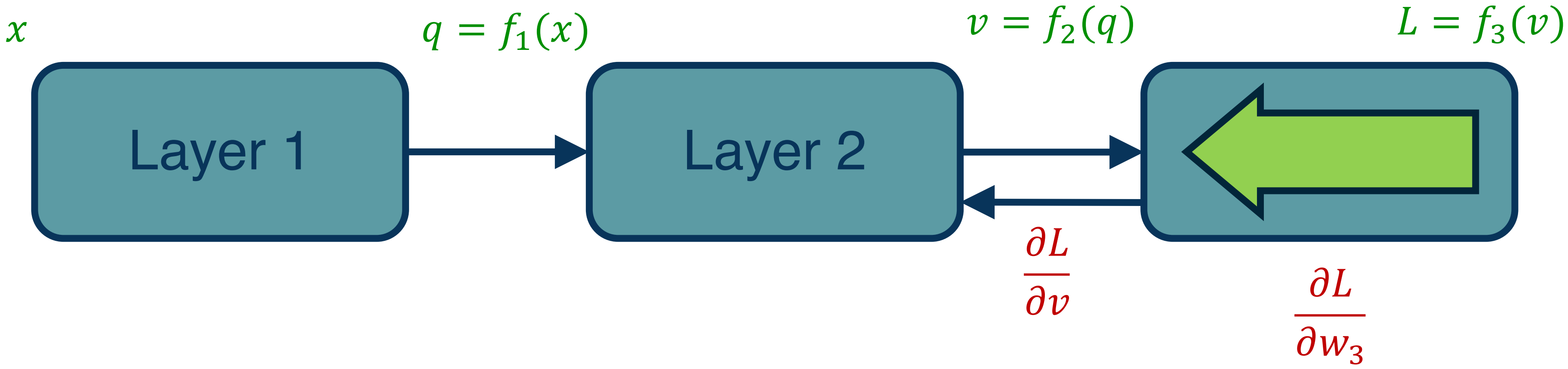

Note that we must store the **intermediate outputs of all layers**!

- This is because we will need them to **compute the gradients** (the gradient equations will have terms with the output values in them)

*Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun*

**Step 1:** Compute Loss on Mini-Batch: **Forward Pass**

**Step 2:** Compute Gradients wrt parameters: **Backward Pass**

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**Step 1:** Compute Loss on Mini-Batch: **Forward Pass**

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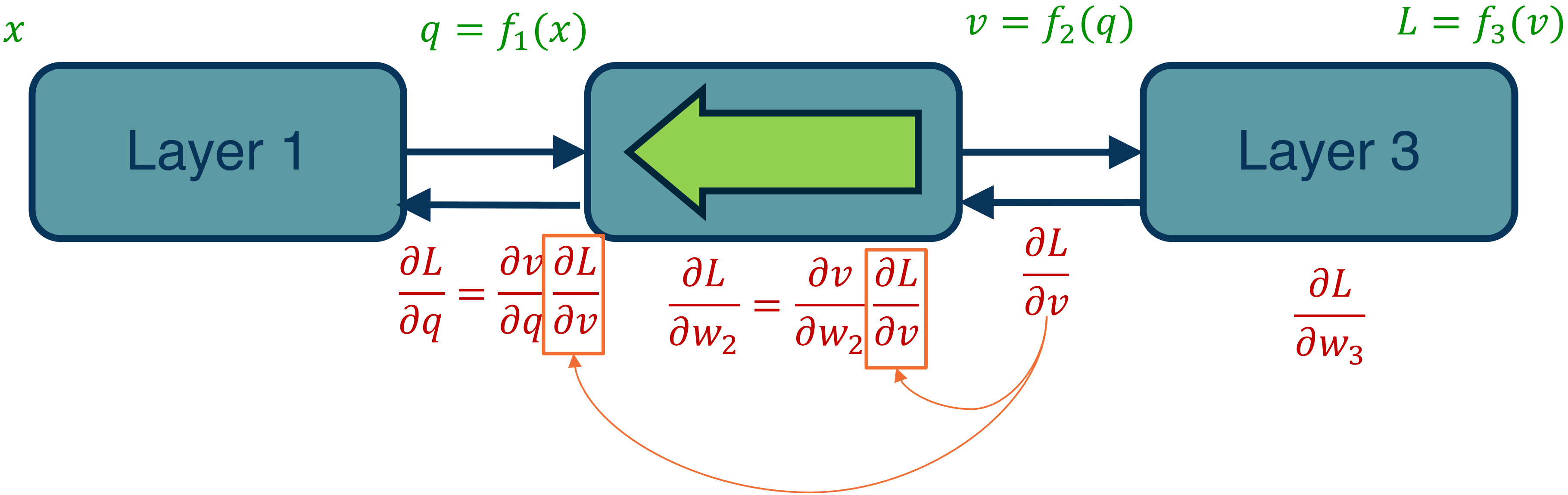


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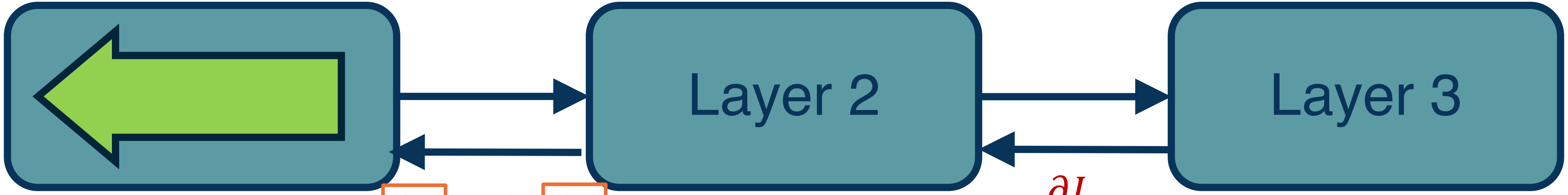
**Step 1:** Compute Loss on Mini-Batch: **Forward Pass**

**Step 2:** Compute Gradients wrt parameters: **Backward Pass**

$x$ $\qquad q = f_1(x) \qquad v = f_2(q) \qquad L = f_3(v)$



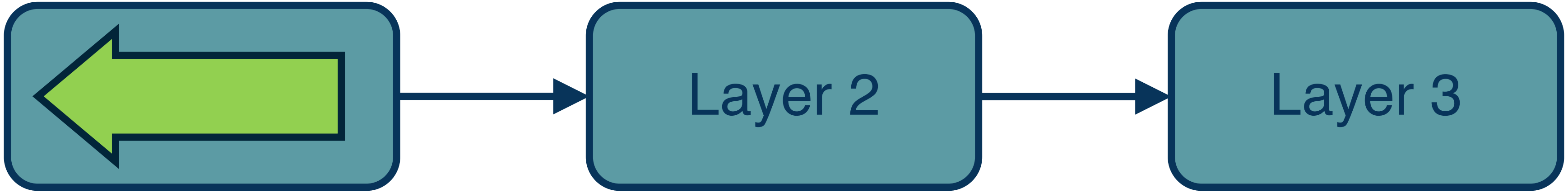

$$\frac{\partial L}{\partial w_3} = \frac{\partial v}{\partial w_3}\boxed{\frac{\partial L}{\partial q}} \qquad \boxed{\frac{\partial L}{\partial q}} = \frac{\partial v}{\partial q}\boxed{\frac{\partial L}{\partial v}} \qquad \frac{\partial L}{\partial w_2} = \frac{\partial v}{\partial w_2}\boxed{\frac{\partial L}{\partial v}} \qquad \frac{\partial L}{\partial v} \qquad \frac{\partial L}{\partial w_3}$$

*Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun*

**Step 1:** Compute Loss on Mini-Batch: **Forward Pass**

**Step 2:** Compute Gradients wrt parameters: **Backward Pass**

**Step 3:** Use **gradient** to update **all parameters** at the end




$$\frac{\partial L}{\partial w_1} \qquad \frac{\partial L}{\partial w_2} \qquad \frac{\partial L}{\partial w_3}$$

$$\boldsymbol{w_i = w_i - \alpha \frac{\partial L}{\partial w_i}}$$

Gradient Descent!

*Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun*

**So far:**

- **Linear classifiers**: a basic model
- **Loss functions**: measures performance of a model
- **Backpropagation**: an algorithm to calculate gradients of loss w.r.t. arbitrary differentiable function
- **Gradient Descent**: an iterative algorithm to perform gradient-based optimization

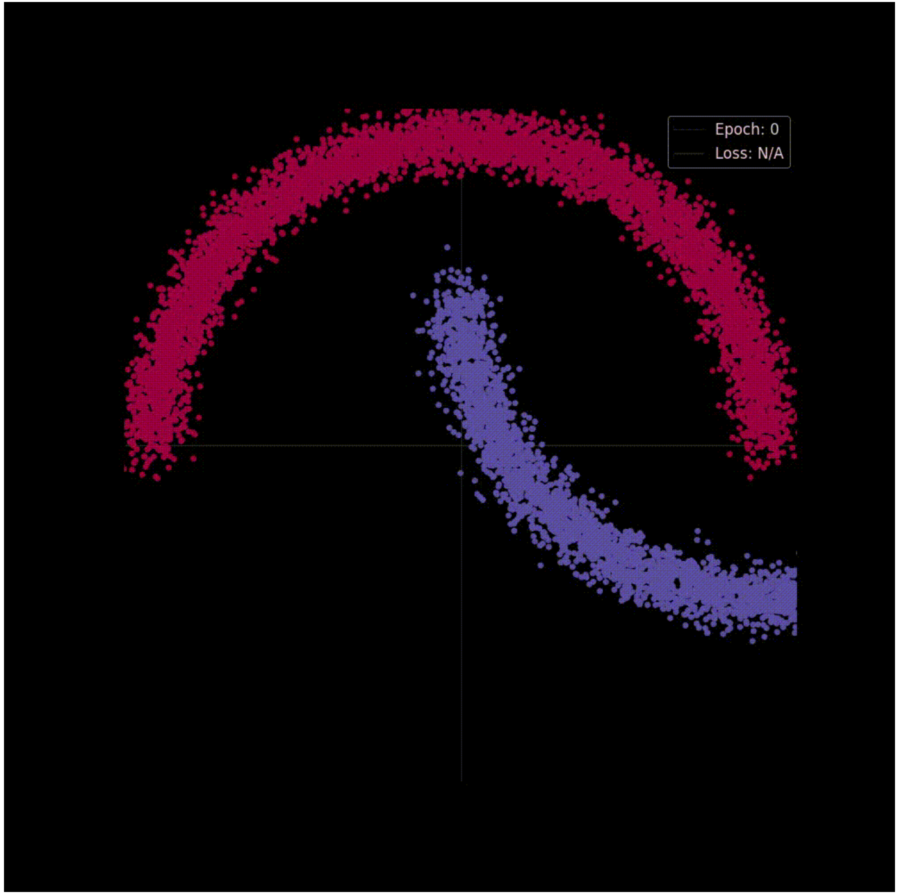
**Next:**

- What are neural networks?
- Non-linear functions
- How do we run backpropagation on neural nets?

# Deep Representation Learning

Want: a function that transforms complex raw data space into a linearly-separable space.

The function needs to be non-linear!


https://khalidsaifullaah.github.io/neural-networks-from-linear-algebraic-perspective

Neural Network

Linear classifier

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# Neural networks: the original linear classifier

(**Before**) Linear score function: $f = Wx$

$$x \in \mathbb{R}^D, W \in \mathbb{R}^{C \times D}$$

*Slide credit: Stanford CS231n Instructors*

# Neural networks: 2 layers

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \boxed{\max}(0, W_1 x)$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

(In practice we will usually add a learnable bias at each layer as well)

*Slide credit: Stanford CS231n Instructors*

# Neural networks: 3 layers

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$
or 3-layer Neural Network

$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

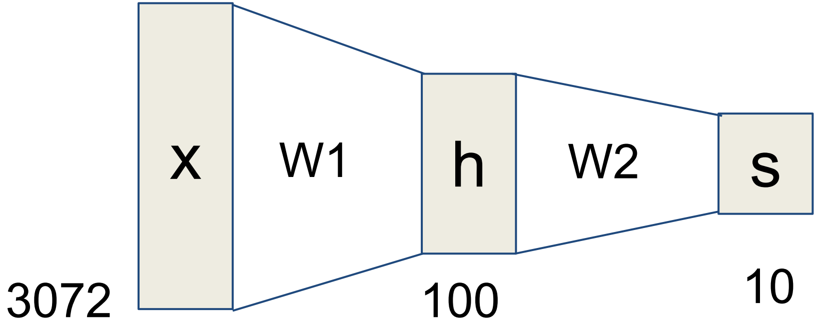
(In practice we will usually add a learnable bias at each layer as well)

*Slide credit: Stanford CS231n Instructors*

# Neural networks: hierarchical computation

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$




$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

*Slide credit: Stanford CS231n Instructors*

# Neural networks: why is max operator important?

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \boxed{\max(0,} W_1 x)$

The function $\max(0, z)$ is called the **activation function.**

**Q:** What if we try to build a neural network without one?

$$f = W_2 W_1 x$$

*Slide credit: Stanford CS231n Instructors*

# Neural networks: why is max operator important?

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \boxed{\max(0,} W_1 x)$

The function $\max(0, z)$ is called the **activation function.**
**Q:** What if we try to build a neural network without one?

$$f = W_2 W_1 x \qquad W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$$

**A**: We end up with a linear classifier again!
(Non-linear) activation function allows us to build non-linear functions with NNs.
NNs with certain non-linear activation functions are known as **Universal Function Approximators.**

*Slide credit: Stanford CS231n Instructors*

# Aside: Universal Function Approximators

**Claim**: Neural Networks with certain non-linear activation functions are universal function approximators.

- What the heck are universal function approximators?
- Why are NNs considered universal function approximators?
- Why does it matter?

# Aside: Universal Function Approximators

**Claim**: Neural Networks with certain non-linear activation functions are universal function approximators.

**A quick primer on approximation theory.**
A branch of mathematics that deals with how functions can be approximated by simpler or more tractable functions, while maintaining some measure of closeness to the original function.

**Example**: approximating $f(x) = e^x$.
$e^x$ are known as *transcendental functions*: you cannot calculate its value with finitely many basic algebraic operations like multiplication, addition, and power.

But we can approximate $e^x$ with a polynomial with bounded error:

$$\sum_{k=1}^{N} \frac{1}{k!} x^k$$

*Adapted from https://tivadardanka.com/blog/universal-approximation-theorem*

# Aside: Universal Function Approximators

**Claim**: Neural Networks with certain non-linear activation functions are universal function approximators.

**NNs as function approximators**

A single layer network with a sigmoid activation $\sigma = \frac{1}{1+e^{-x}}$ can be written as

$$F(x) = \sum_{i=1}^{M} v_i \sigma(w_i^T x + b_i)$$

Is the family of single layer network with sigmoid activation enough to approximate any reasonable function (more on this next slide)?

$$\mathcal{F} = \{\sum_{i=1}^{M} v_i \sigma\left(w_i^T x + b_i\right) : w_i, b_i \in \mathbb{R}^N, v_i \in \mathbb{R}\}$$

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# Aside: Universal Function Approximators

**Claim**: Neural Networks with certain non-linear activation functions are universal function approximators.

**The universal approximation theorem** (Cybenko, G. 1989)

**Theorem 1.** *Let $\sigma$ be any continuous discriminatory function. Then finite sums of the form*

$$G(x) = \sum_{j=1}^{N} \alpha_j \sigma(y_j^T x + \theta_j) \tag{2}$$

*are dense in $C(I_n)$. In other words, given any $f \in C(I_n)$ and $\varepsilon > 0$, there is a sum, $G(x)$, of the above form, for which*

$$|G(x) - f(x)| < \varepsilon \qquad \textit{for all} \quad x \in I_n.$$

**Plain English:** as long as the activation function is <u>sigmoid-like</u> and the function to be approximated is <u>continuous</u>, a neural network with a single hidden layer can approximate it as precisely as you want.

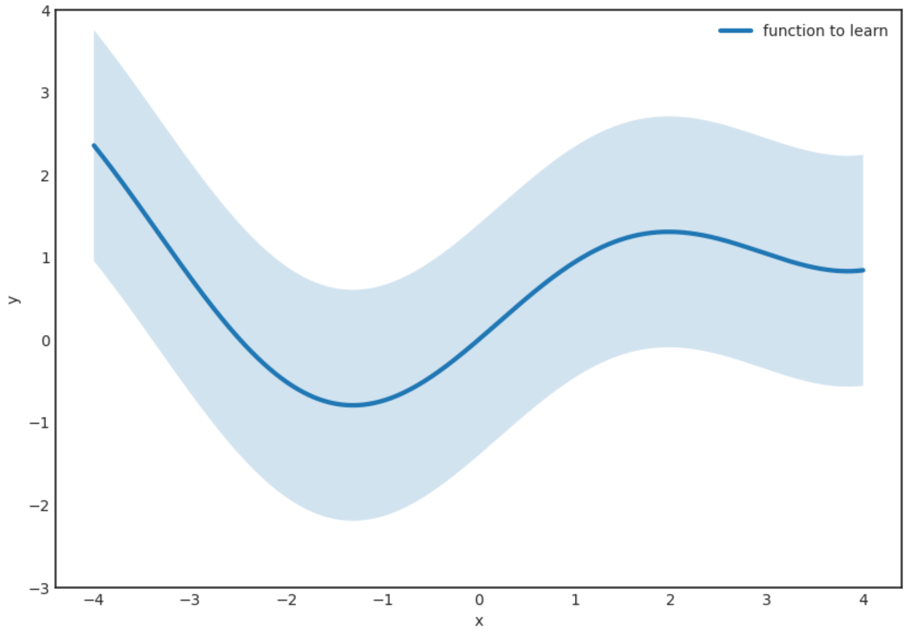
*Adapted from https://tivadardanka.com/blog/universal-approximation-theorem*

# Aside: Universal Function Approximators

**Claim**: Neural Networks with certain non-linear activation functions are universal function approximators.

**A 1-D example of the universal approximation theorem**

We want to approximate $g(x)$ bounded by some small error $\epsilon$ (shaded band) with a single layer NN $F(x)$

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# Aside: Universal Function Approximators

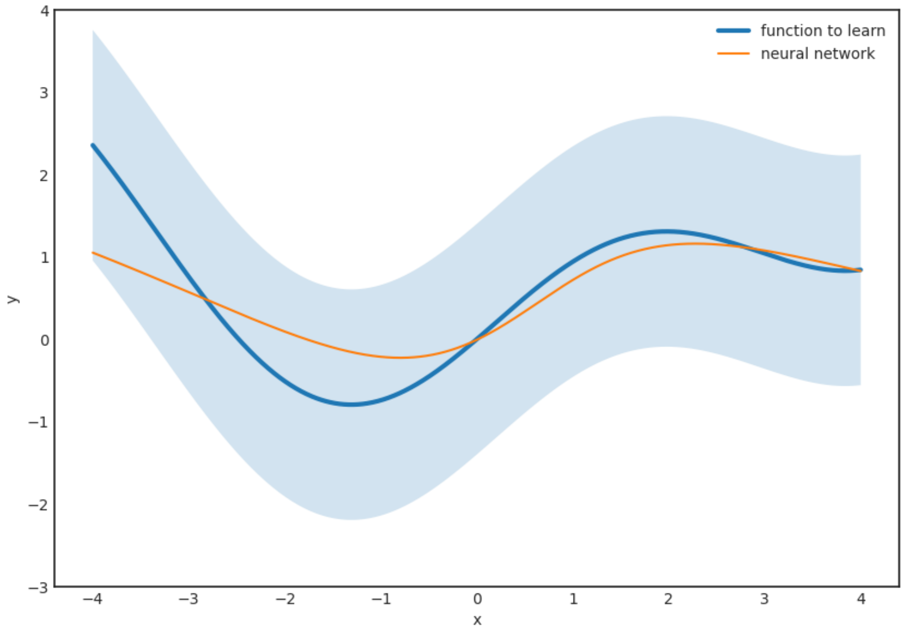
**Claim**: Neural Networks with certain non-linear activation functions are universal function approximators.

**A 1-D example of the universal approximation theorem**

We want to approximate $g(x)$ bounded by some small error $\epsilon$ (shaded band) with a single layer NN $F(x)$

The universal approximation theorem <u>guarantees the existence</u> of such an $F(x)$

… but it doesn't tell us how to get it or what the size of the model ($M$) should be

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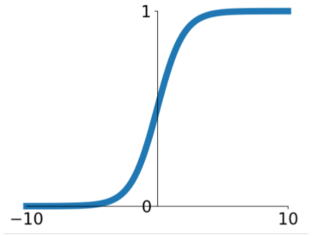
# Activation functions

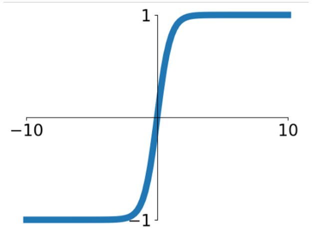
**Sigmoid**

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



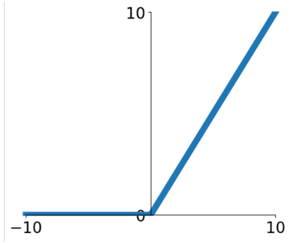

**tanh**

$$\tanh(x)$$



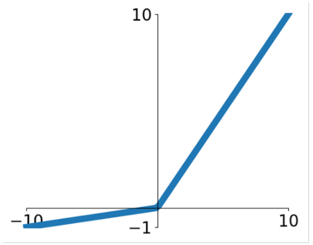

**ReLU**

$$\max(0, x)$$




**Leaky ReLU**

$$\max(0.1x, x)$$

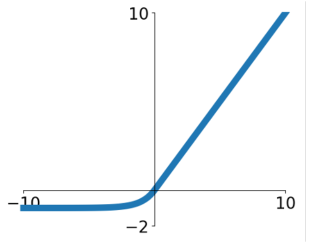



**Maxout**

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

**ELU**

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$

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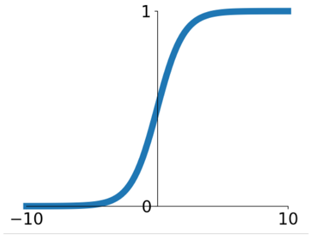
# Activation functions

ReLU is a good default choice for most problems

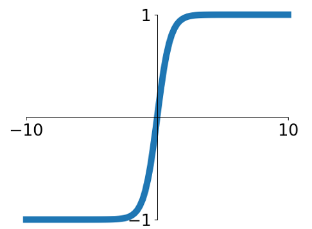
**Sigmoid**

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



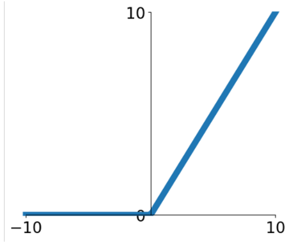

**tanh**

$\tanh(x)$



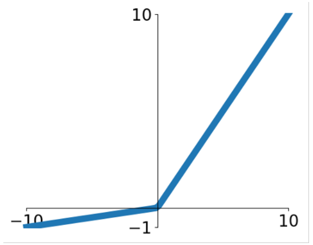

**ReLU**

$\max(0, x)$




**Leaky ReLU**

$\max(0.1x, x)$

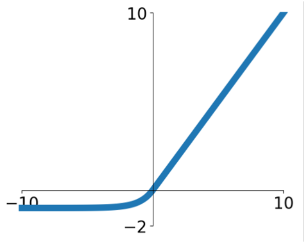



**Maxout**

$\max(w_1^T x + b_1, w_2^T x + b_2)$

**ELU**

$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$

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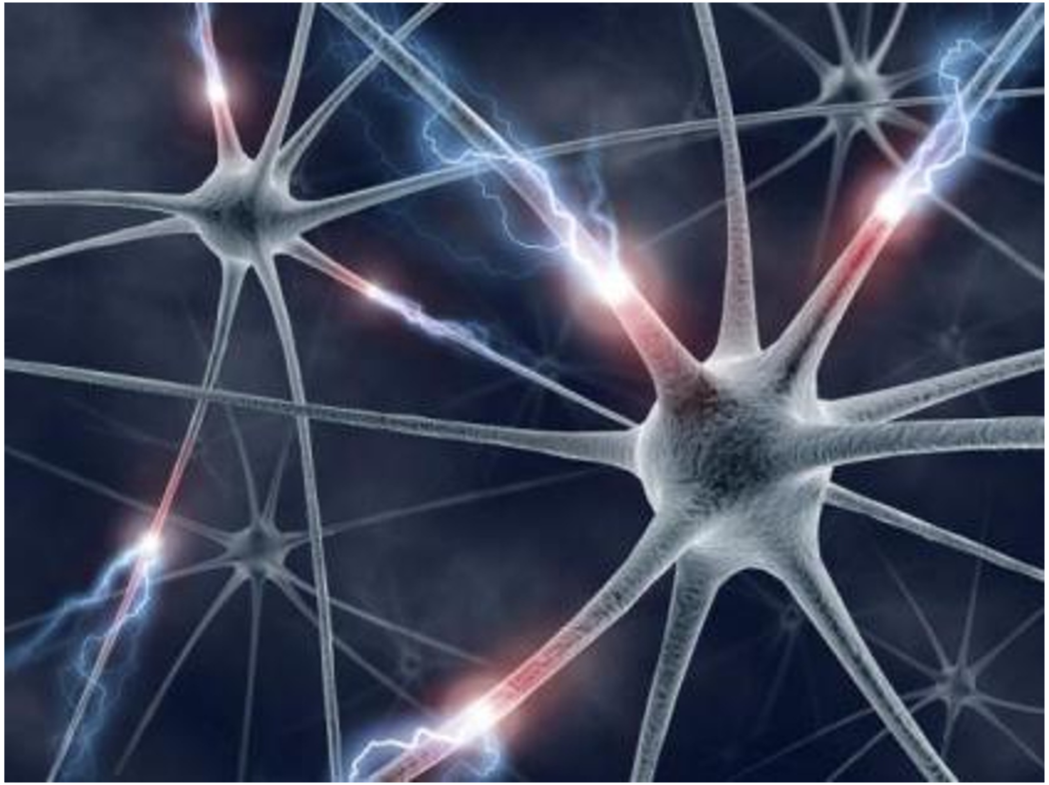
# Why are they called Neural Networks, anyway?





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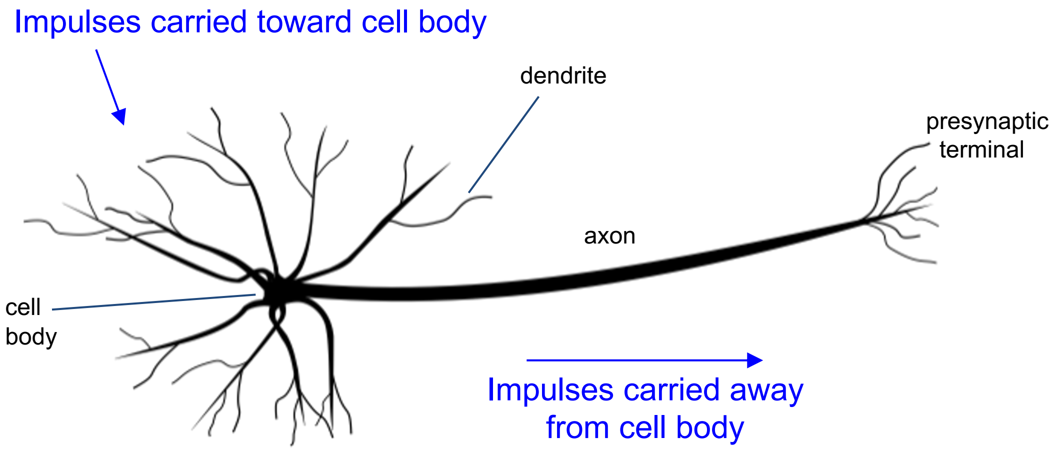
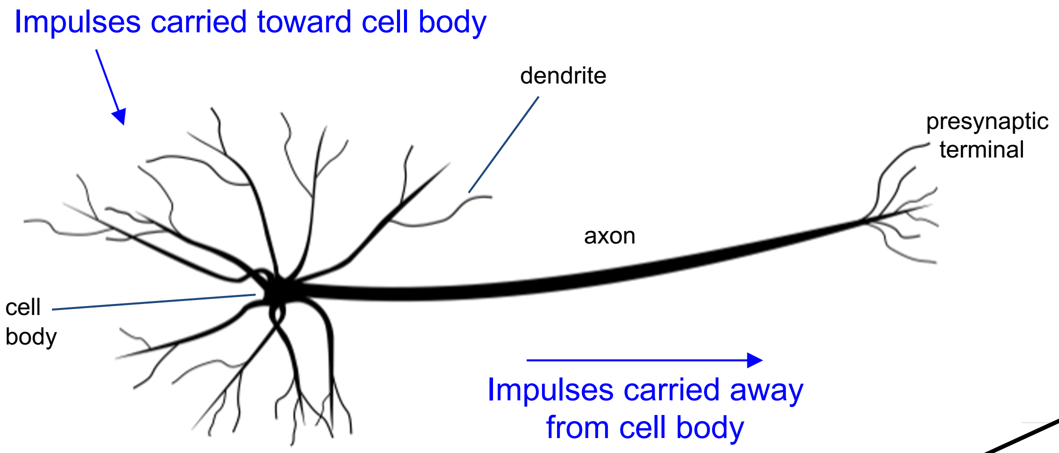
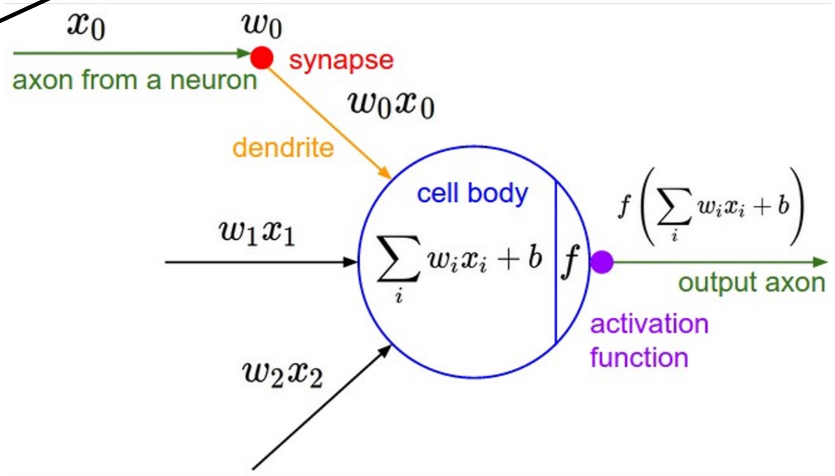

Impulses carried toward cell body
dendrite
presynaptic
terminal
axon
cell
body
Impulses carried away
from cell body



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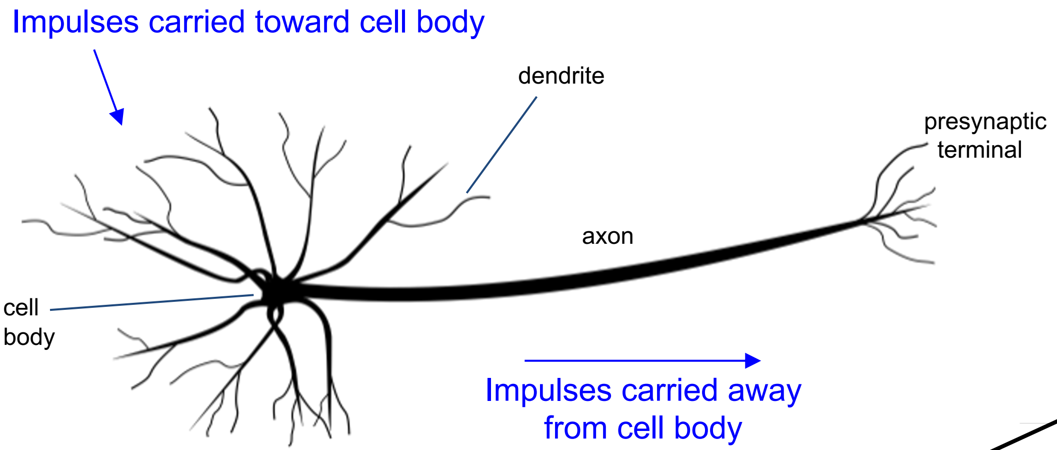
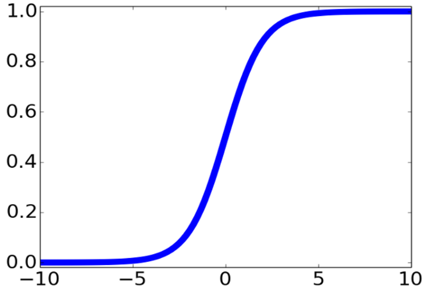
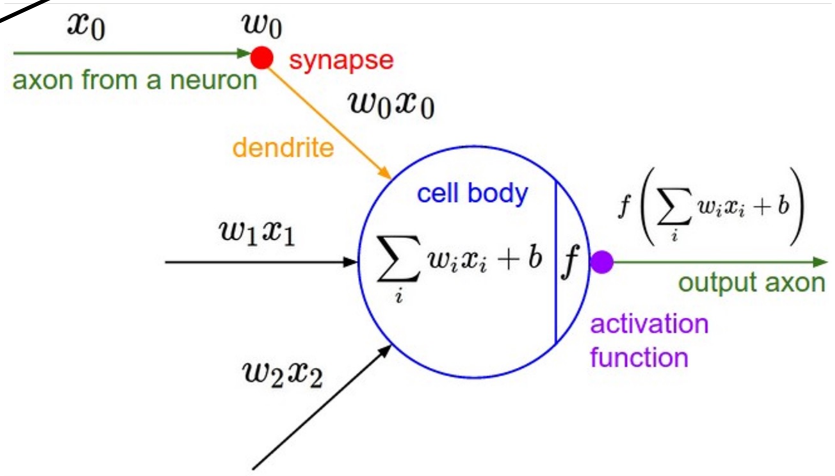





sigmoid activation function

$$\frac{1}{1+e^{-x}}$$

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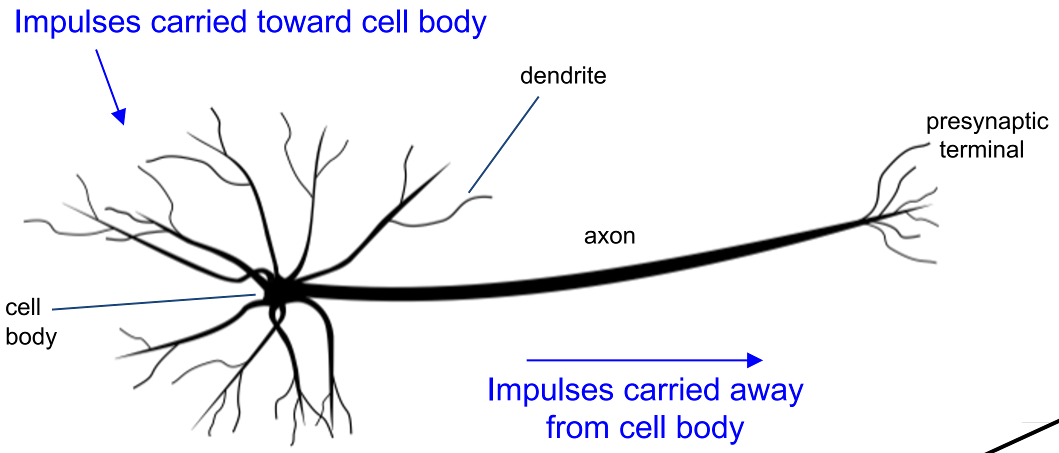
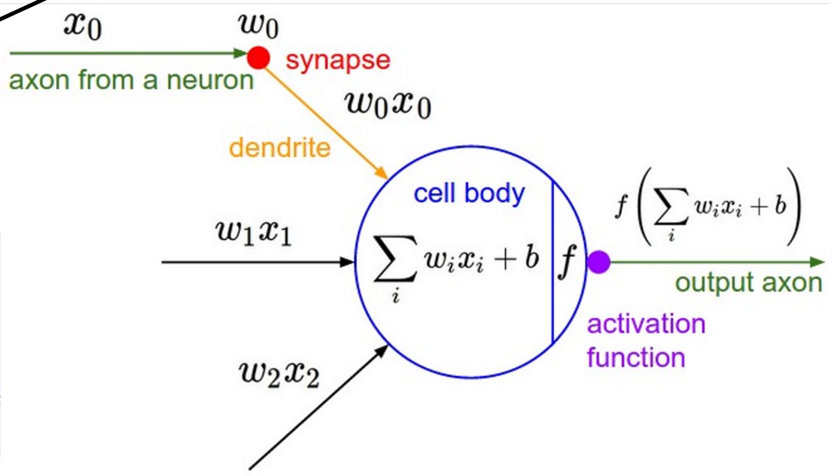





```python
class Neuron:
  # ...
  def neuron_tick(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation func
    return firing_rate
```

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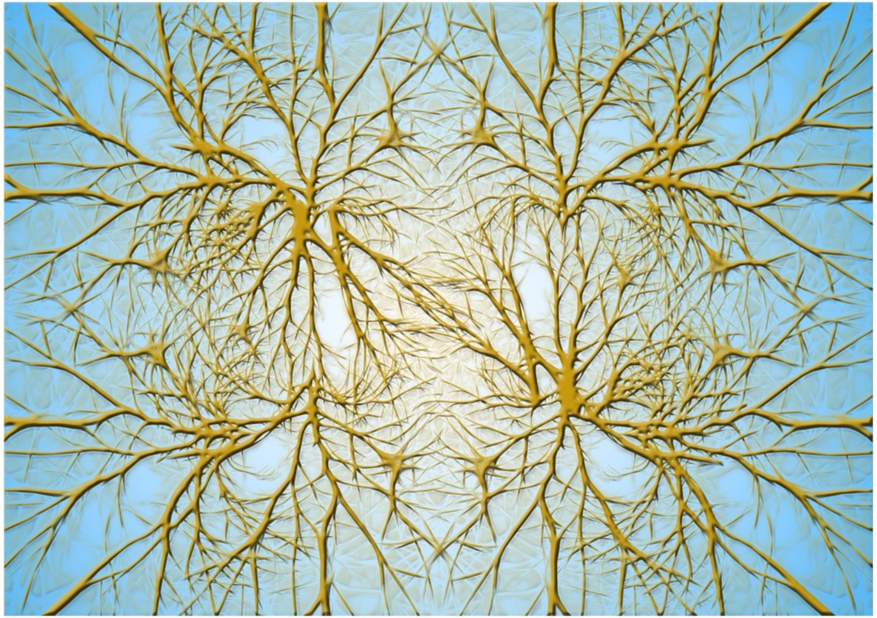
Biological Neurons:
Complex connectivity patterns



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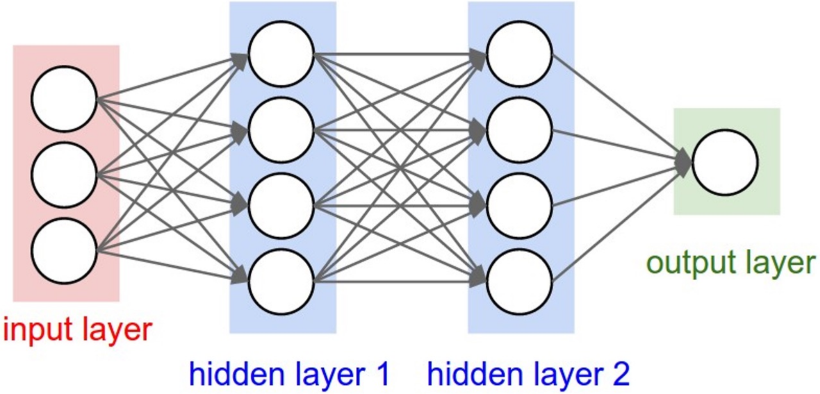
Neurons in a neural network:
Organized into regular layers for computational efficiency

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Biological Neurons:
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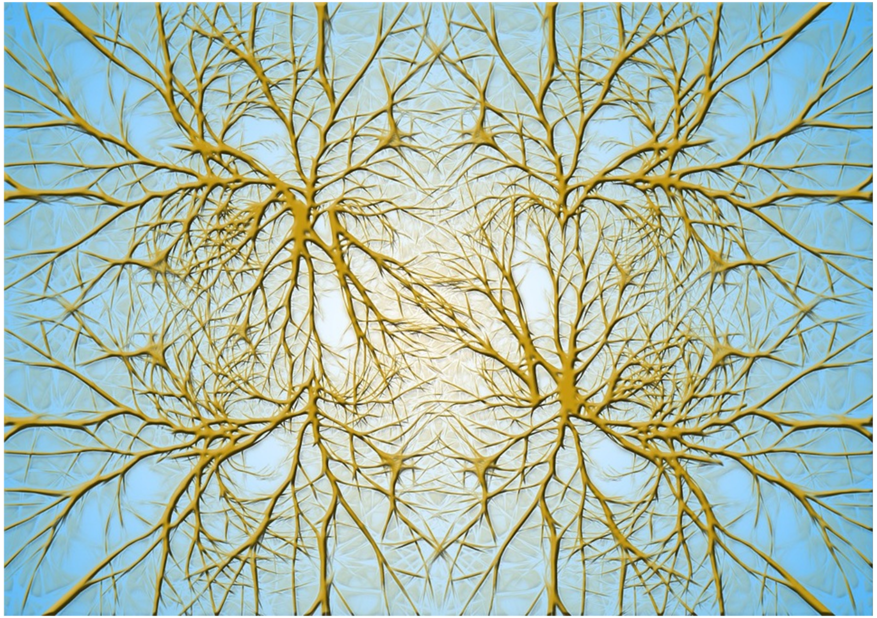

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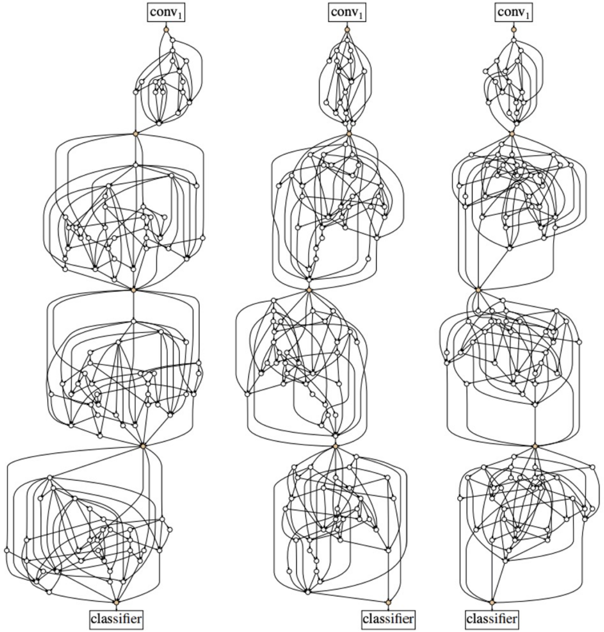
But neural networks with random connections can work too!




Xie et al, “Exploring Randomly Wired Neural Networks for Image Recognition”, arXiv 2019

*Slide credit: Stanford CS231n Instructors*

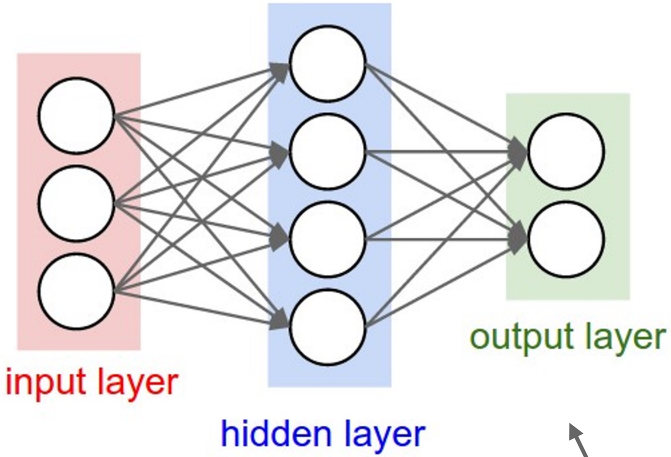
# Be very careful with your brain analogies!

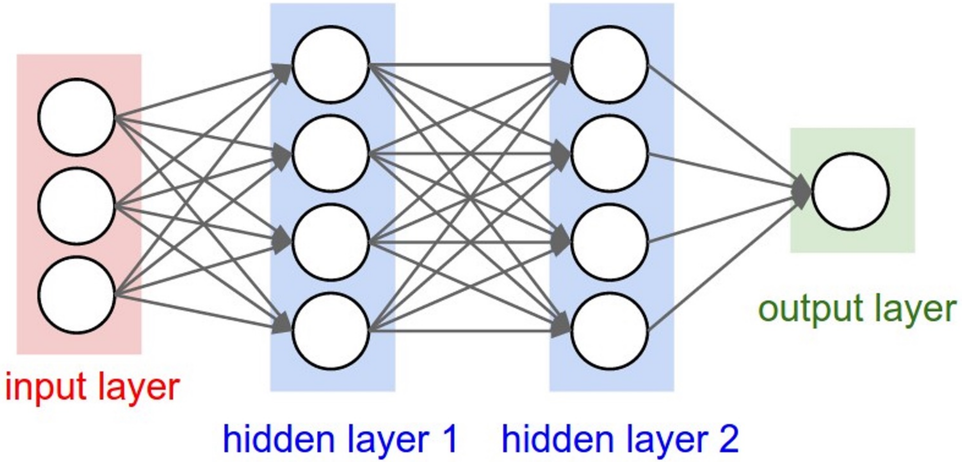
**Biological Neurons:**

- Many different types
- Dendrites can perform complex non-linear computations
- Synapses are not a single weight but a complex non-linear dynamical system

[Dendritic Computation. London and Hausser]

# Neural networks: Architectures




"2-layer Neural Net", or
"1-hidden-layer Neural Net"

"3-layer Neural Net", or
"2-hidden-layer Neural Net"

**"Fully-connected" layers**

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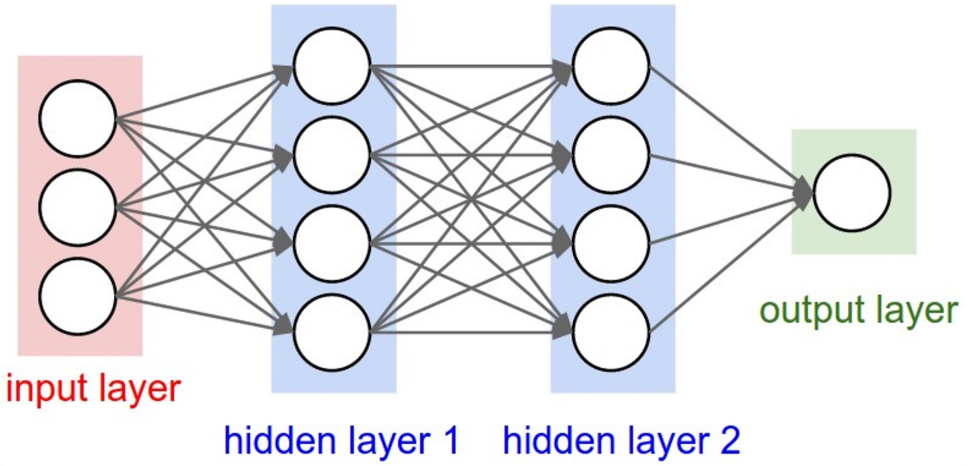
# Example feed-forward computation of a neural network




```
# forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```

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# Full implementation of training a 2-layer Neural Network needs ~20 lines:

```
import numpy as np
from numpy.random import randn

N, D_in, H, D_out = 64, 1000, 100, 10
x, y = randn(N, D_in), randn(N, D_out)
w1, w2 = randn(D_in, H), randn(H, D_out)

for t in range(2000):
  h = 1 / (1 + np.exp(-x.dot(w1)))
  y_pred = h.dot(w2)
  loss = np.square(y_pred - y).sum()
  print(t, loss)

  grad_y_pred = 2.0 * (y_pred - y)
  grad_w2 = h.T.dot(grad_y_pred)
  grad_h = grad_y_pred.dot(w2.T)
  grad_w1 = x.T.dot(grad_h * h * (1 - h))

  w1 -= 1e-4 * grad_w1
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```

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Define the network

*Slide credit: Stanford CS231n Instructors*

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Forward pass

Calculate the analytical gradients

*Slide credit: Stanford CS231n Instructors*

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Forward pass

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Gradient descent

*Slide credit: Stanford CS231n Instructors*

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```

matrix

Calculate the analytical gradients

How?

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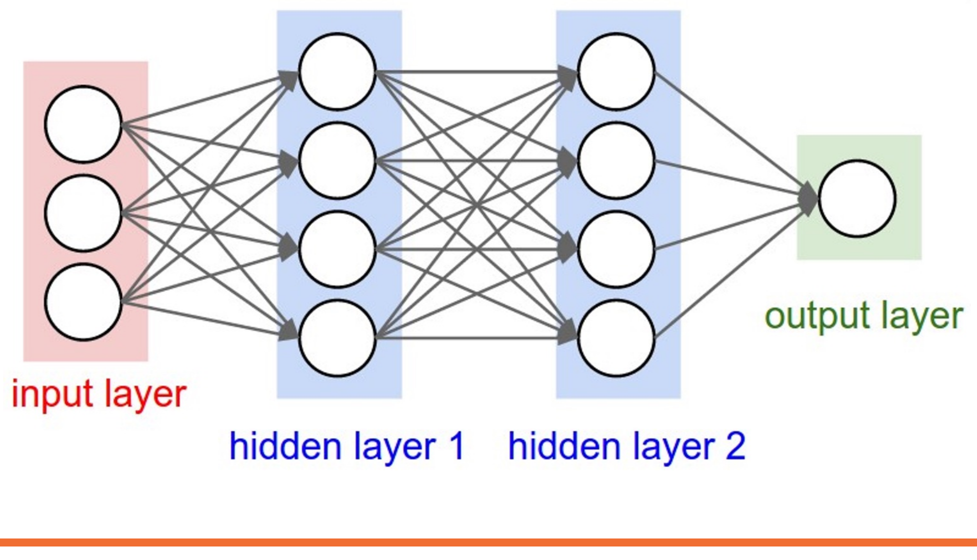
# Next: Vector Calculus!




How do we do backpropagation with neural nets?

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# Recap: Vector derivatives

## Scalar to Scalar

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

Regular derivative:

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

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

Slide credit: Stanford CS231n Instructors

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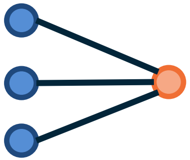
## Vector to Scalar

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

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, how much will y change?





*Slide credit: Stanford CS231n Instructors*

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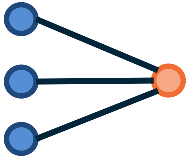


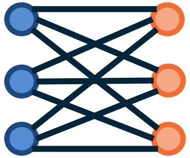
## Vector to Vector

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

Derivative is **Jacobian**:

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

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





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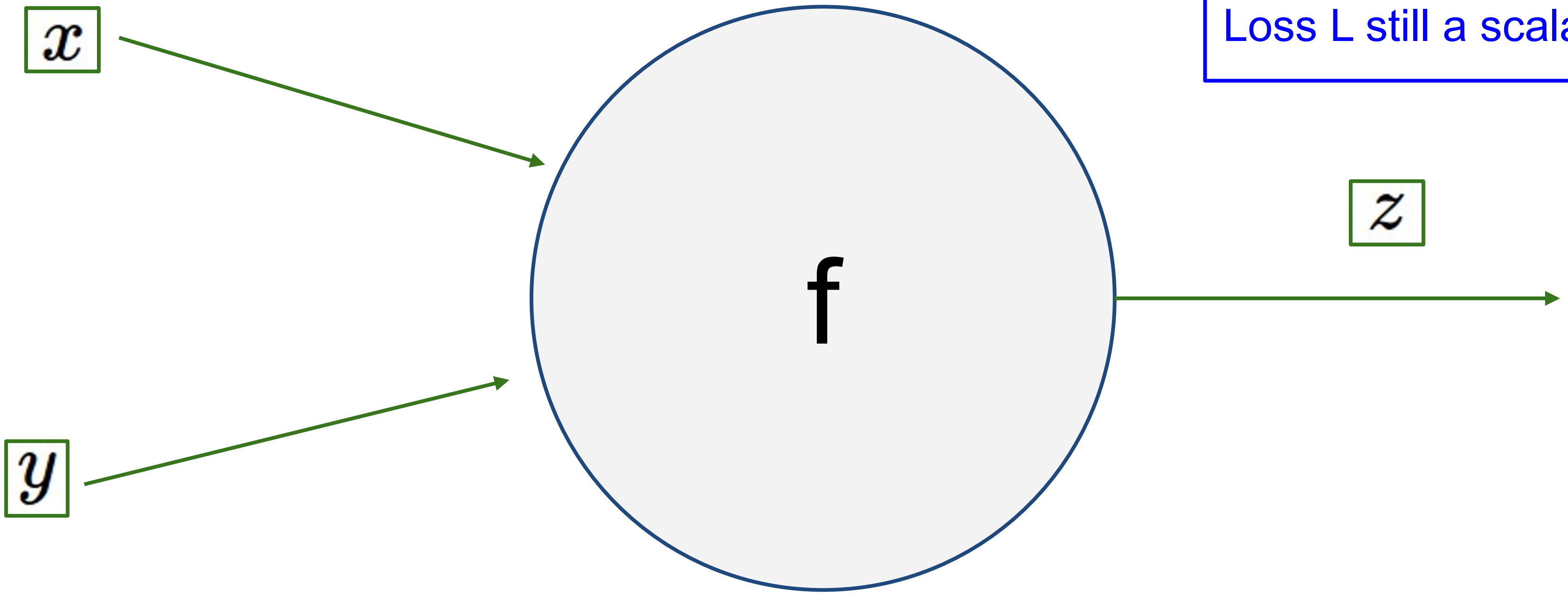
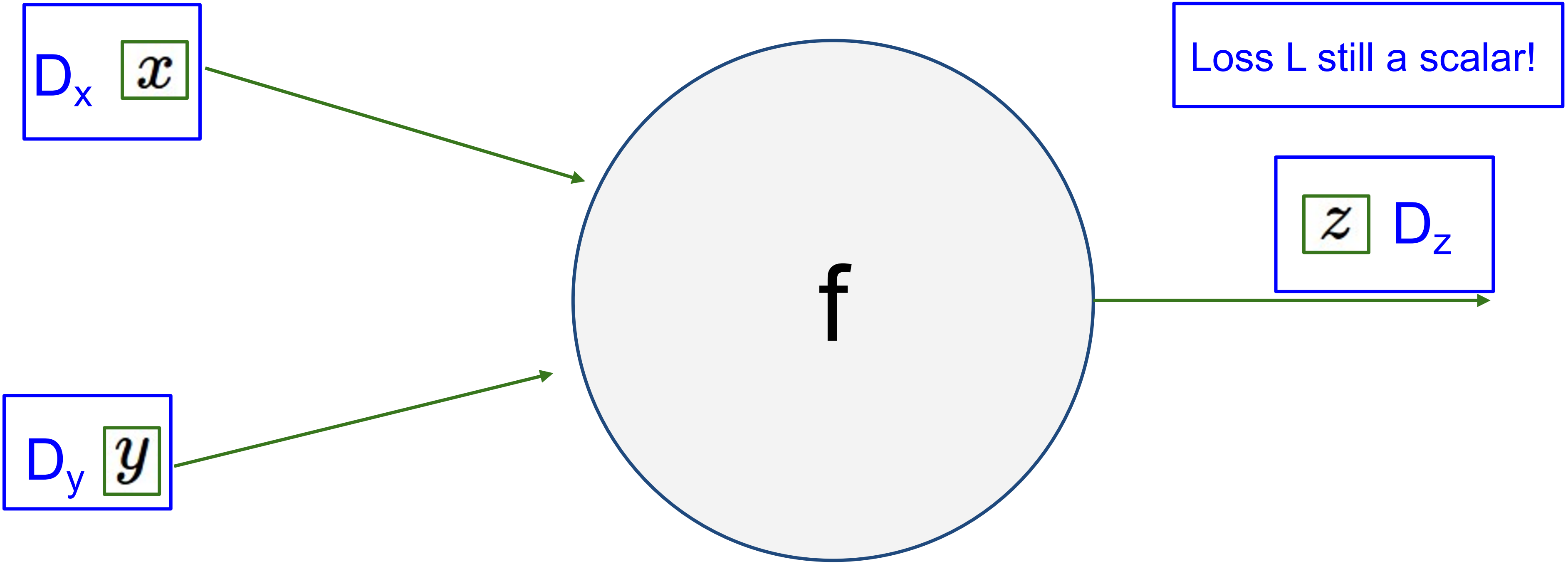
# Backprop with Vectors




Loss L still a scalar!

# Backprop with Vectors

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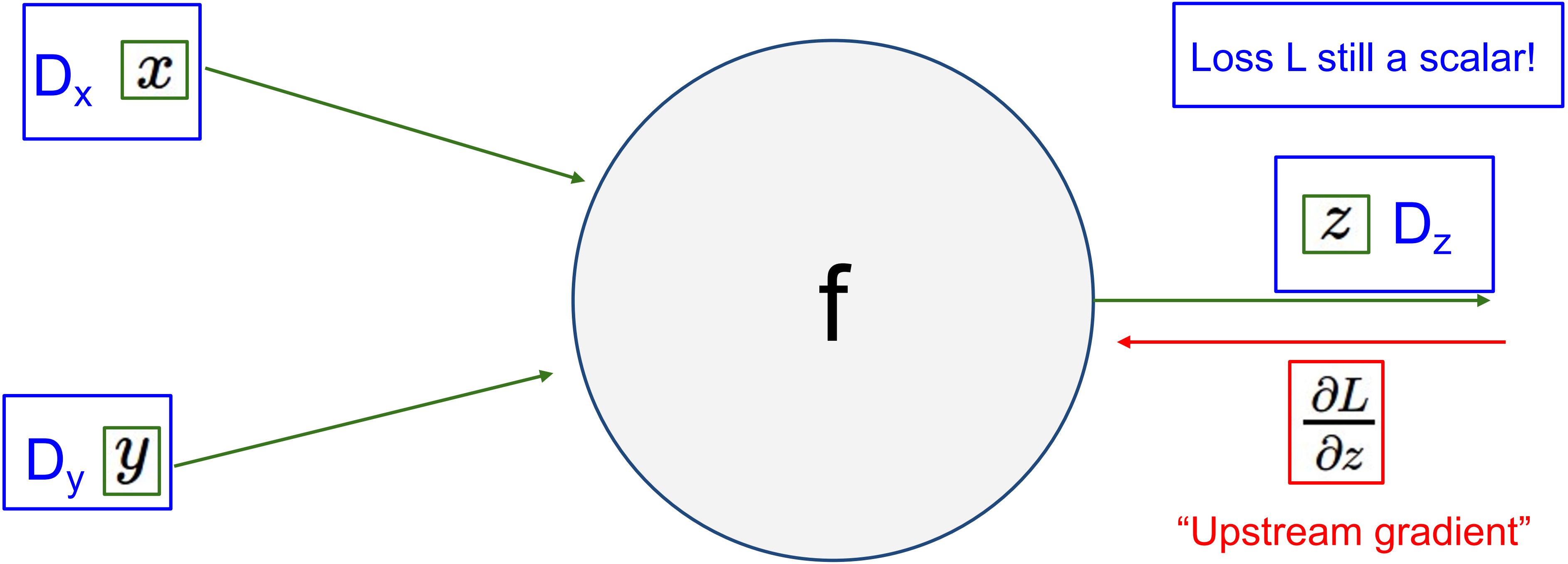


What's the shape of $\frac{\partial L}{\partial z}$?

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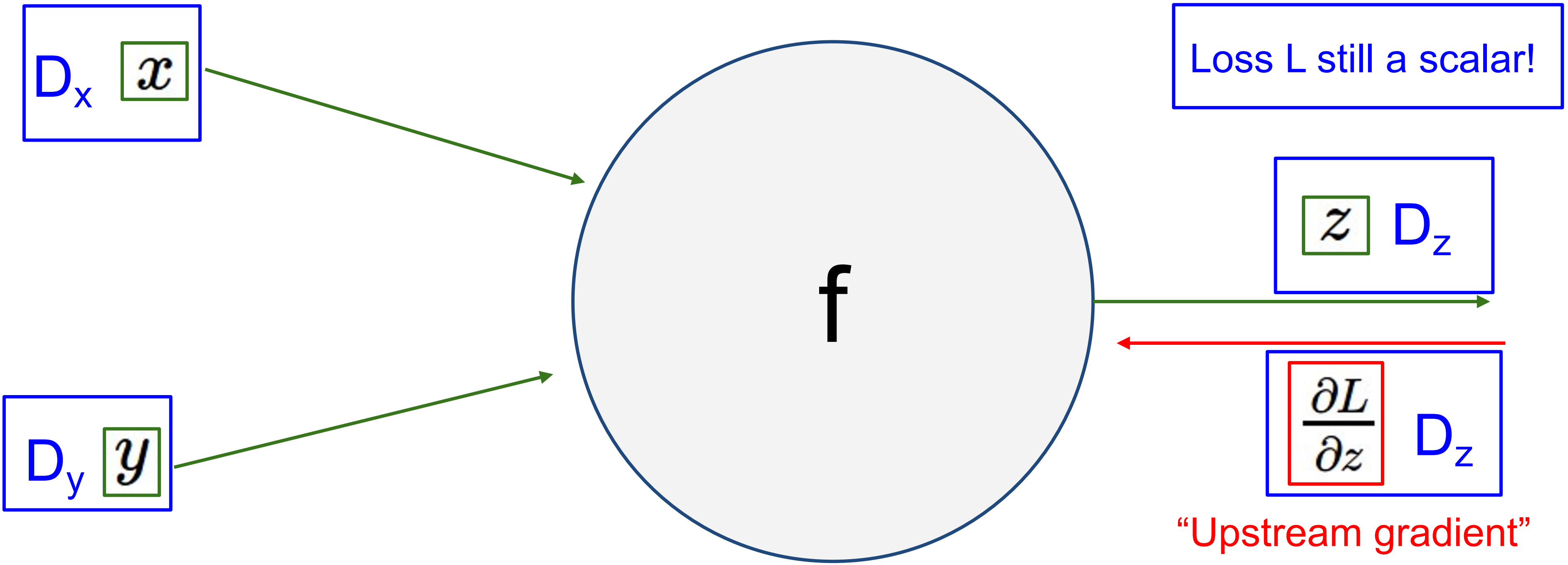
# Backprop with Vectors




"Upstream gradient"

It's a vector of size $D_z$ !

Intuitively: for each element of z, how much does it influence L?

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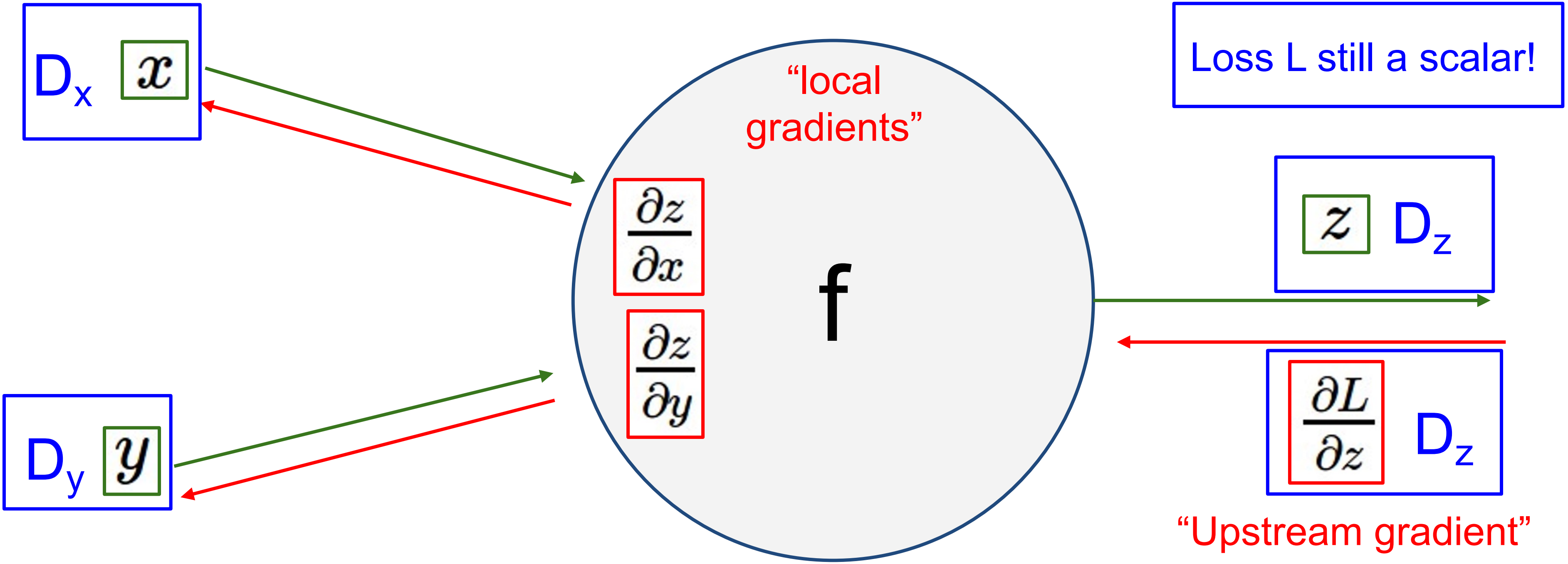
# Backprop with Vectors




What about $\frac{\partial z}{\partial x}$ and $\frac{\partial z}{\partial y}$ ?

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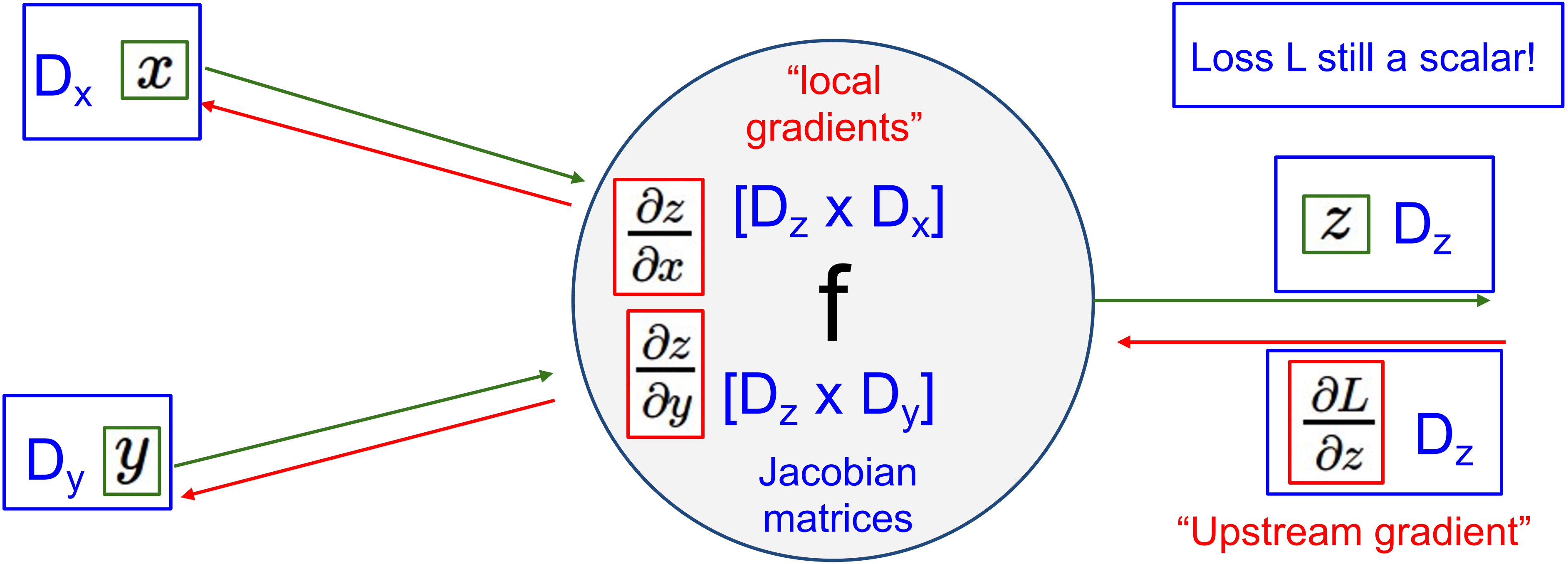
# Backprop with Vectors




What about $\frac{\partial z}{\partial x}$ and $\frac{\partial z}{\partial y}$ ?

How much does each element in $x$ influence each element in $z$

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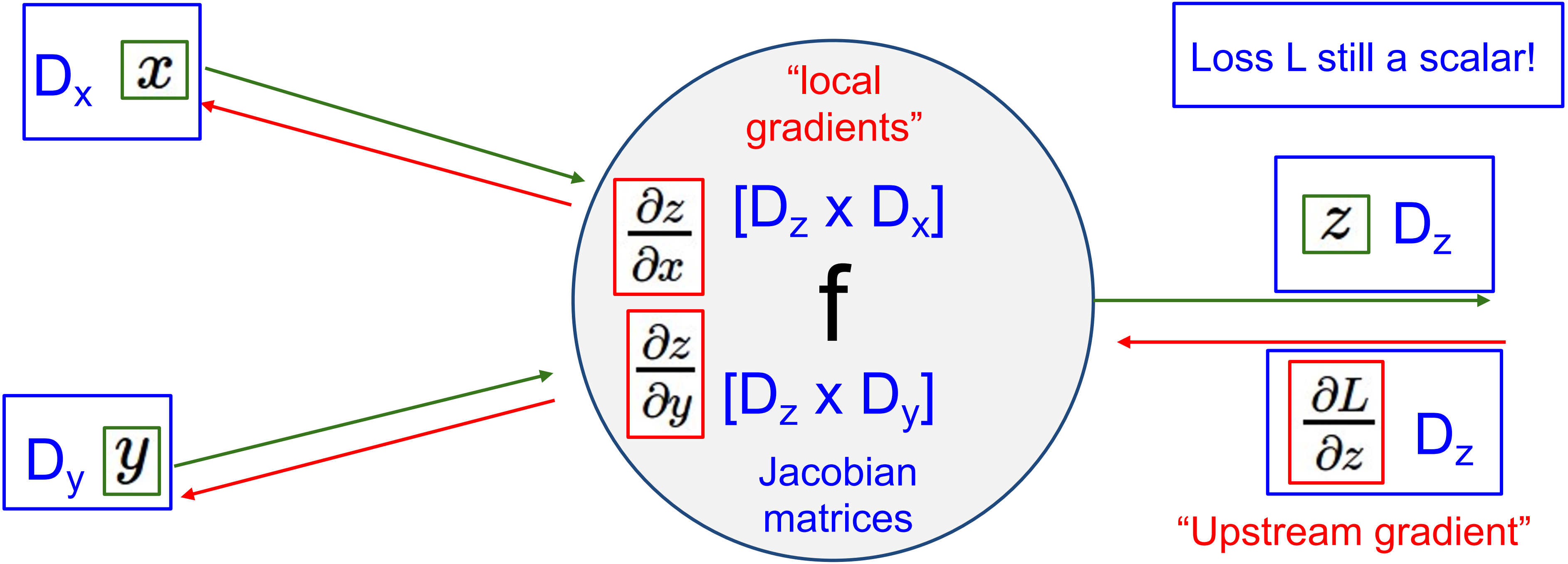
# Backprop with Vectors

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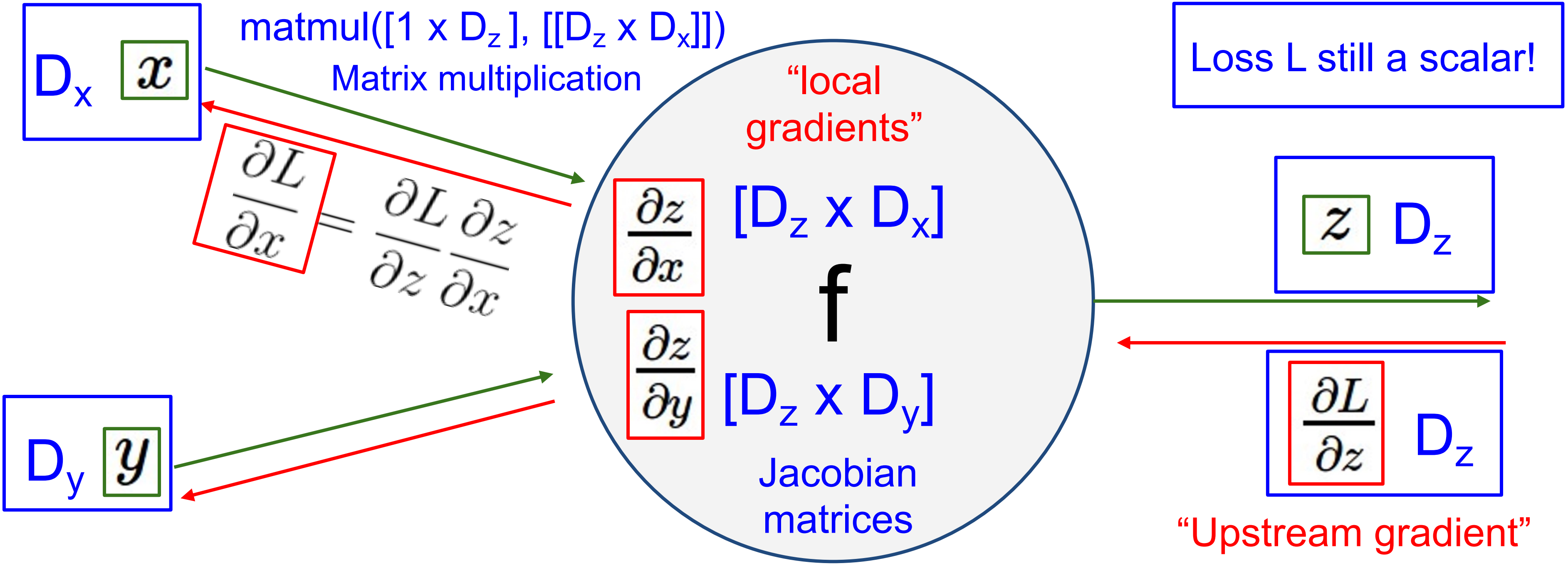


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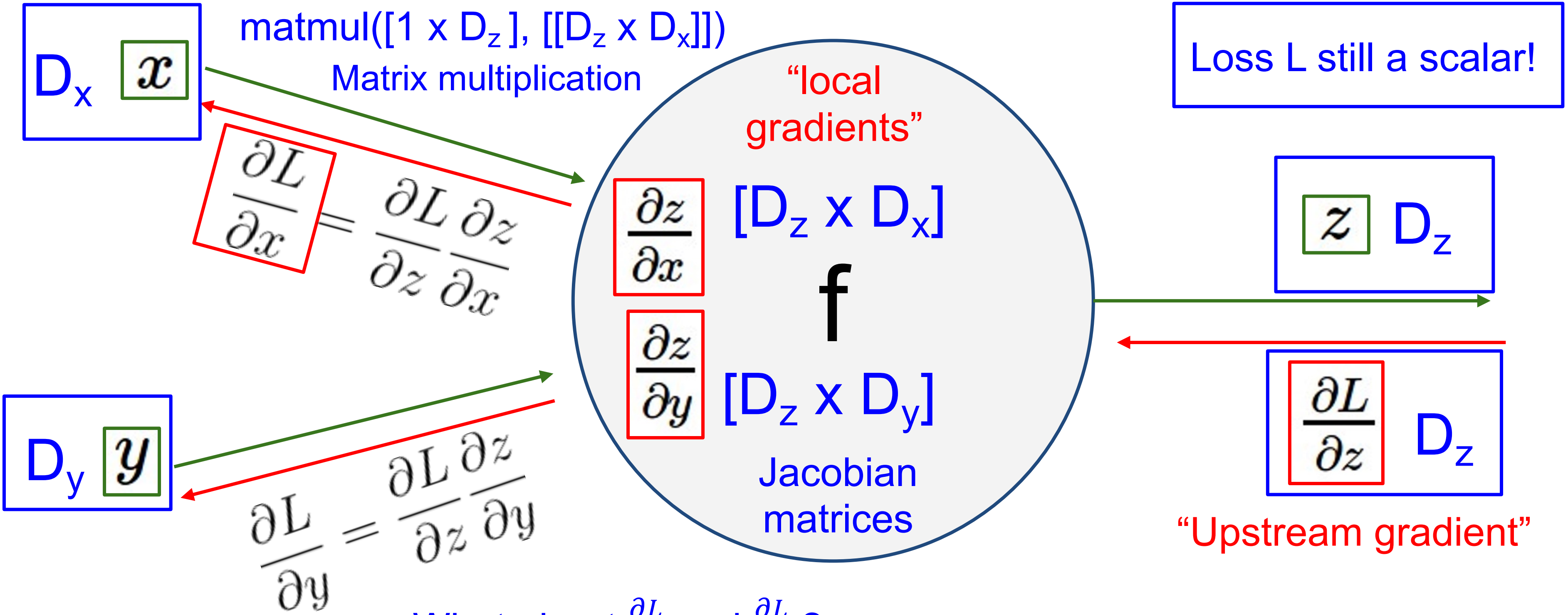


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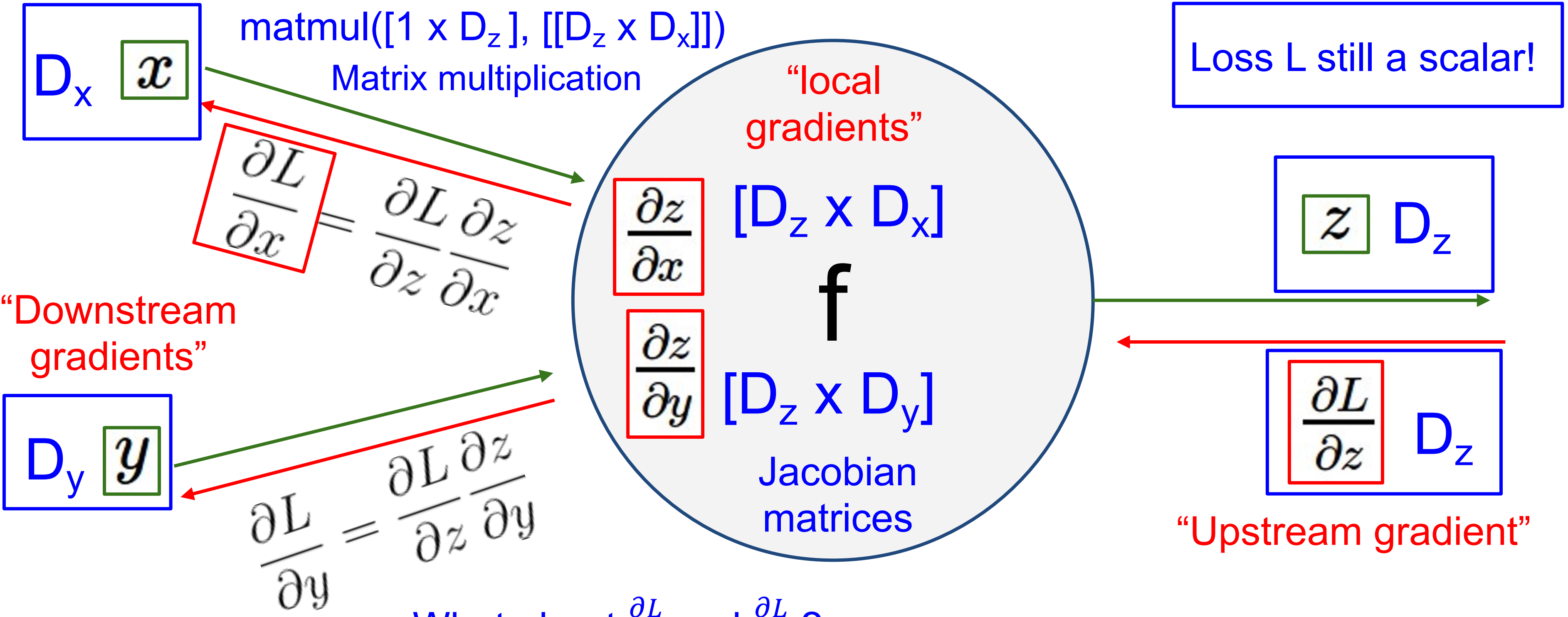


What about $\frac{\partial L}{\partial x}$ and $\frac{\partial L}{\partial y}$ ?

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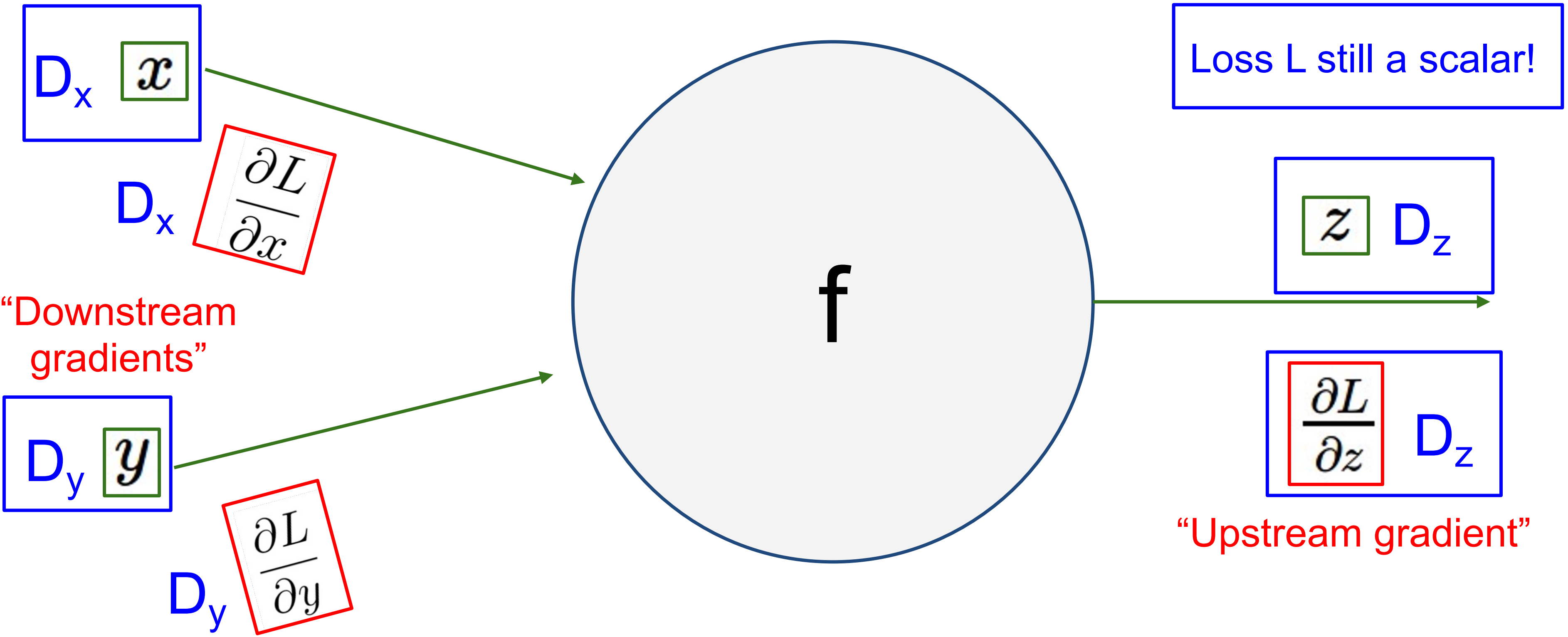
# Gradients loss of wrt a variable have same dims as the original variable

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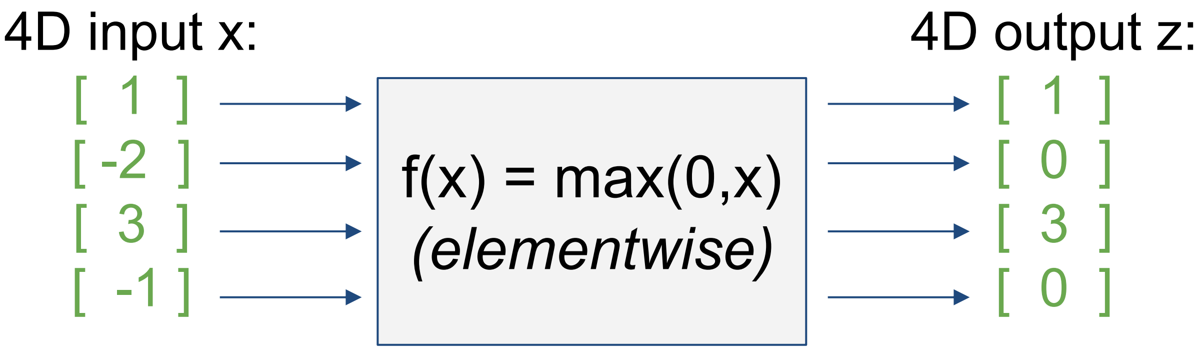
# Jacobians

Given a function $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$, we have the Jacobian matrix $\mathbf{J}$ of shape $\boldsymbol{m} \times \boldsymbol{n}$, where $\mathbf{J}_{i,j} = \frac{\partial f_i}{\partial x_j}$

$$\mathbf{J} = \begin{bmatrix} \dfrac{\partial \mathbf{f}}{\partial x_1} & \cdots & \dfrac{\partial \mathbf{f}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \nabla^{\mathrm{T}} f_1 \\ \vdots \\ \nabla^{\mathrm{T}} f_m \end{bmatrix} = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_1} & \cdots & \dfrac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \dfrac{\partial f_m}{\partial x_1} & \cdots & \dfrac{\partial f_m}{\partial x_n} \end{bmatrix}$$

Figure source: https://en.wikipedia.org/wiki/Jacobian_matrix_and_determinant

# Backprop with Vectors

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# Backprop with Vectors

4D input x:

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

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

4D output z:

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

What does $\frac{\partial z}{\partial x}$ look like?

[dL/dz]
[4 -1 5 9]

Upstream gradient

Slide credit: Stanford CS231n Instructors

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[dz/dx]

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

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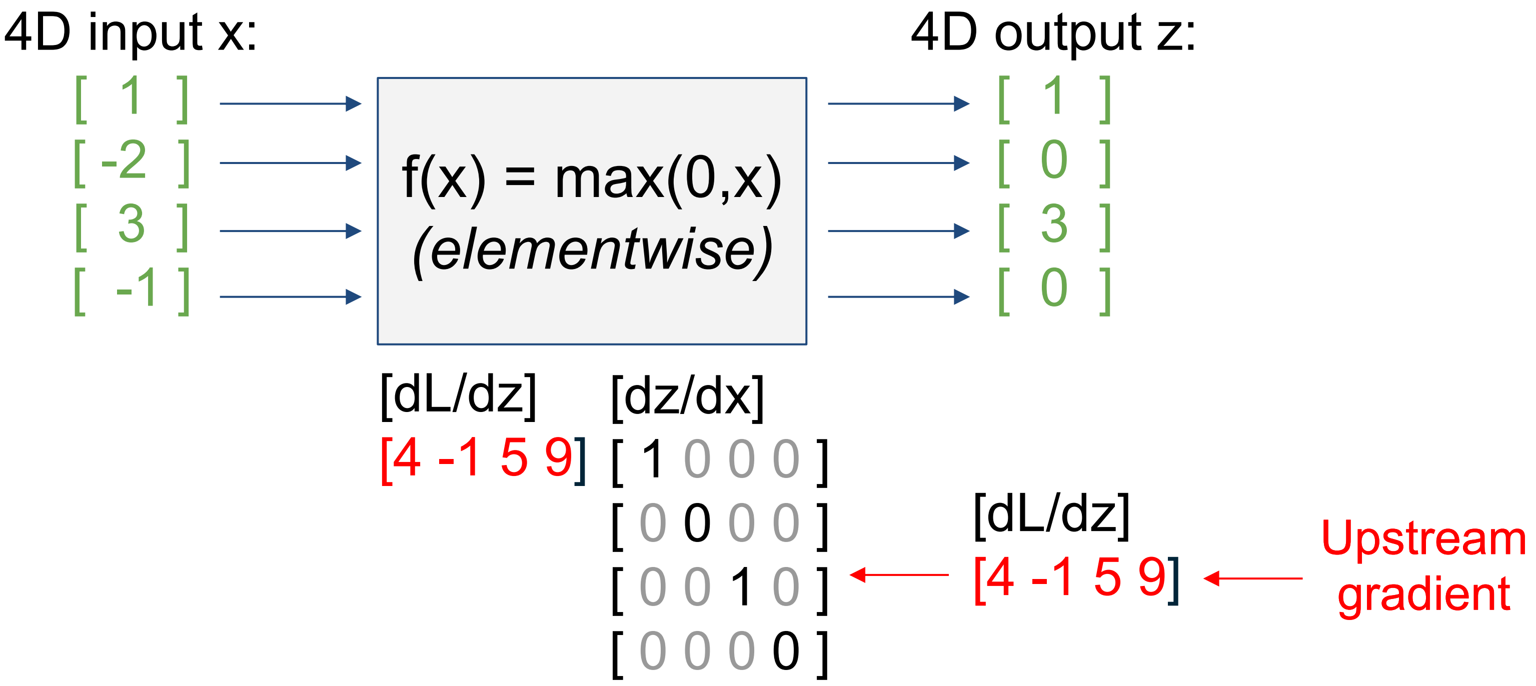


*Slide credit: Stanford CS231n Instructors*

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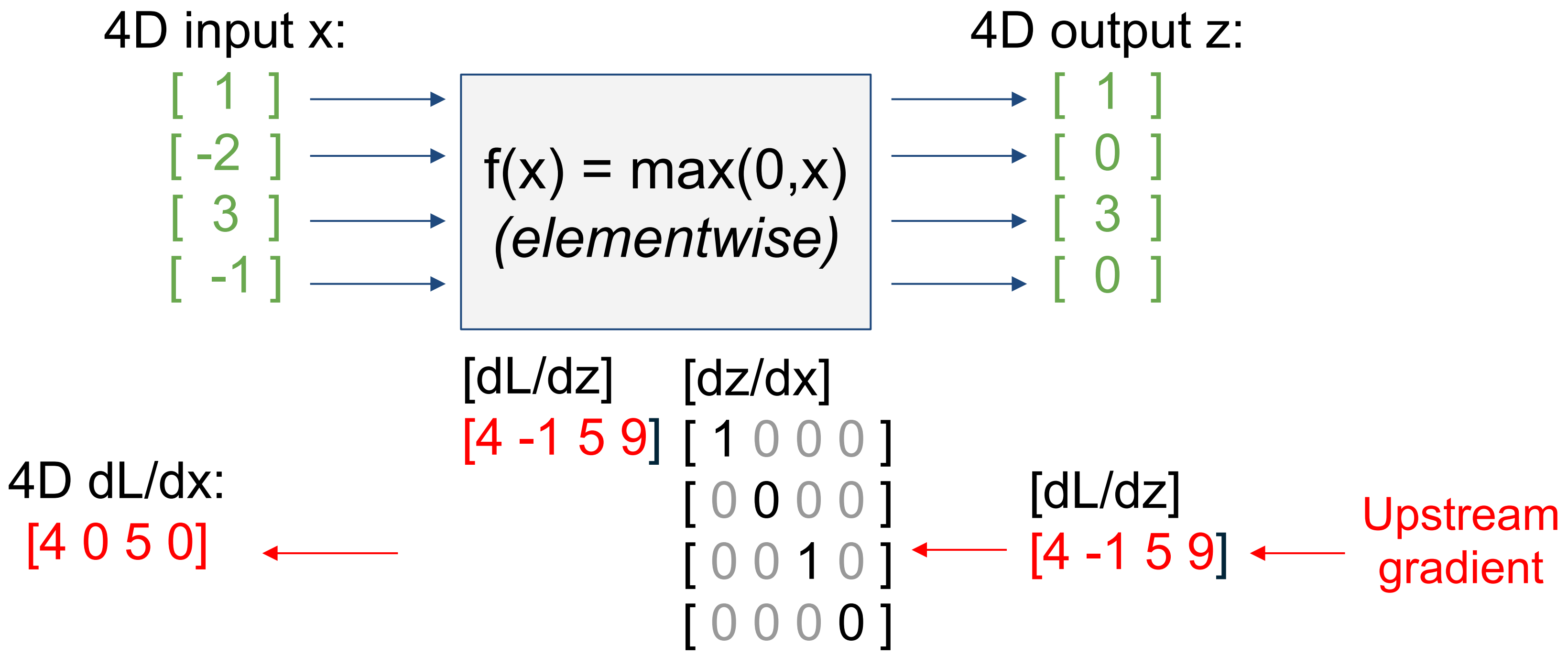


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# Backprop with Vectors

For element-wise ops, jacobian is **sparse**: off-diagonal entries always zero! Never **explicitly** form Jacobian -- instead use Hadamard (element-wise) multiplication

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[dL/dz] [dz/dx]

[4 -1 5 9]

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

4D dL/dx:

[4 0 5 0]

[dL/dz]

[4 -1 5 9]

Upstream gradient

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

4D output z:

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

4D dL/dx:
[4 0 5 0]

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

[dL/dz]
[4 -1 5 9]

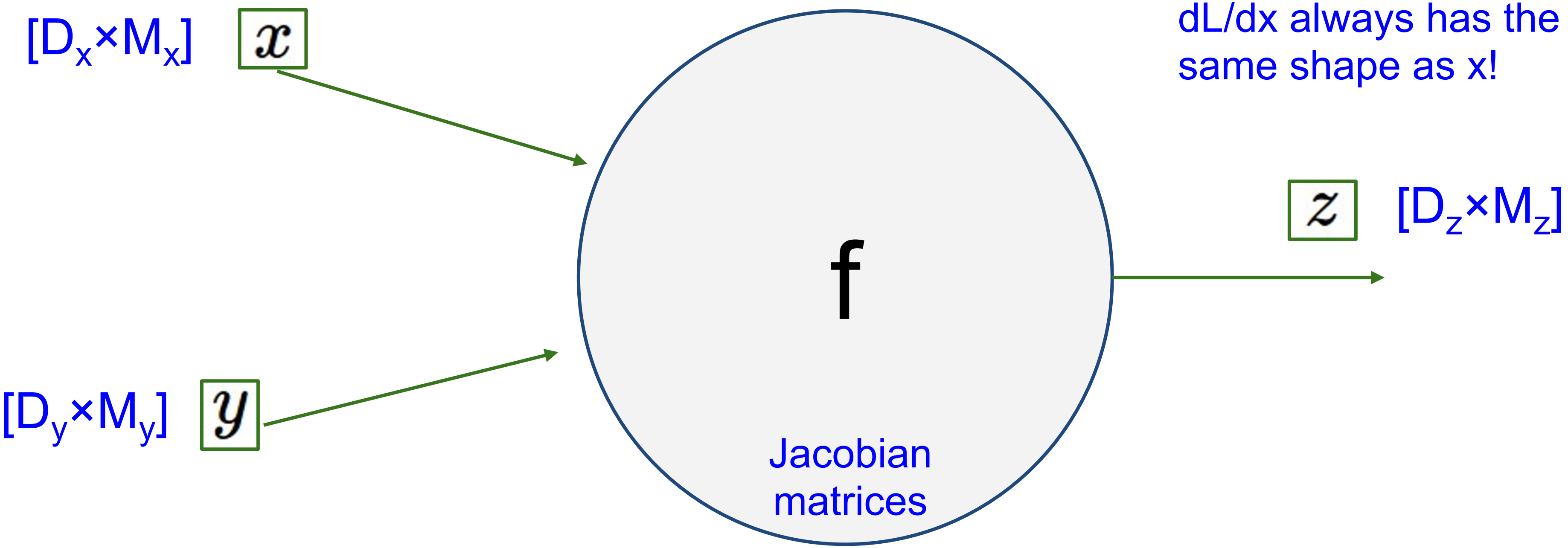
Upstream gradient

*Slide credit: Stanford CS231n Instructors*

# Backprop with Matrices (or Tensors)

Loss L still a scalar!

dL/dx always has the same shape as x!




Slide credit: Stanford CS231n Instructors

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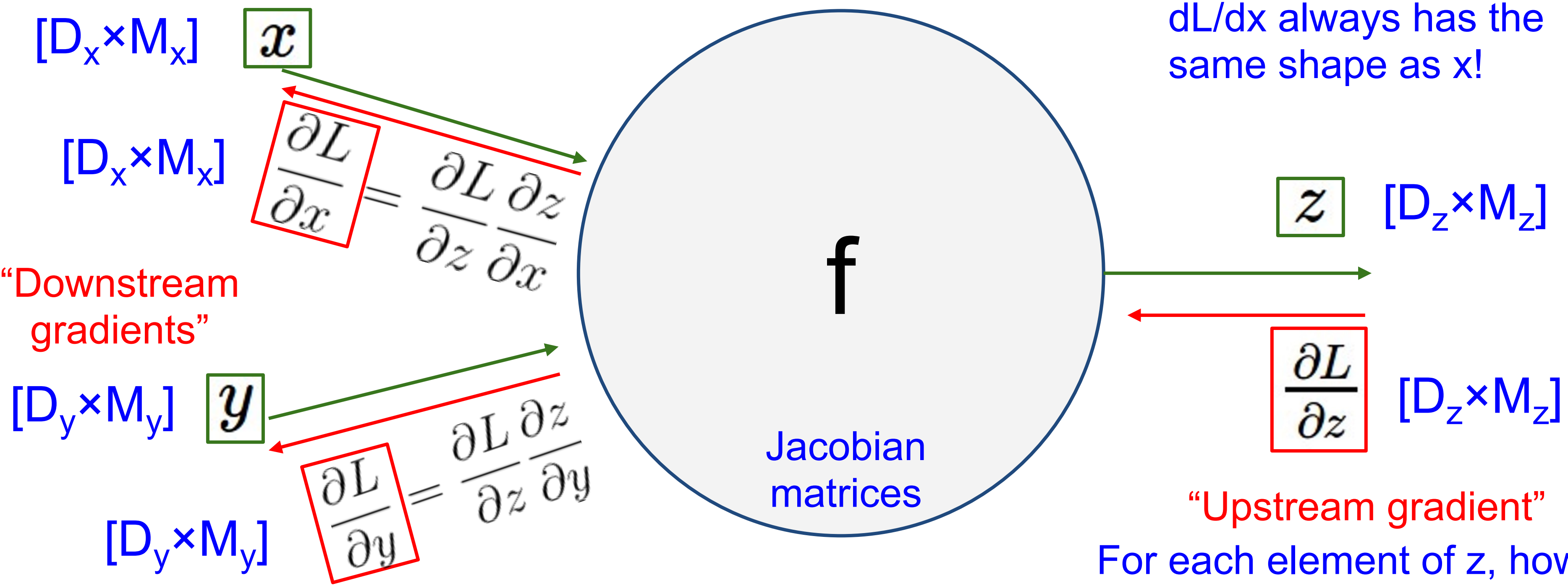


For each element of z, how much does it influence L?

*Slide credit: Stanford CS231n Instructors*

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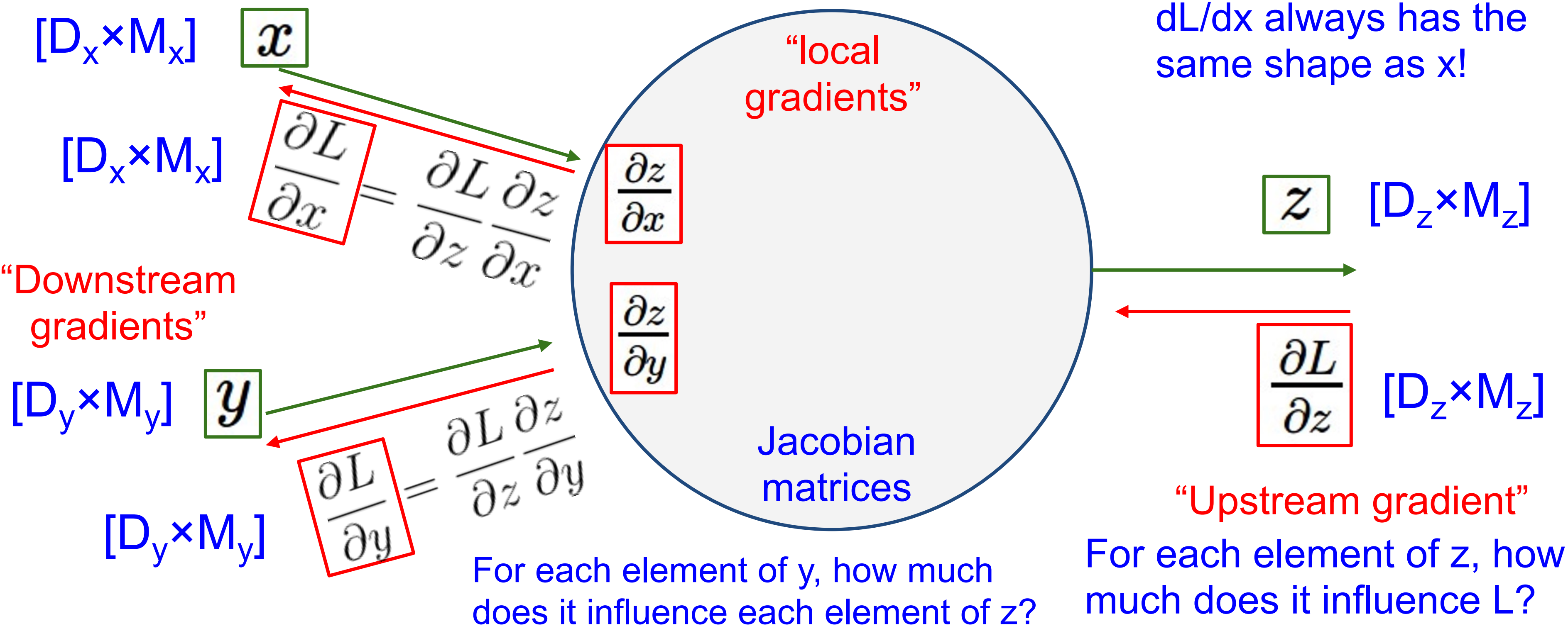


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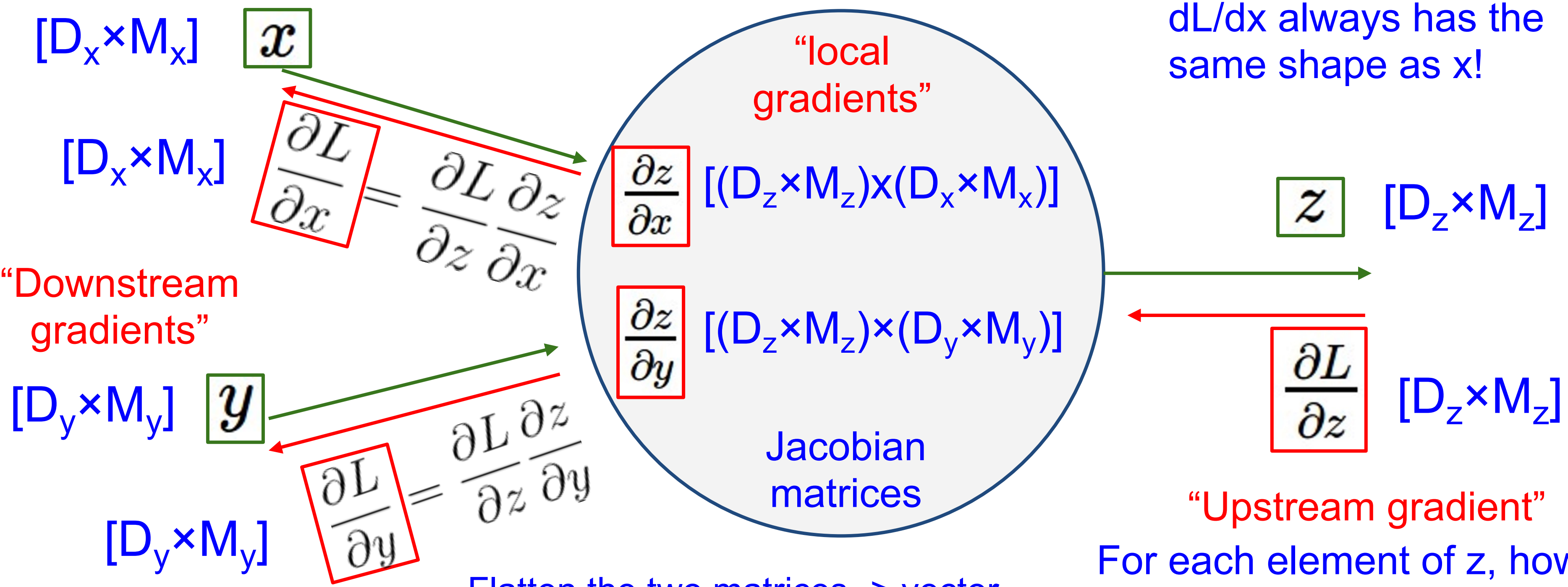
# Backprop with Matrices (or Tensors)

Loss L still a scalar!

dL/dx always has the same shape as x!




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

Flatten the two matrices -> vector-vector gradients -> jacobian matrices!

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# Backprop with Matrices

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**

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

y: [N×M]
**[13 9 -2 -6 ]**
[ 5 2 17 1 ]

dL/dy: [N×M]
[ 2 3 -3 9 ]
[ -8 1 4 6 ]



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# Backprop with Matrices

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**

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

y: [N×M]

$$\begin{bmatrix} 13 & 9 & -2 & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

dL/dy: [N×M]

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

**Jacobians**:

dy/dx: [(N×M)x(N×D)]

dy/dw: [(N×M)x(D×M)]

What does the jacobian matrix look like?



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# Backprop with Matrices

x: [N×D]
[ 2 1 -3 ]
[ -3 4 2 ]

w: [D×M]
[ 3 2 1 -1]
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**Matrix Multiply**

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y: [N×M]
**[13 9 -2 -6 ]**
[ 5 2 17 1 ]

dL/dy: [N×M]
[ 2 3 -3 9 ]
[ -8 1 4 6 ]

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

For a neural net with
N=64, D=M=4096
Each Jacobian takes 256 GB of memory!
Must exploit its sparsity!



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# Backprop with Matrices

x: [N×D]

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

w: [D×M]

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

## Matrix Multiply

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

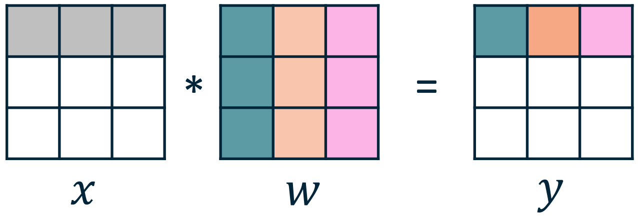
y: [N×M]

$$\begin{bmatrix} \mathbf{13} & \mathbf{9} & \mathbf{-2} & \mathbf{-6} \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

dL/dy: [N×M]

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

**Q**: What parts of y are affected by one element of x?



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# Backprop with Matrices

x: [N×D]

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

w: [D×M]

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**Matrix Multiply**

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$$\begin{bmatrix} \boxed{13 \quad 9 \quad -2 \quad -6} \\ 5 \quad 2 \quad 17 \quad 1 \end{bmatrix}$$

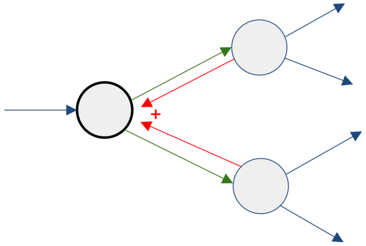
dL/dy: [N×M]

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

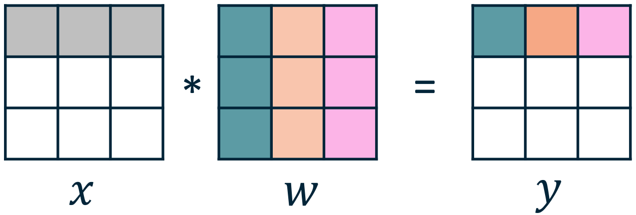
**Q**: What parts of y are affected by one element of x?

**A**: $\boxed{x_{n,d}}$ affects the whole row $y_{n,\cdot}$

$$\frac{\partial L}{\partial x_{n,d}} = \boxed{\sum_m} \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}}$$




Recall the branching gradient rule!






Slide credit: Stanford CS231n Instructors

# Backprop with Matrices

x: [N×D]

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**Matrix Multiply**

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

y: [N×M]

$$\begin{bmatrix} \boxed{13 \quad 9 \quad -2 \quad -6} \\ 5 \quad 2 \quad 17 \quad 1 \end{bmatrix}$$

dL/dy: [N×M]

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

**Q**: What parts of y are affected by one element of x?

**A**: $\boxed{x_{n,d}}$ affects the whole row $y_{n,\cdot}$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \underbrace{\frac{\partial L}{\partial y_{n,m}}}_{\text{Upstream gradient}} \underbrace{\boxed{\frac{\partial y_{n,m}}{\partial x_{n,d}}}}_{\text{local gradient}}$$



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# Backprop with Matrices

x: [N×D]

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

w: [D×M]

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

**Matrix Multiply**

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

y: [N×M]

[ 13 9 $\boxed{-2}$ -6 ]
[ 5 2 17 1 ]

dL/dy: [N×M]

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

**Q**: What parts of y are affected by one element of x?

**A**: $\boxed{x_{n,d}}$ affects the whole row $y_{n,\cdot}$

**Q**: How much does $\boxed{x_{n,d}}$ affect $\boxed{y_{n,m}}$?

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \boxed{\frac{\partial y_{n,m}}{\partial x_{n,d}}}$$

How do we calculate this?



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# Backprop with Matrices

x: [N×D]

[ 2 $\boxed{1}$ -3 ]
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**A**: $\boxed{x_{n,d}}$ affects the whole row $y_{n,\cdot}$

**Q**: How much does $\boxed{x_{n,d}}$ affect $\boxed{y_{n,m}}$?

$$y_{n,m} = \sum_{i=1}^{D} x_{n,i} w_{i,m}$$

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

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \boxed{\frac{\partial y_{n,m}}{\partial x_{n,d}}}$$

How do we calculate this?



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**A**: $\boxed{w_{d,m}}$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}}$$

$\boxed{w_{d,m}}$



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# Backprop with Matrices

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w: [D×M]

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

**Matrix Multiply**

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**A:** $\boxed{w_{d,m}}$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \underbrace{\frac{\partial y_{n,m}}{\partial x_{n,d}}}_{\boxed{w_{d,m}}} = \sum_m \frac{\partial L}{\partial y_{n,m}} w_{d,m} = \frac{\partial L}{\partial y_n} w_d^T$$

Just a dot product!



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# Backprop with Matrices

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**A:** $\boxed{w_{d,m}}$

[N×D] [N×M] [M×D]

$$\boxed{\frac{\partial L}{\partial x} = \left(\frac{\partial L}{\partial y}\right) w^T}$$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} w_{d,m} = \frac{\partial L}{\partial y_n} w_d^T$$

Just a matrix multiplication

No jacobian matrix needed!



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# Backprop with Matrices

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dL/dy: [N×M]

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

By similar logic:

[N×D] [N×M] [M×D]

$$\boxed{\frac{\partial L}{\partial x} = \left(\frac{\partial L}{\partial y}\right) w^T}$$

[D×M] [D×N] [N×M]

$$\boxed{\frac{\partial L}{\partial w} = x^T \left(\frac{\partial L}{\partial y}\right)}$$



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# Backprop with Matrices

x: [N×D]

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dL/dy: [N×M]

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

By similar logic:

[N×D] [N×M] [M×D]

$$\boxed{\frac{\partial L}{\partial x} = \left(\frac{\partial L}{\partial y}\right) w^T}$$

[D×M] [D×N] [N×M]

$$\boxed{\frac{\partial L}{\partial w} = x^T \left(\frac{\partial L}{\partial y}\right)}$$

For a neural net layer with N=64, D=M=4096

The larges matrix ($W$) takes up to 0.13 GB memory



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Summary:

- Review backpropagation
- Neural networks, activation functions
- NNs as universal function approximators
- Neurons as biological inspirations to DNNs
- Vector Calculus
- Backpropagation through vectors / matrices

# Next Time: How to Pick a Project!