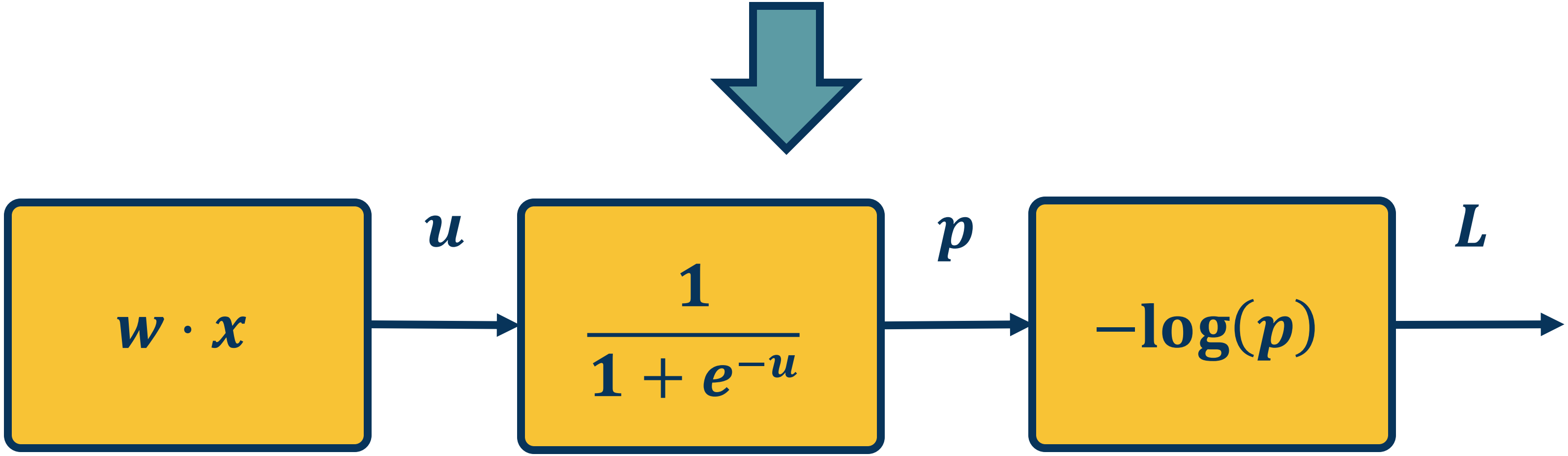
CS 4644 / 7643-A: LECTURE 5
DANFEI XU

Topics:

- Backpropagation
- Neural Networks
- Jacobians

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



Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

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

Chain rule and Backpropagation!

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

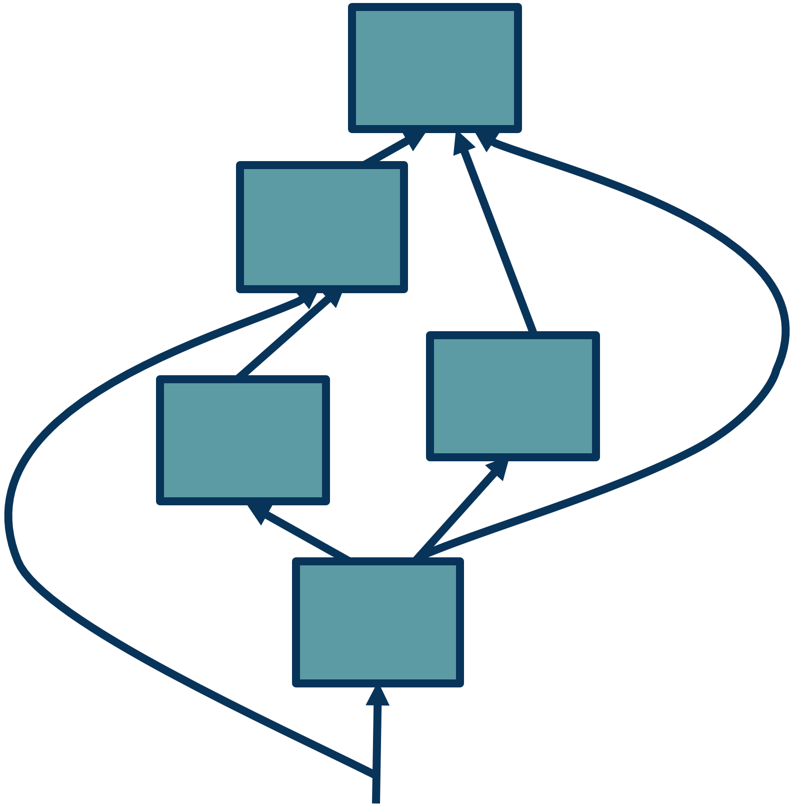
Recap: Computation Graph

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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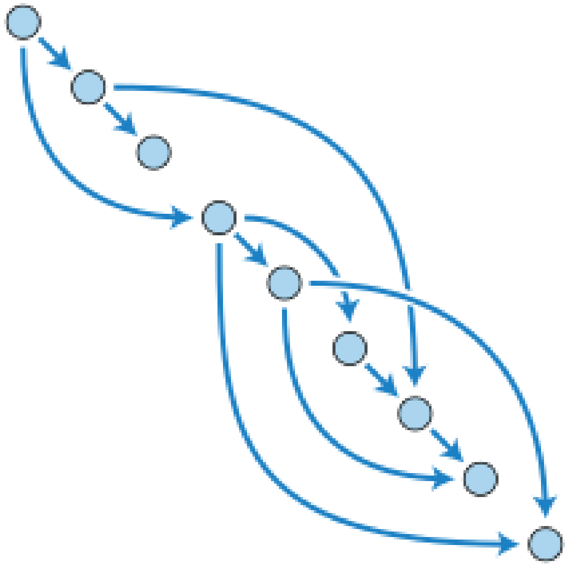
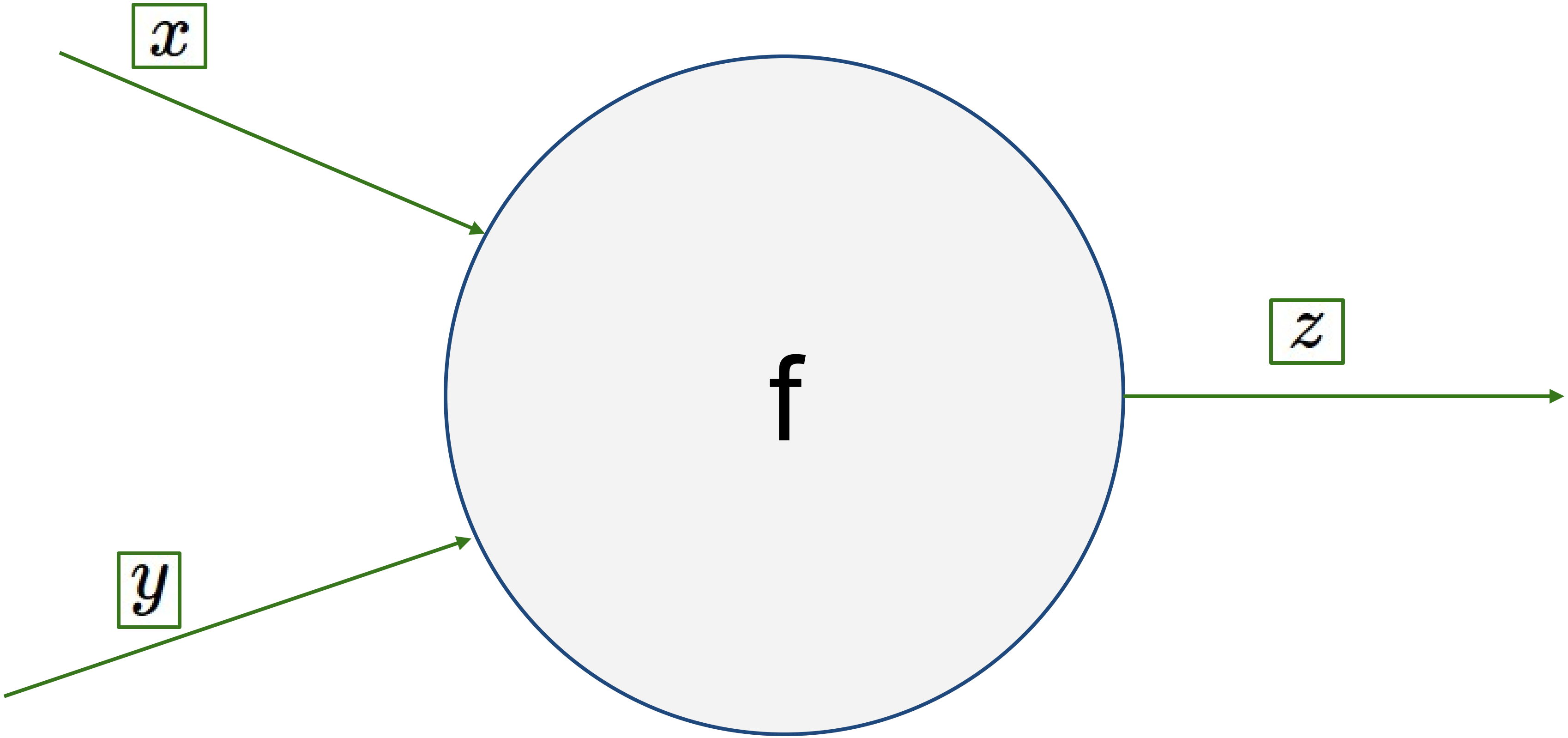
Directed Acyclic Graphs (DAGs)



A computation node



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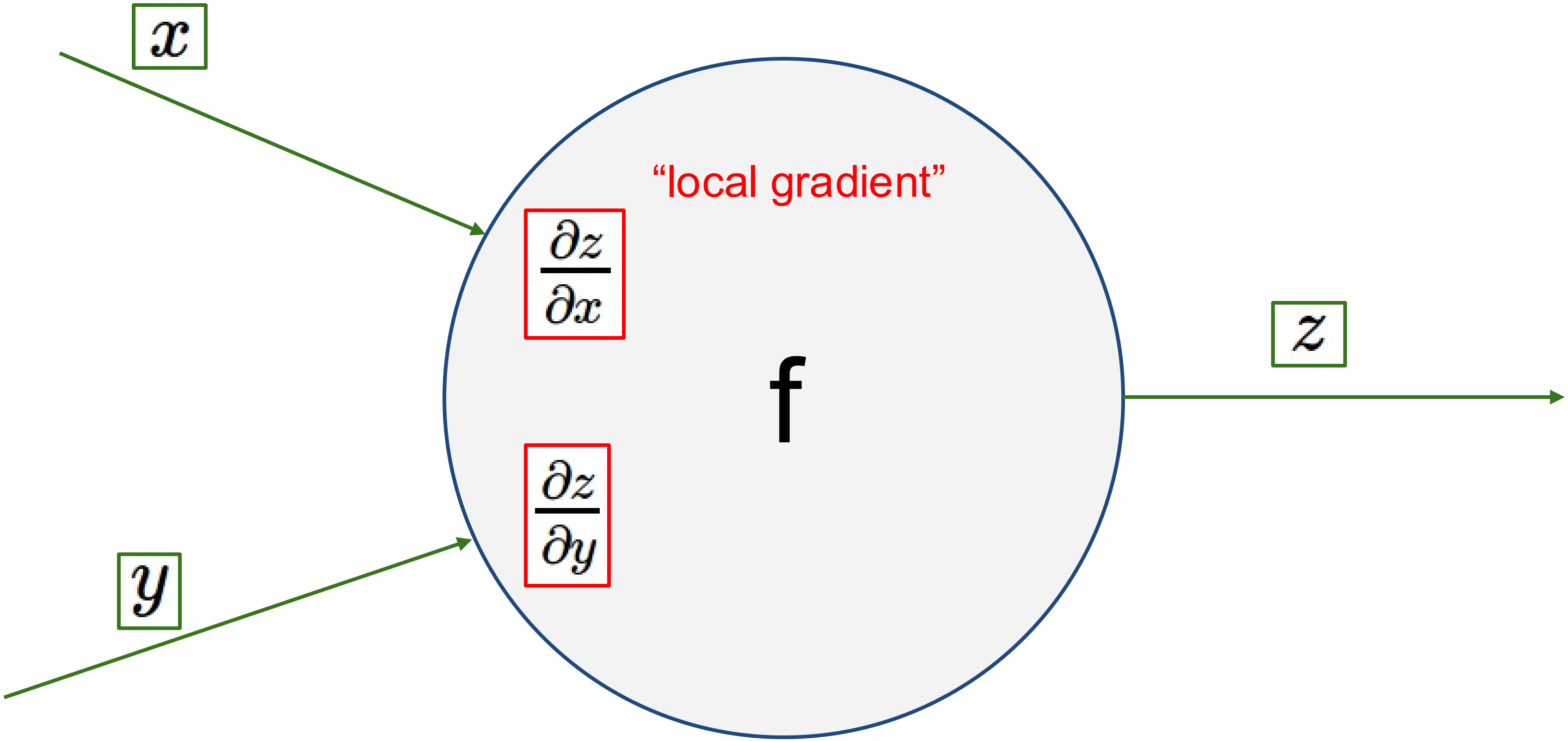
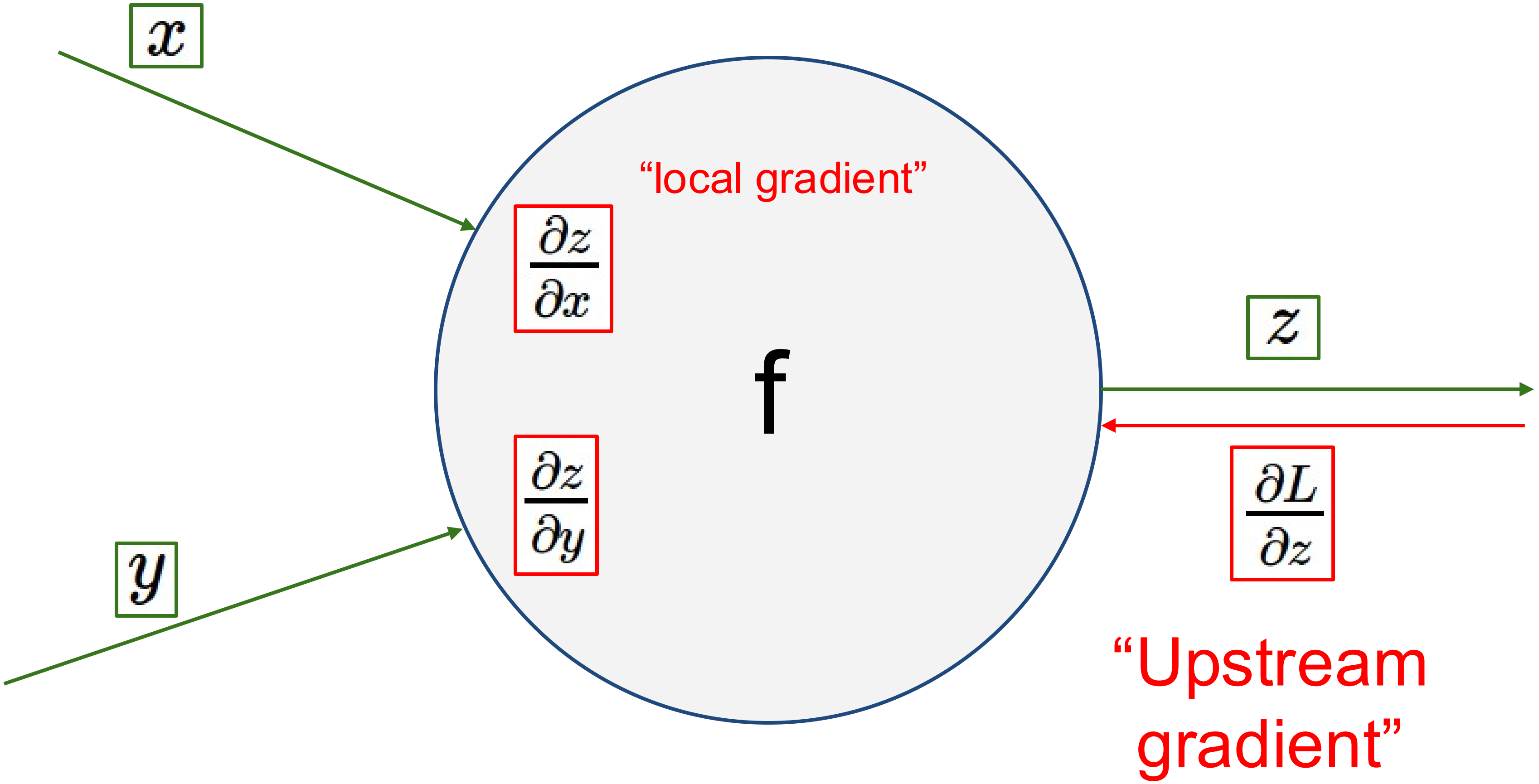

x
"local gradient"
$\frac{\partial z}{\partial x}$
z
f
$\frac{\partial z}{\partial y}$
y



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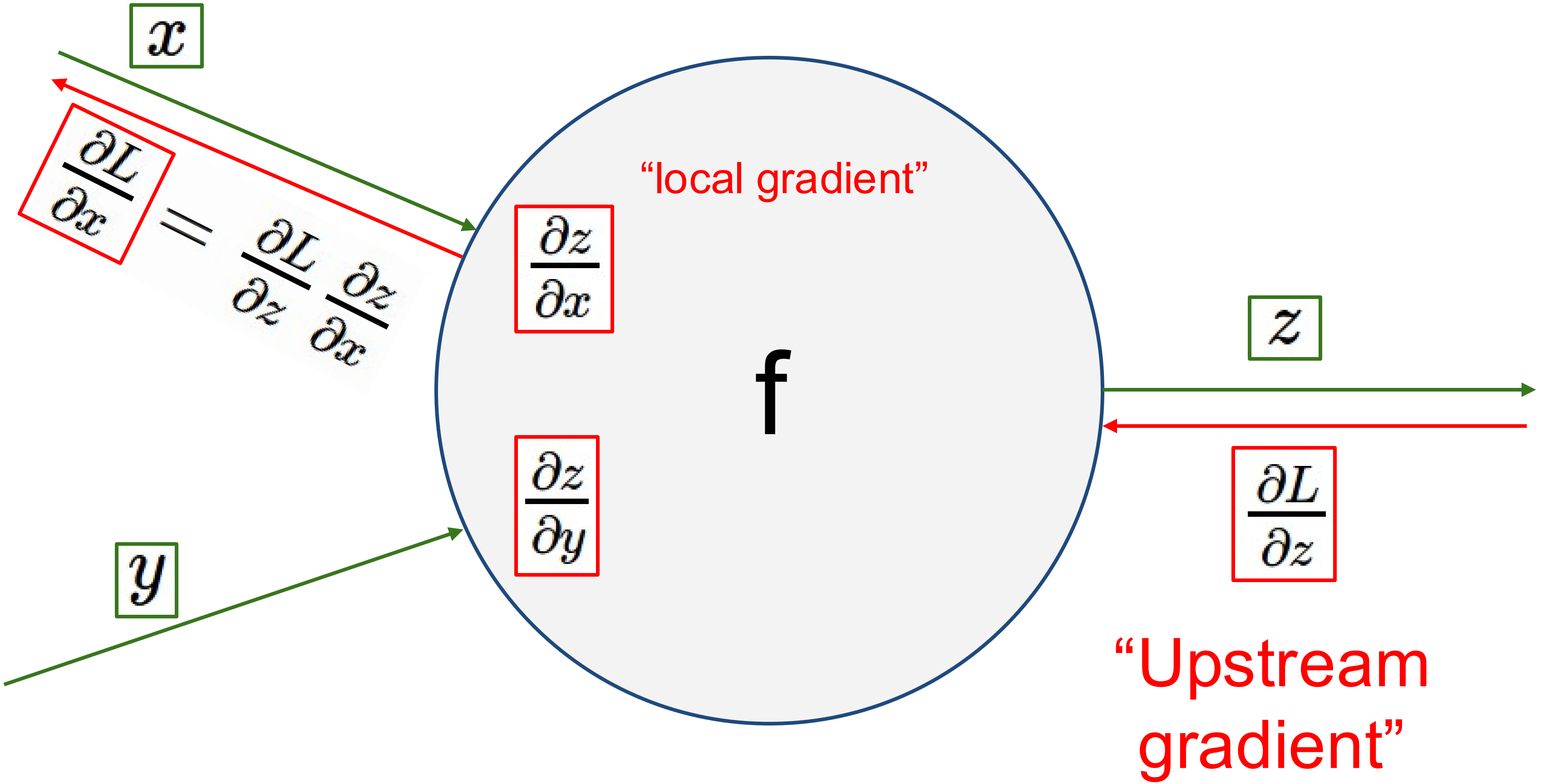

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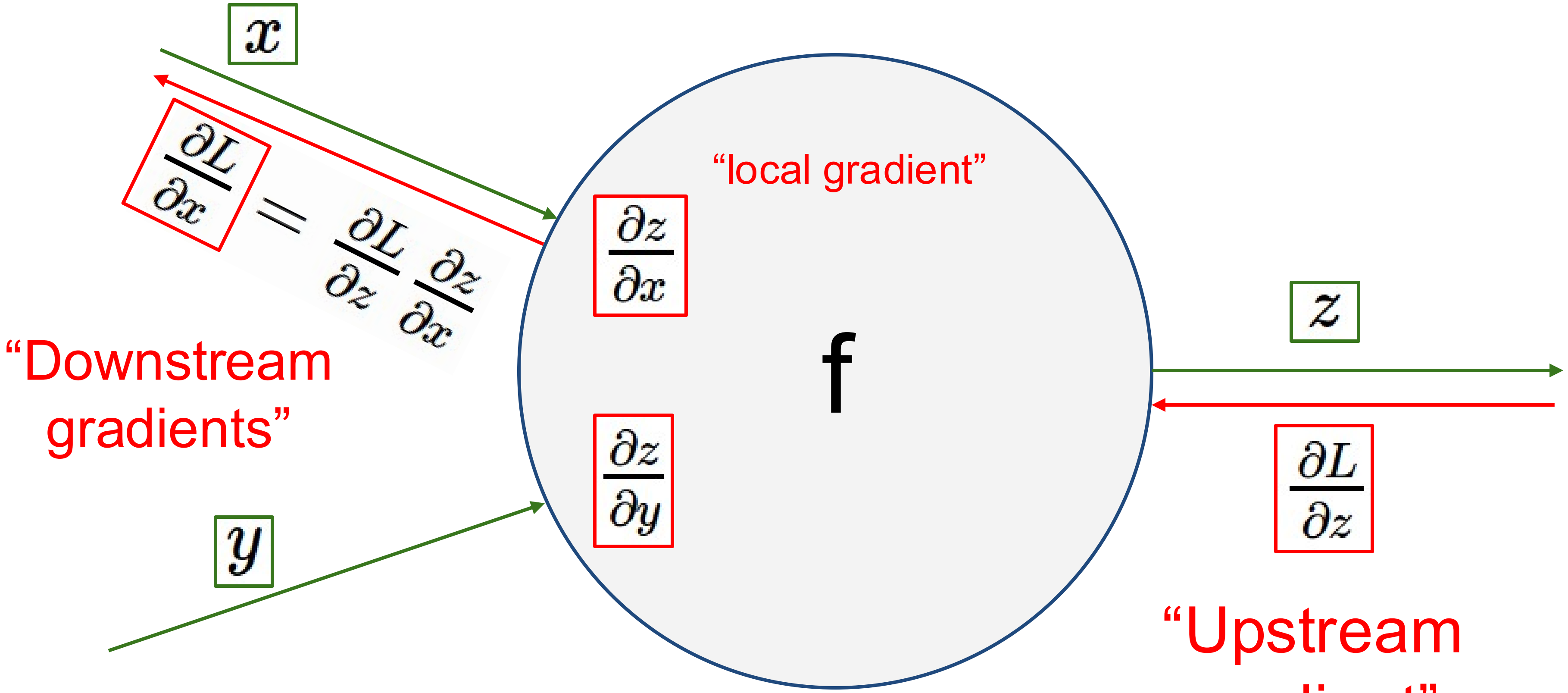

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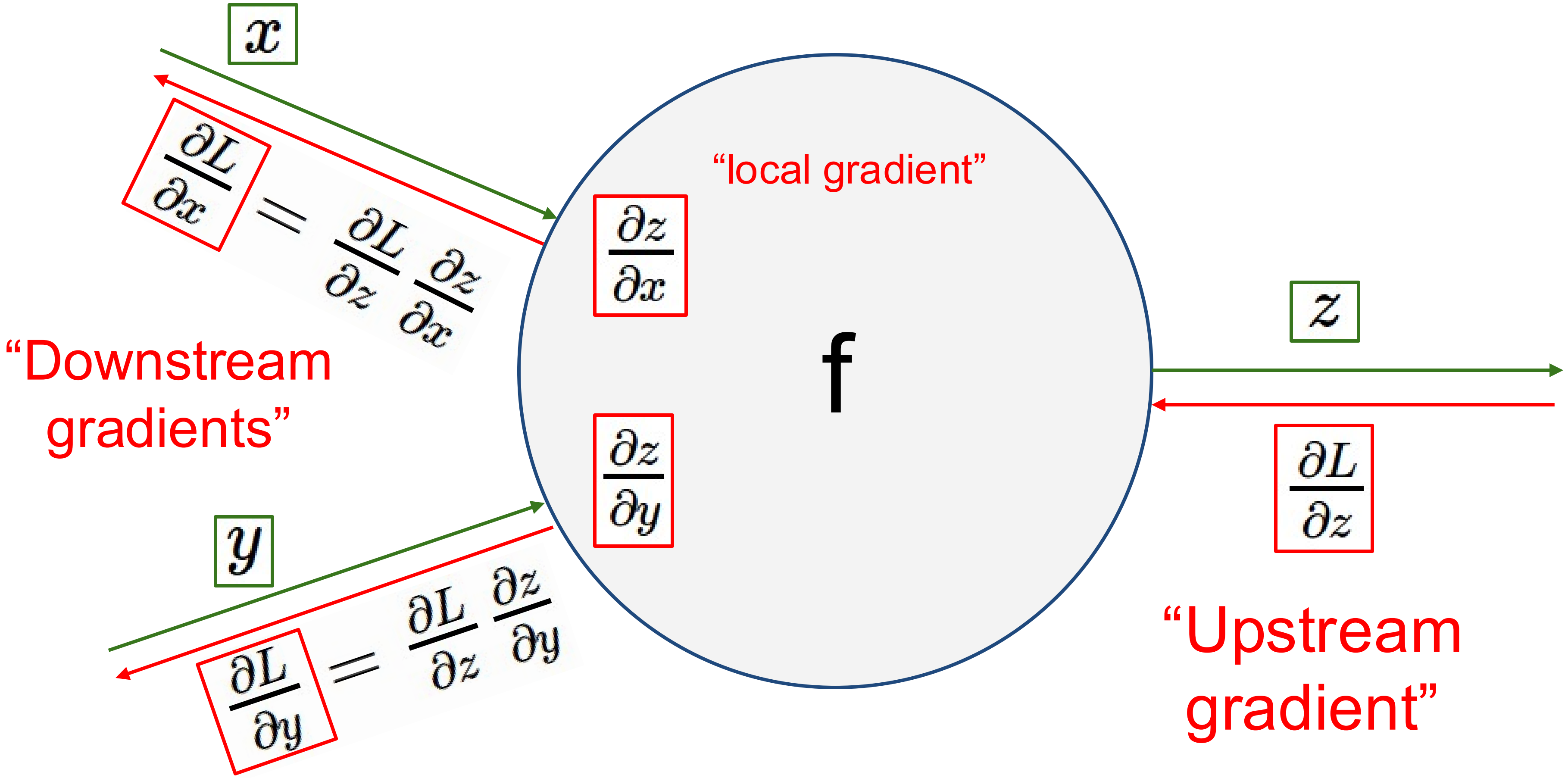

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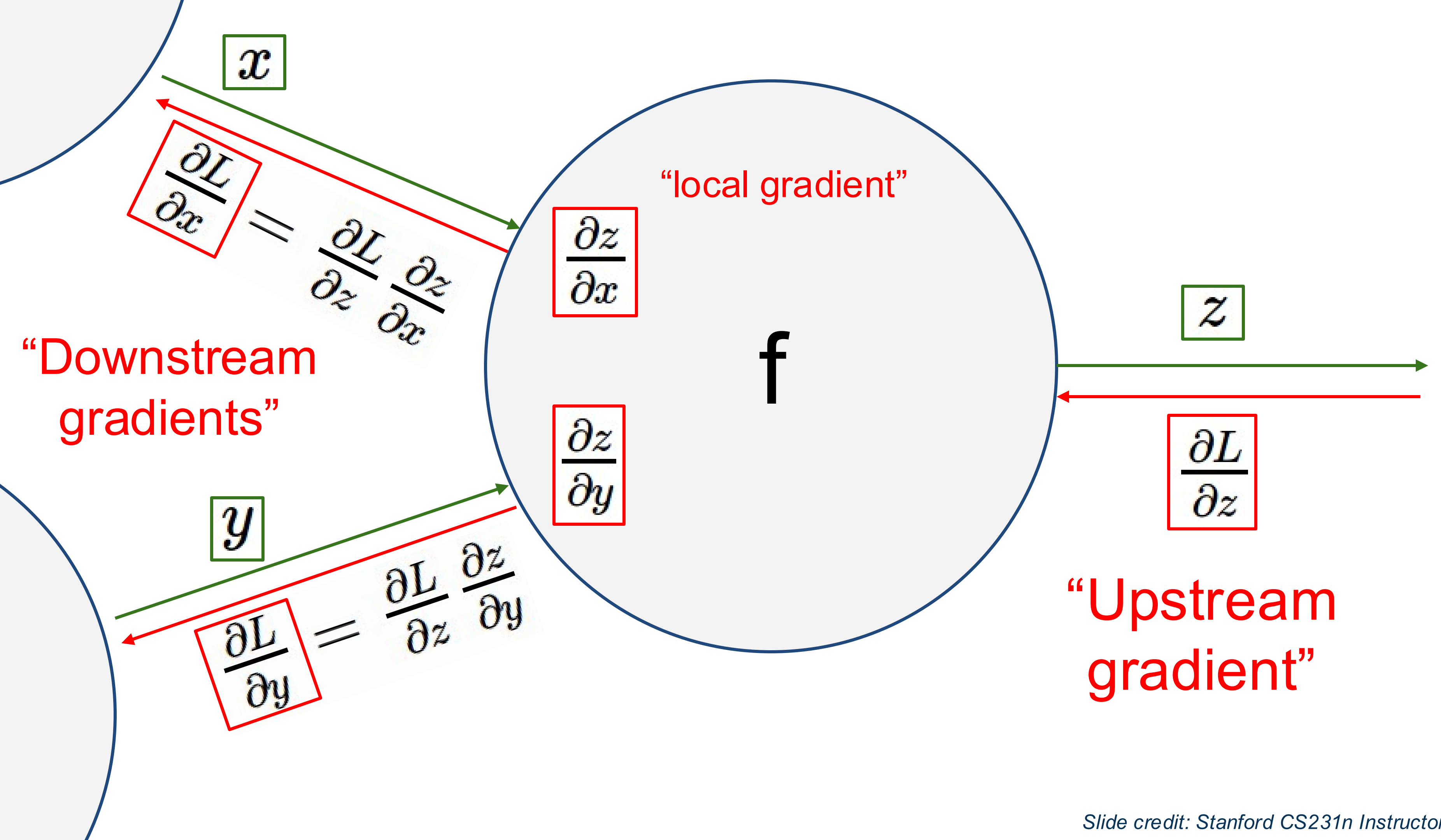

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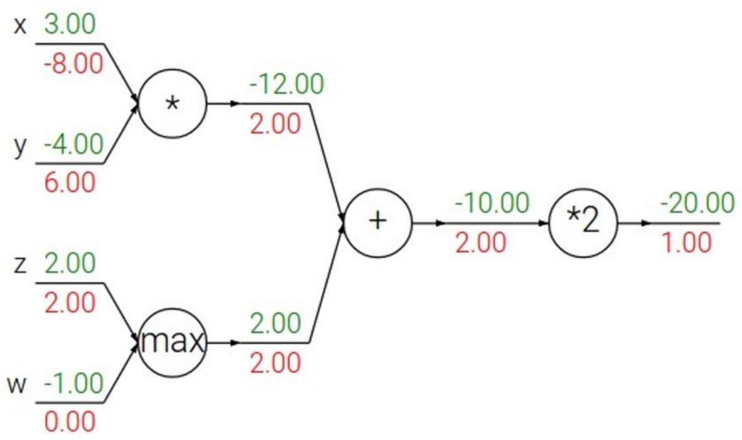
Patterns in backward flow

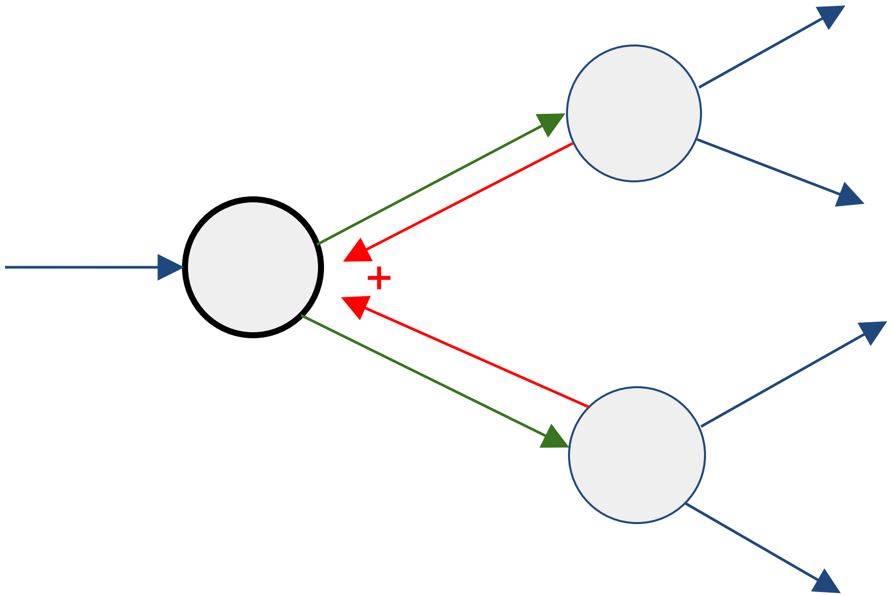
add gate: gradient distributor

max gate: gradient router

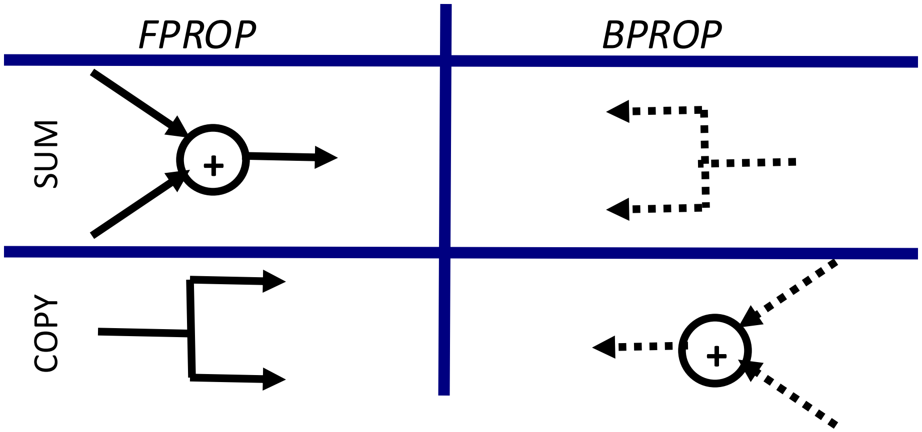
mul gate: gradient switcher



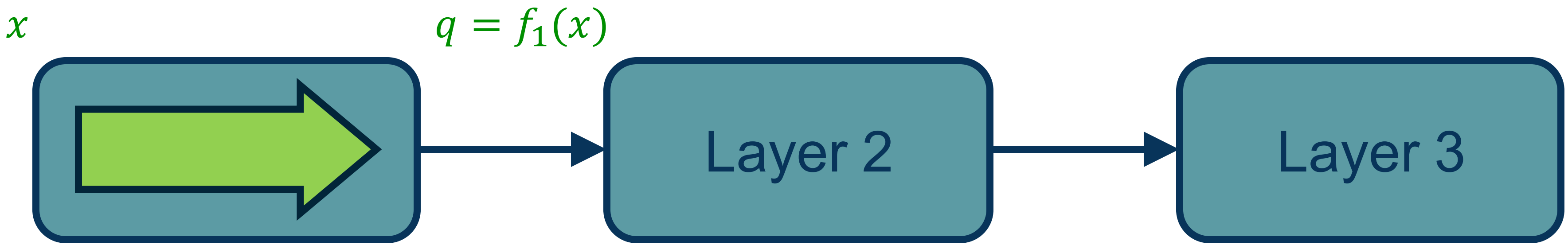
Gradients add at branches



Duality in Fprop and Bprop



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



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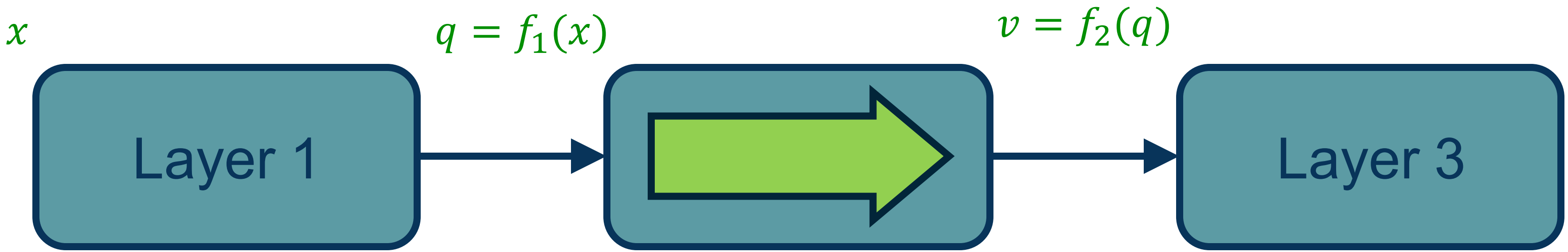

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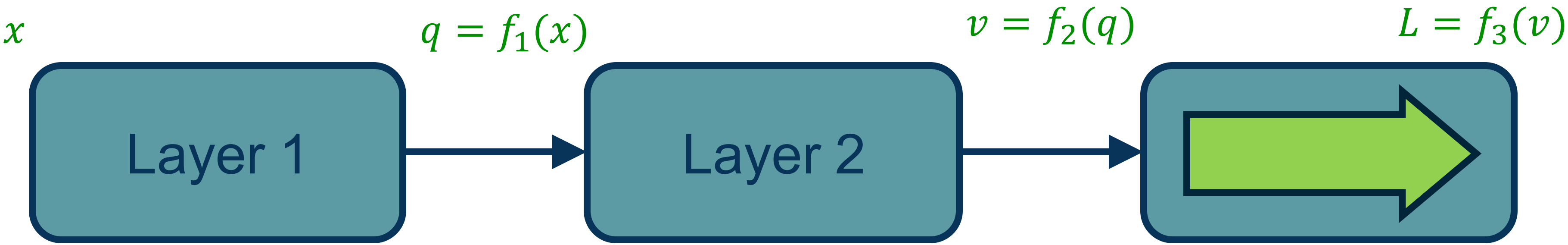


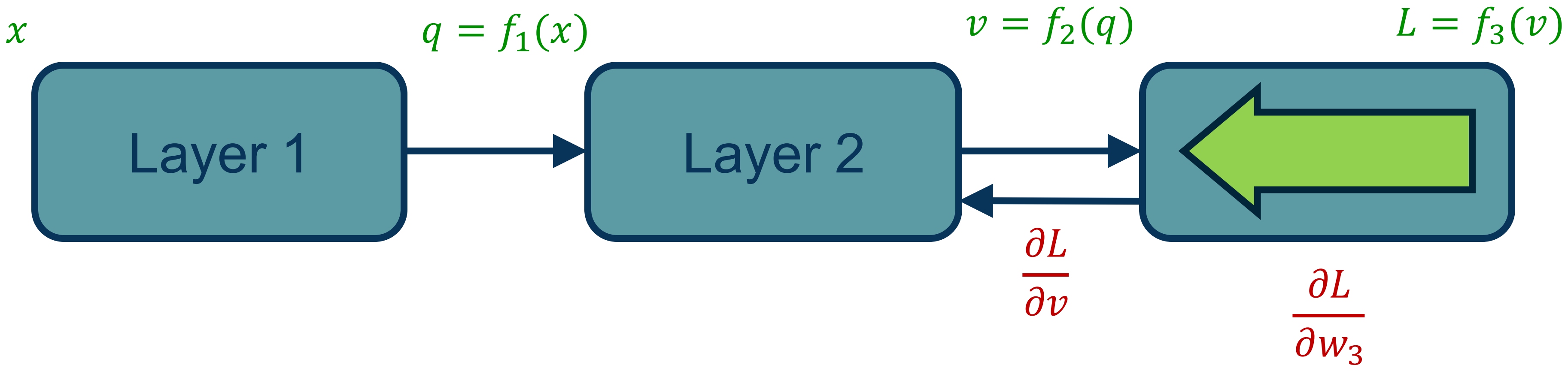
Note that we must store the **intermediate outputs of all layers**!

- 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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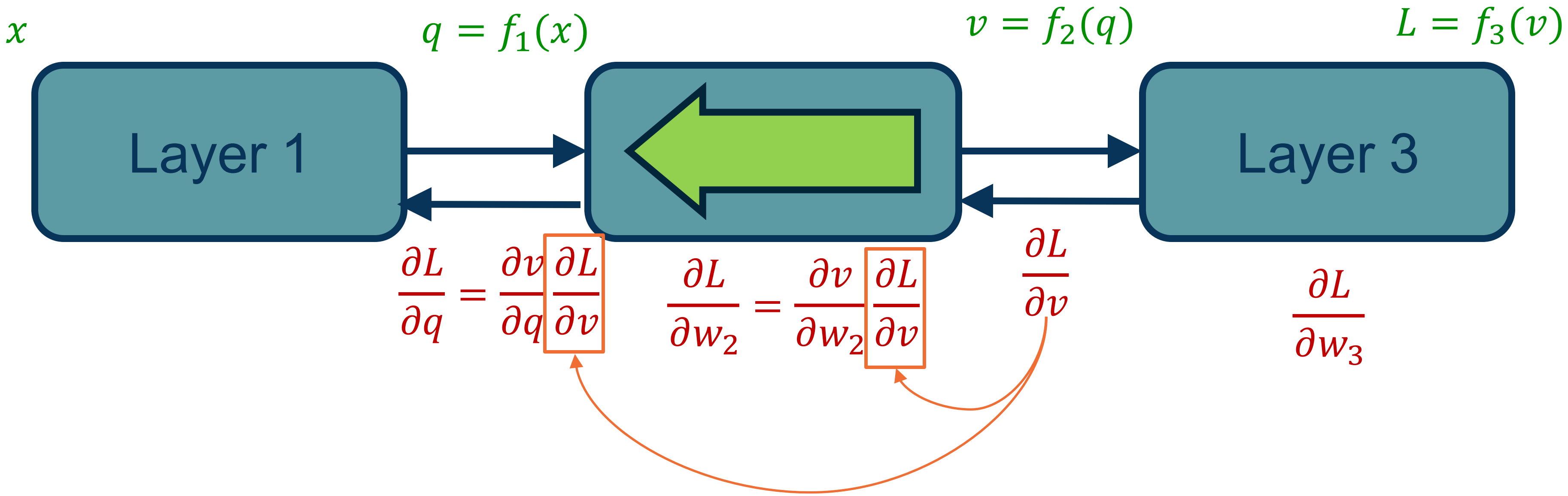

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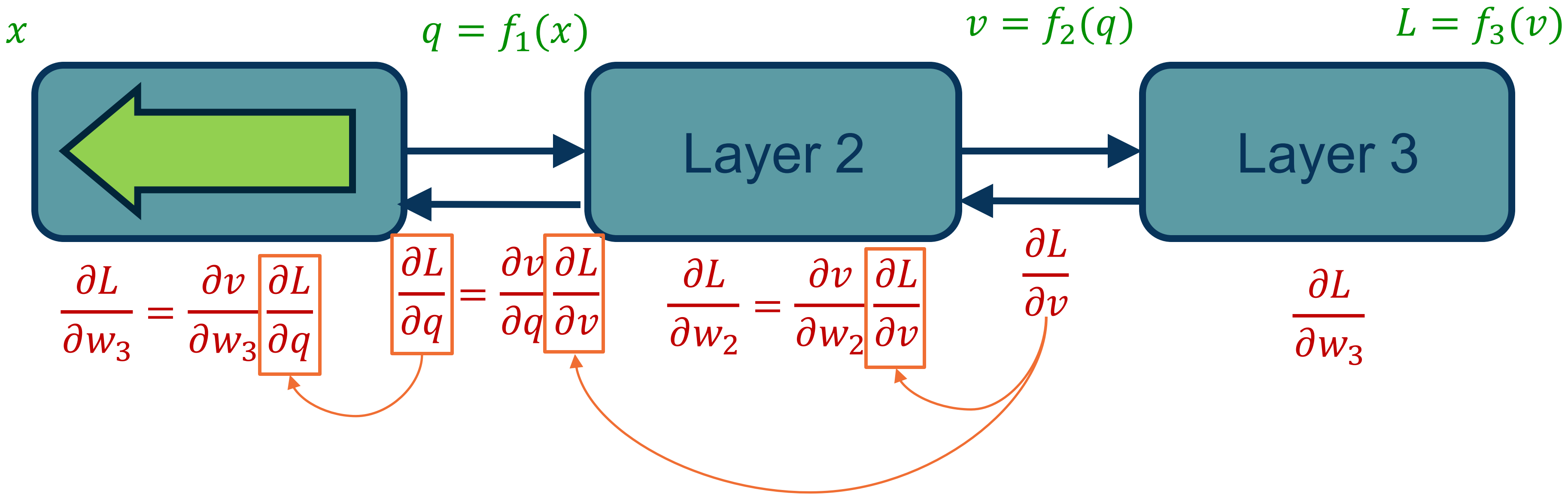
Step 1: Compute Loss on Mini-Batch: **Forward Pass**

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

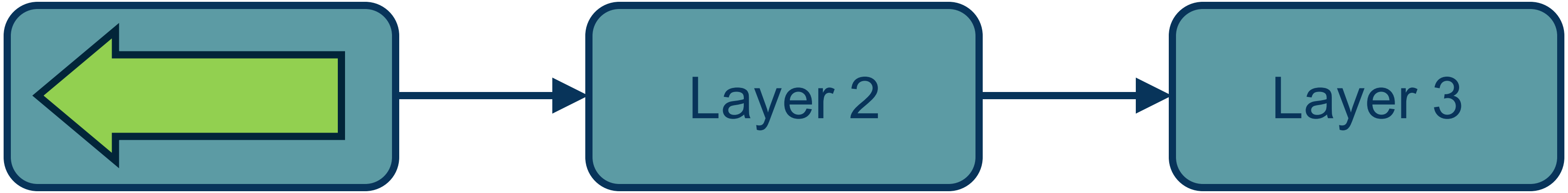


Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

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



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

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

Gradient Descent!

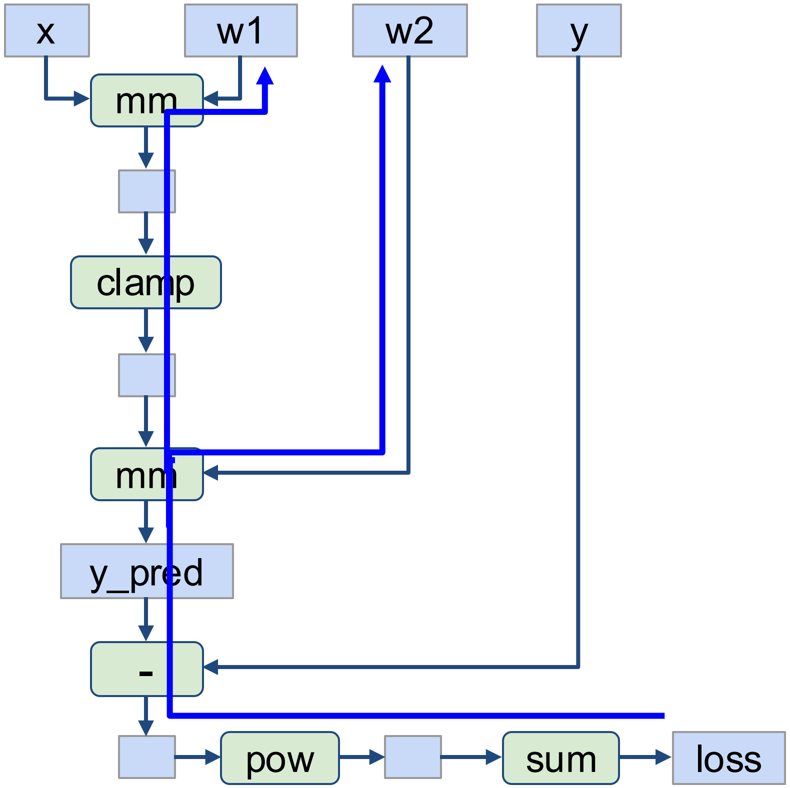
Adapted from figure by Marc'Aurelio Ranzato, Yann LeCun

Deep Learning Framework = Differentiable Programming Engine

- Computation = Graph
  - Input = Data + Parameters
  - Output = Loss
  - Scheduling = Topological ordering

- What do we need to do?
  - Generic code for representing the graph of modules
  - Specify modules (both forward and backward function)

PyTorch: **Dynamic** Computation Graphs




```python
import torch

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

learning_rate = 1e-6
for t in range(500):
    y_pred = x.mm(w1).clamp(min=0).mm(w2)
    loss = (y_pred - y).pow(2).sum()

    loss.backward()
```

Search for path between loss and w1, w2 (for backprop) AND perform computation

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:

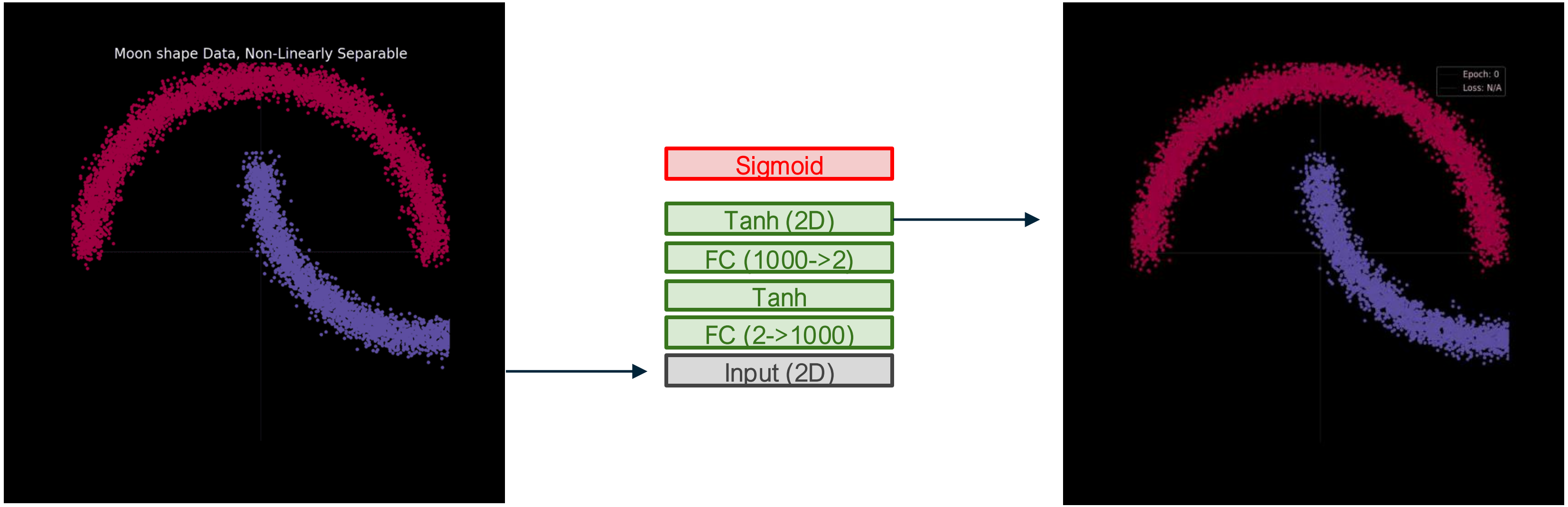
- What are neural networks?
- Non-linear functions
- How do we run backpropagation on neural nets? (Matrix Calculus!)

Neural Network

Linear classifier

(Deep) Representation Learning for Classification

A function that transforms raw data space into a linearly-separable space



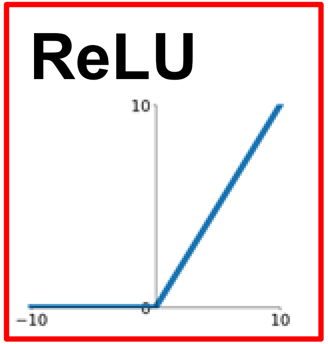
https://khalidsaifullaah.github.io/neural-networks-from-linear-algebraic-perspective

Neural networks: the original linear classifier

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

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

Neural networks: 2 layers



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

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

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

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

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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

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

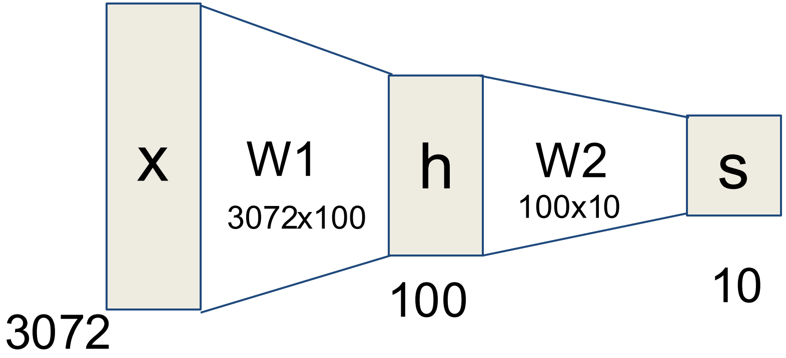
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

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

Neural networks: hierarchical computation

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

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



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

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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?

$$f = W_2 W_1 x$$

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Neural networks: why is max operator important?

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

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

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.

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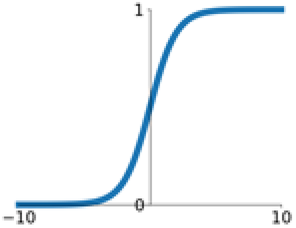
Activation functions

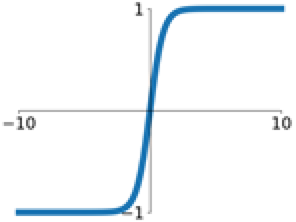
Sigmoid

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



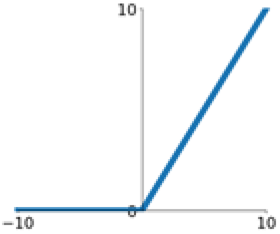
tanh

$\tanh(x)$



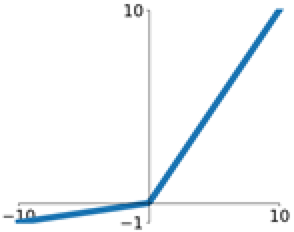
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

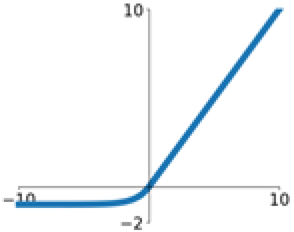


Maxout

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

ELU

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



More on this in week 6…

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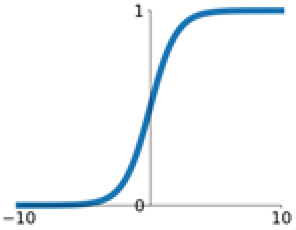
Activation functions

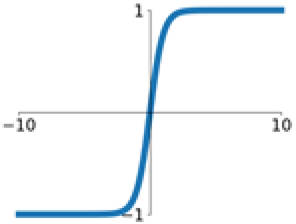
Sigmoid

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



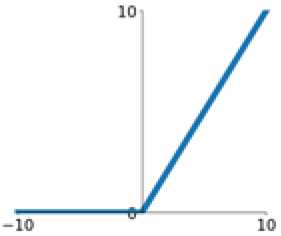
tanh

$\tanh(x)$



ReLU

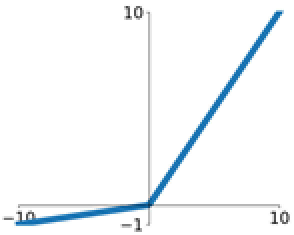
$\max(0, x)$



ReLU is a good default choice for most problems

Leaky ReLU

$\max(0.1x, x)$



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

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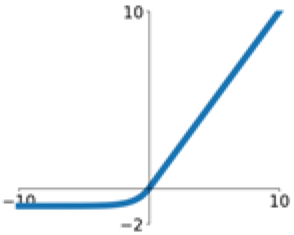
$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



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Neural Networks are 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?

Neural Networks are 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 exact 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

Neural Networks are 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)?

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

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

Neural Networks are 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 σ be any continuous discriminatory function. Then finite sums of the form*

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

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

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

Plain English: as long as the activation function is <u>sigmoid-like</u> and the function to be approximated is <u>continuous</u>, there exists a neural network with a single hidden layer that can approximate it with certain error (bounded uniform norm).

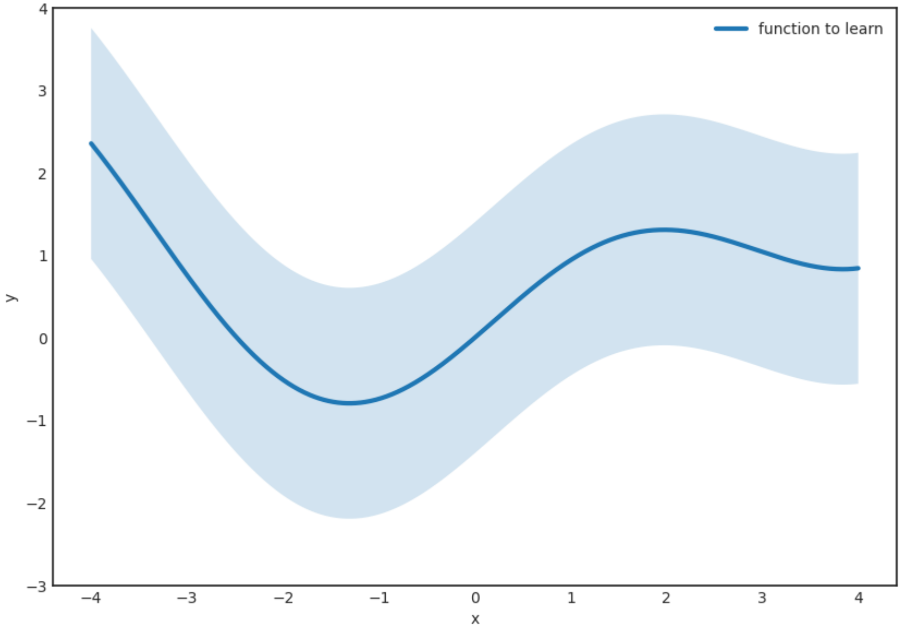
Adapted from https://tivadardanka.com/blog/universal-approximation-theorem

Neural Networks are 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 ϵ (shaded band) with a single layer NN $F(x)$



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Neural Networks are Universal Function Approximators

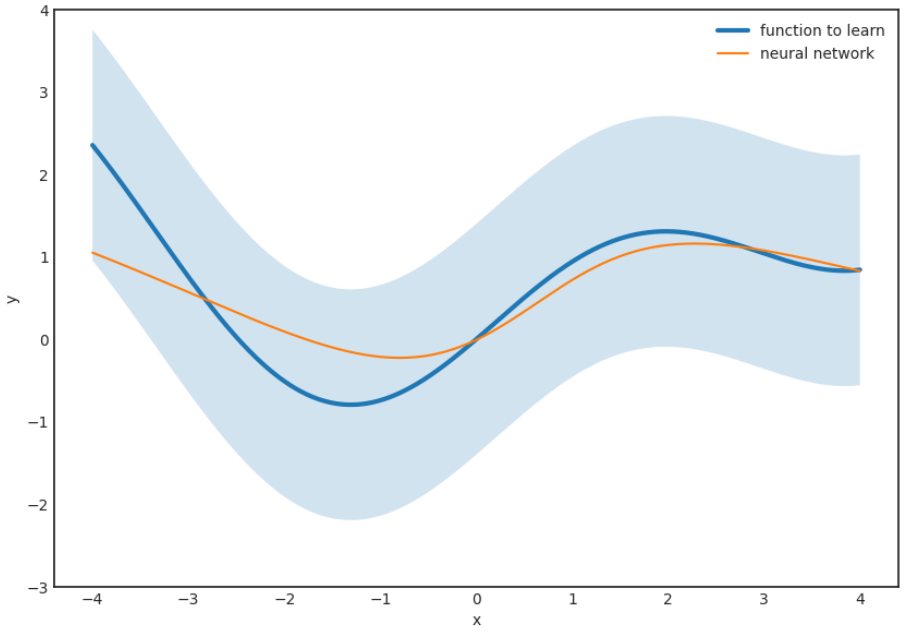
Claim: Neural Networks with certain non-linear activation functions are universal function approximators.

A 1-D example of the universal approximation theorem

We want to approximate $g(x)$ bounded by some small error ϵ (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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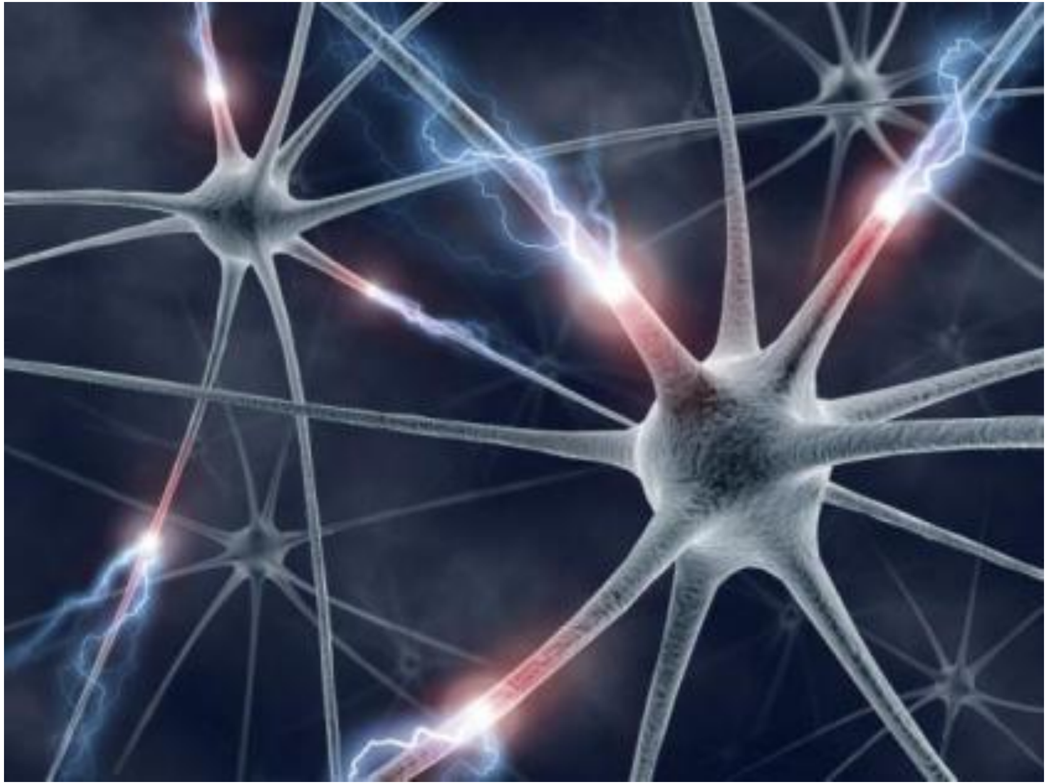
Why are they called Neural Networks, anyway?



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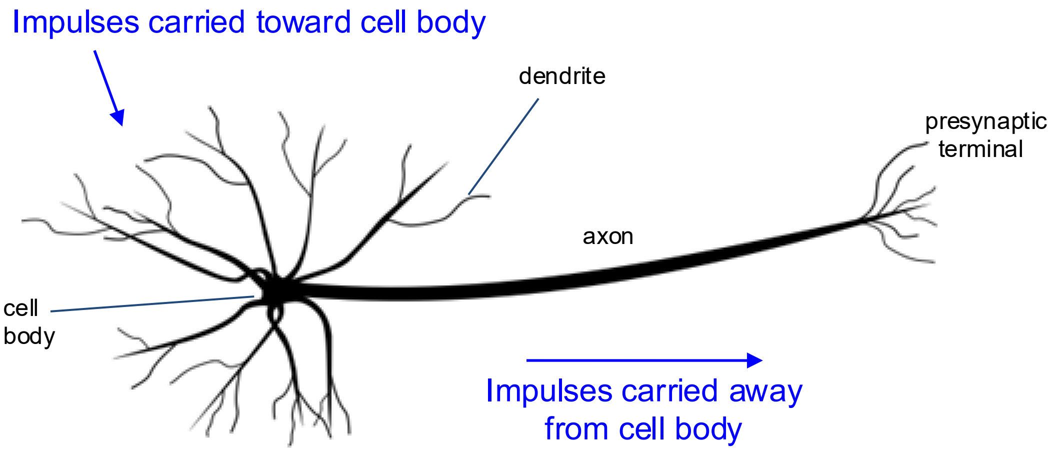
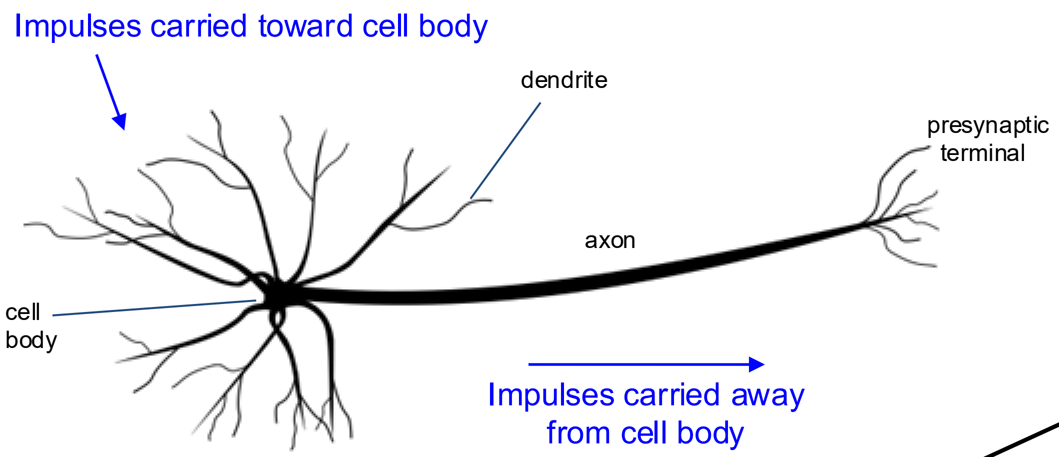
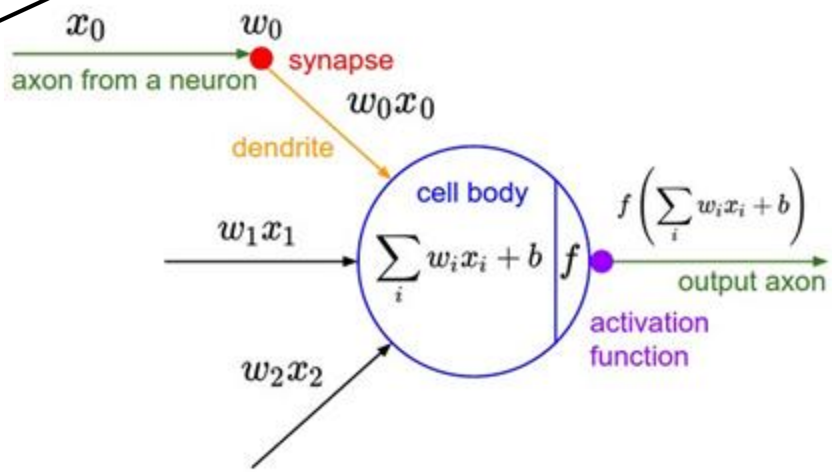

Impulses carried toward cell body
dendrite
presynaptic
terminal
axon
cell
body
Impulses carried away
from cell body





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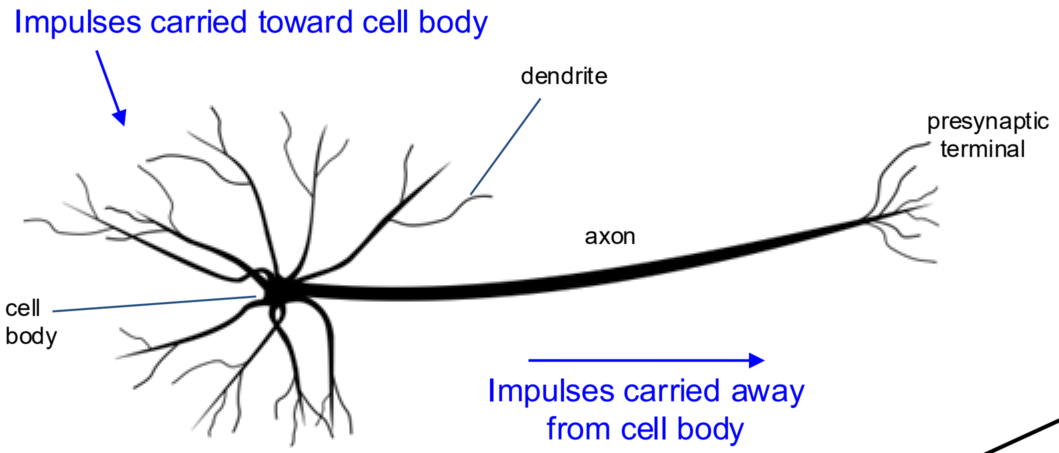
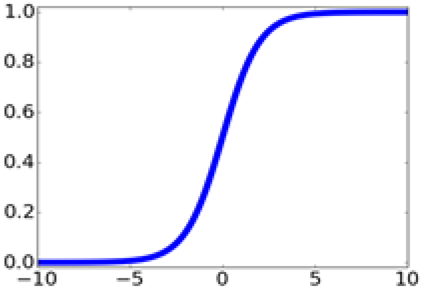
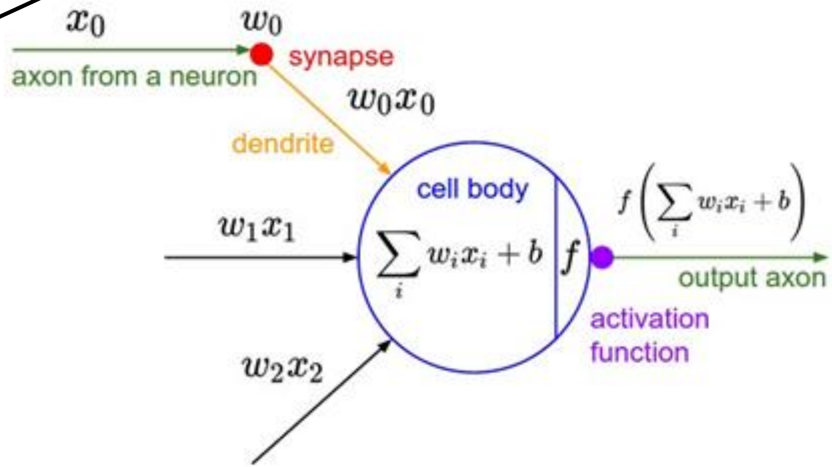




sigmoid activation function

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



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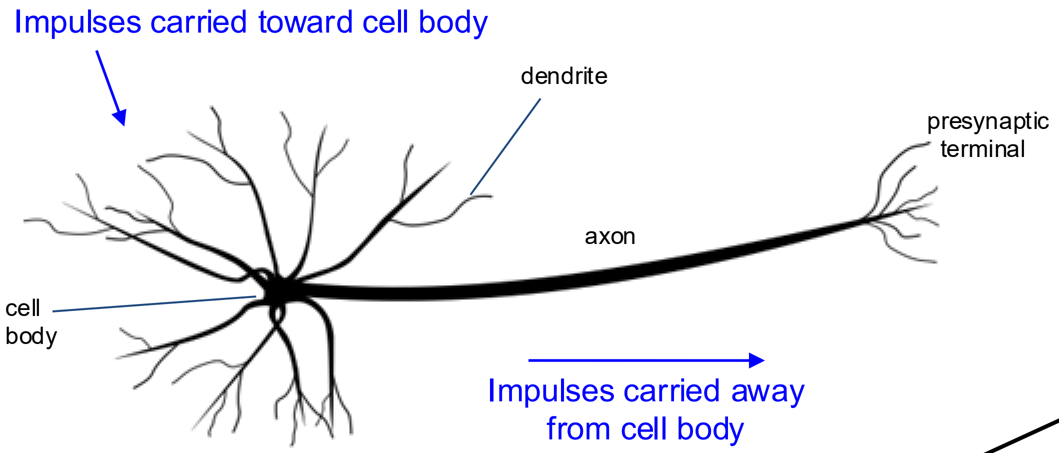
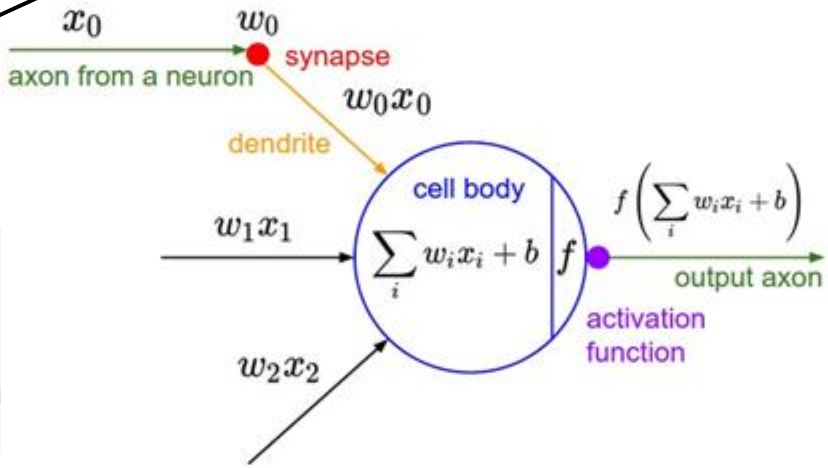



```python
class Neuron:
  # ...
  def neuron_tick(inputs):
    """ assume inputs and weights are 1-D numpy arrays and bias is a number """
    cell_body_sum = np.sum(inputs * self.weights) + self.bias
    firing_rate = 1.0 / (1.0 + math.exp(-cell_body_sum)) # sigmoid activation func
    return firing_rate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



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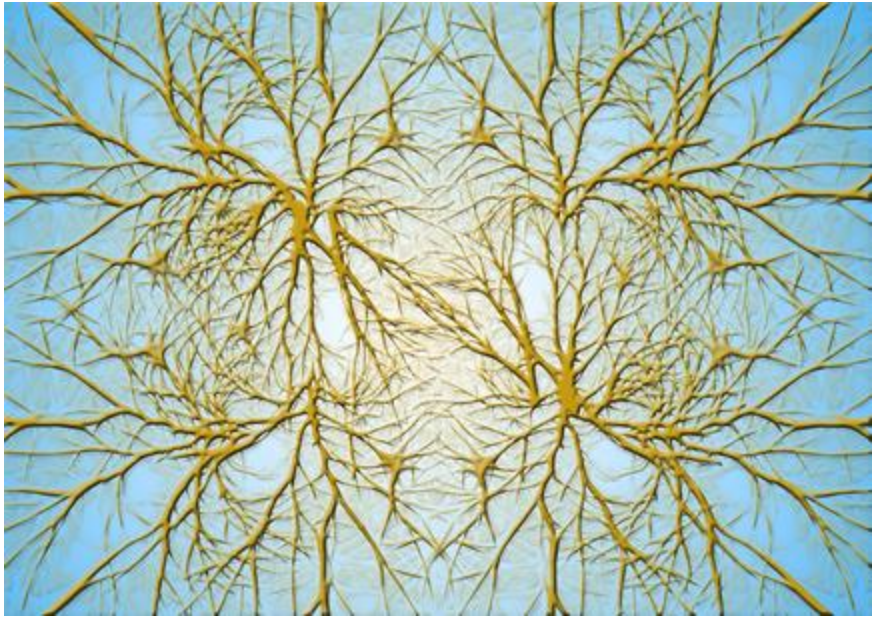
Biological Neurons:
Complex connectivity patterns



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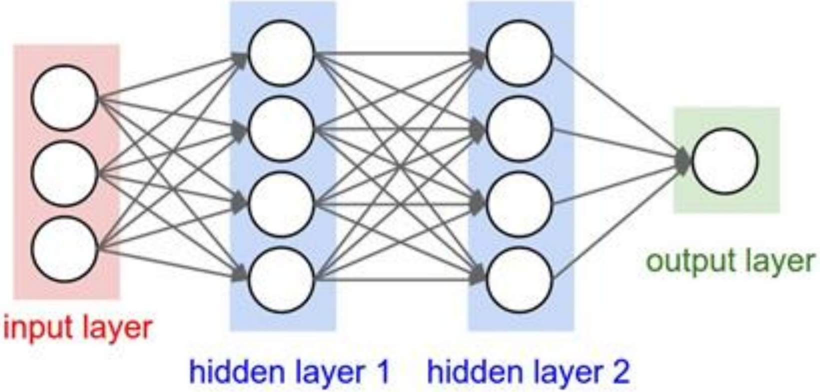
Neurons in a neural network:
Organized into regular layers for computational efficiency



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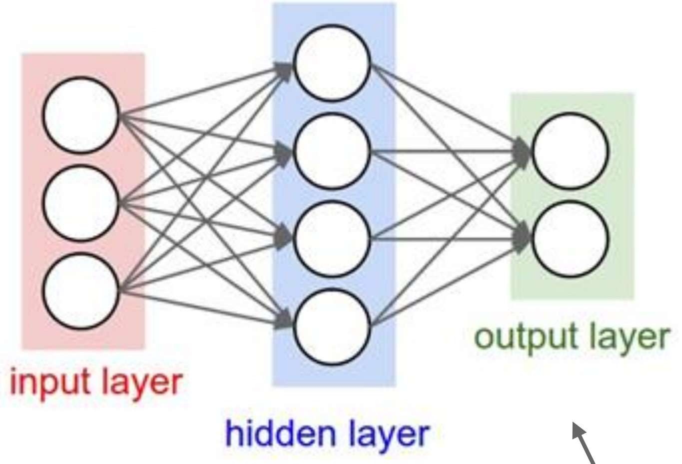
Be very careful with your brain analogies!

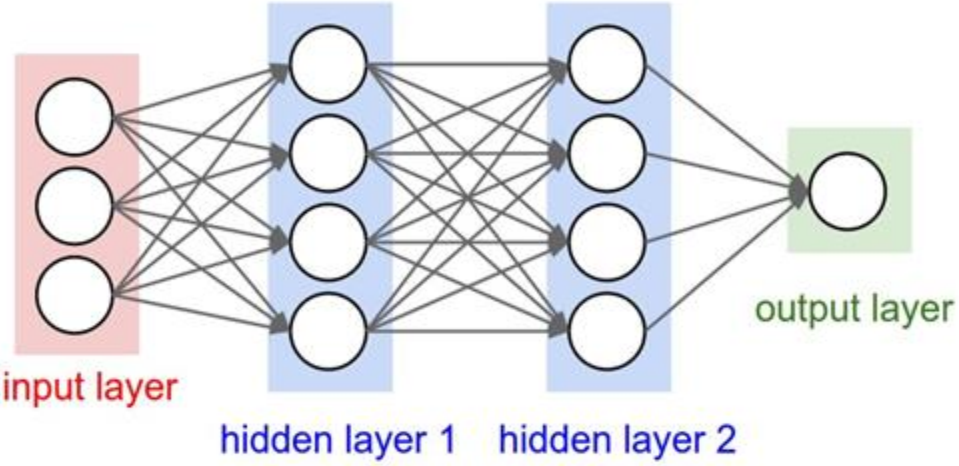
Biological Neurons:

- 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"

"Fully-connected" layers

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

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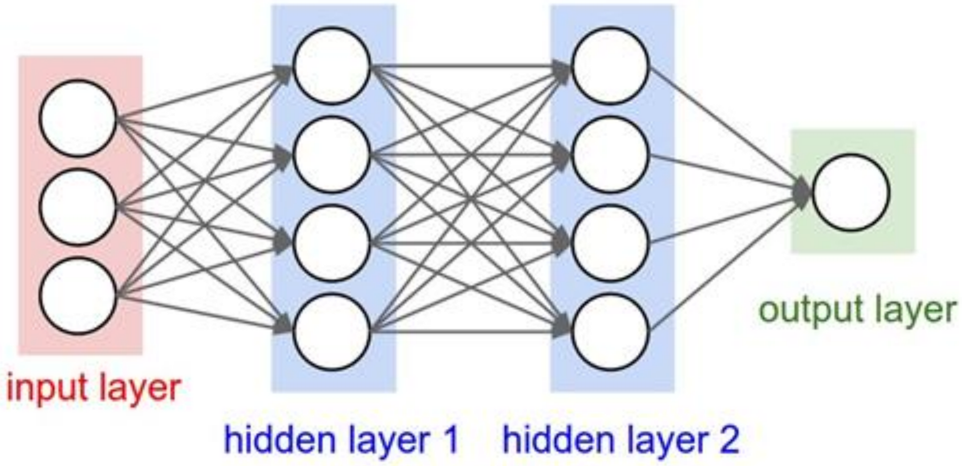
Example feed-forward computation of a neural network




```
# 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:

```python
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
  w2 -= 1e-4 * grad_w2
```

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Define the network

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Define the network

Forward pass

Slide credit: Stanford CS231n Instructors

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```

Define the network

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  grad_h = grad_y_pred.dot(w2.T)
  grad_w1 = x.T.dot(grad_h * h * (1 - h))
```

Calculate the analytical gradients

```python
  w1 -= 1e-4 * grad_w1
  w2 -= 1e-4 * grad_w2
```

Slide credit: Stanford CS231n Instructors

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```

Define the network

Forward pass

Calculate the analytical gradients

Gradient descent

Slide credit: Stanford CS231n Instructors

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  w1 -= 1e-4 * grad_w1
  w2 -= 1e-4 * grad_w2
```

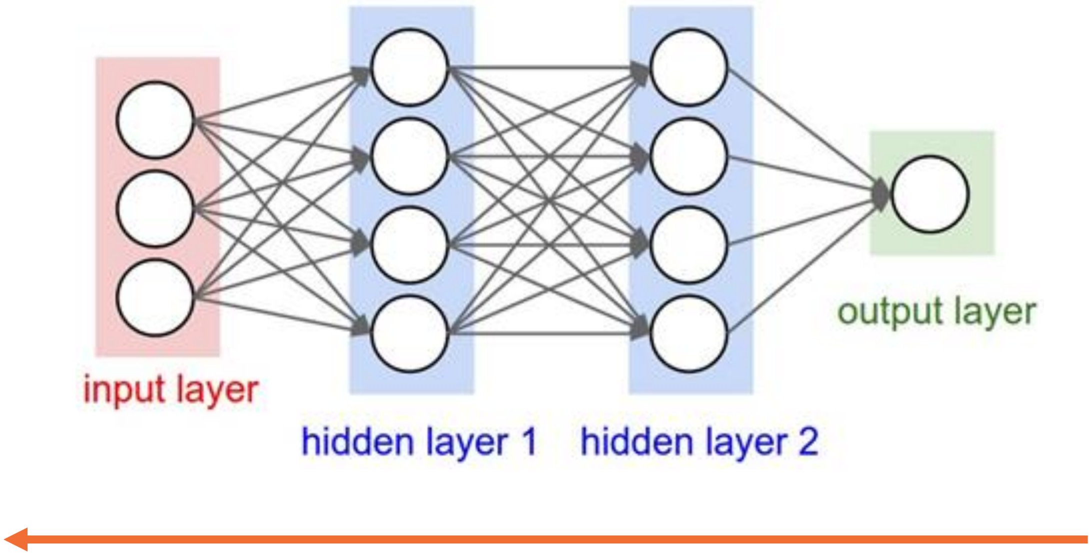
matrix

Calculate the analytical gradients

How to derive this?

Slide credit: Stanford CS231n Instructors

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?

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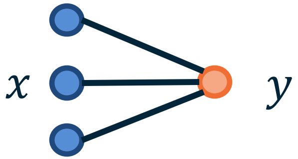
Vector to Scalar

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

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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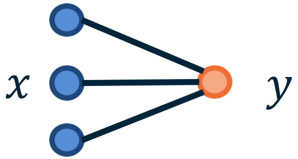


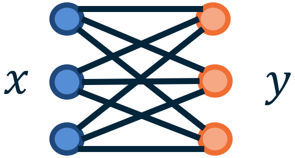
Vector to Vector

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

Derivative is **Jacobian**:

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

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



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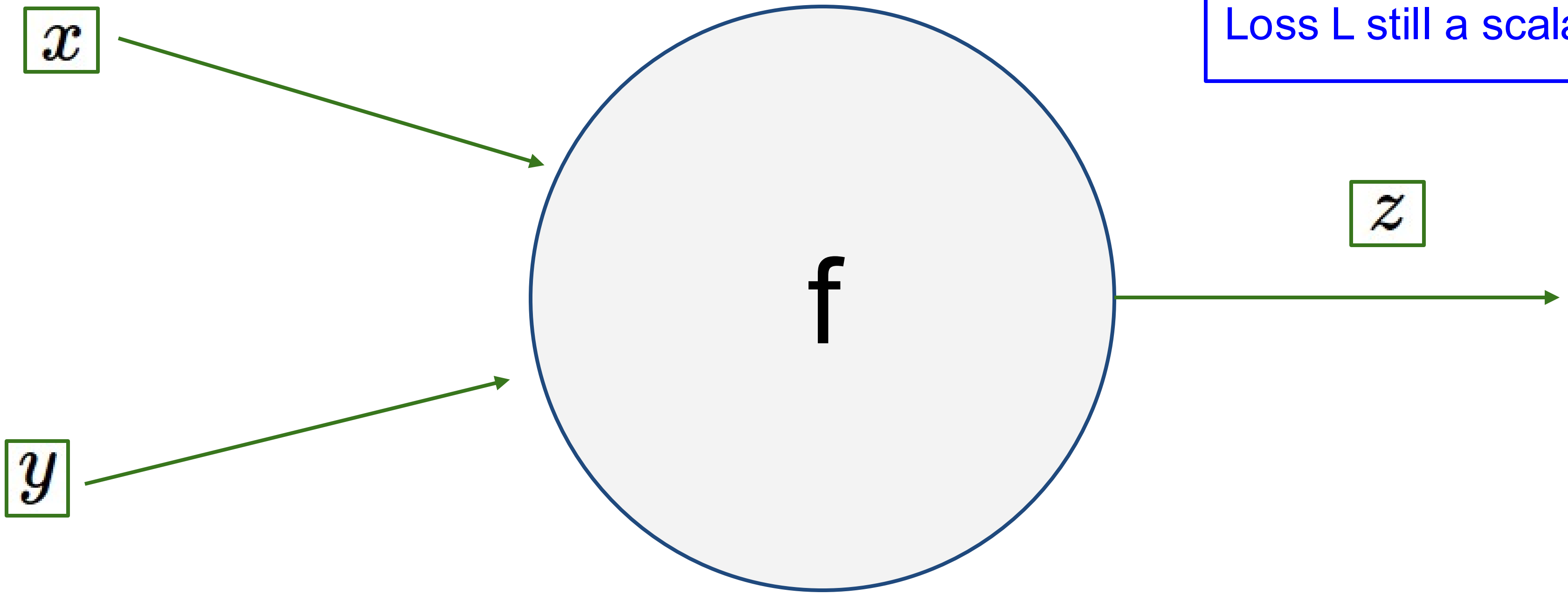
Jacobians

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

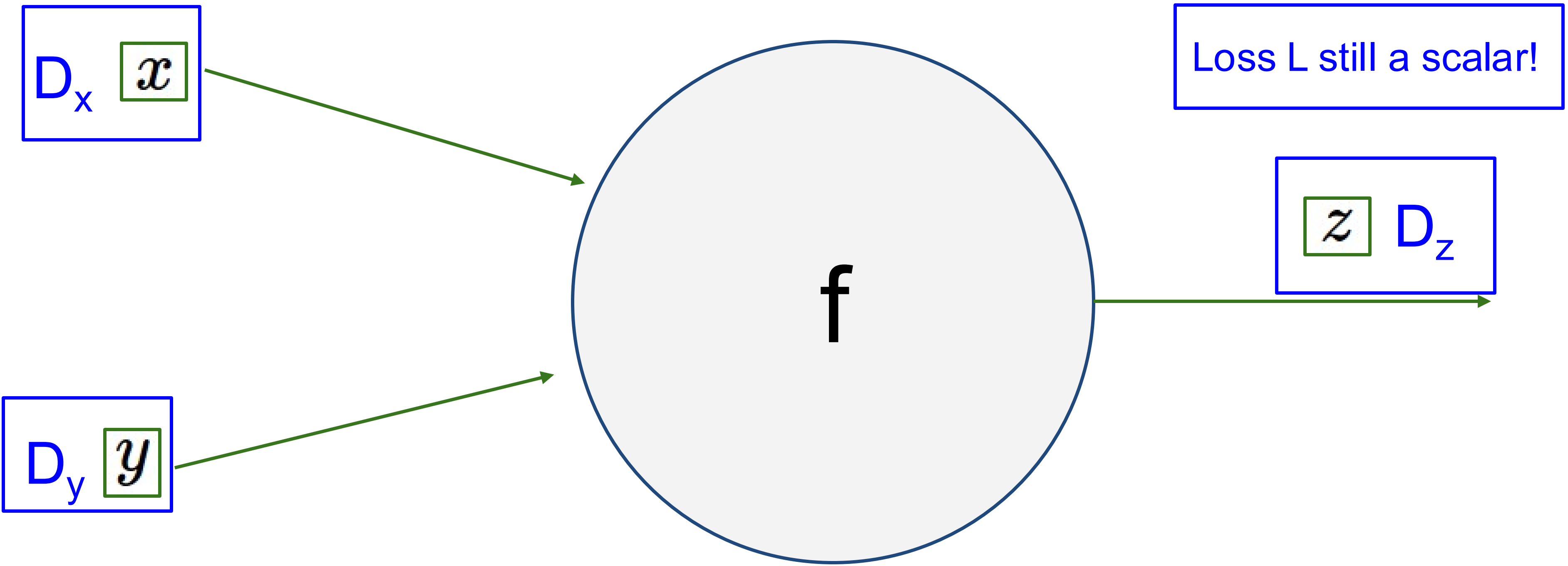
Backprop with Vectors



Loss L still a scalar!

Slide credit: Stanford CS231n Instructors

Backprop with Vectors



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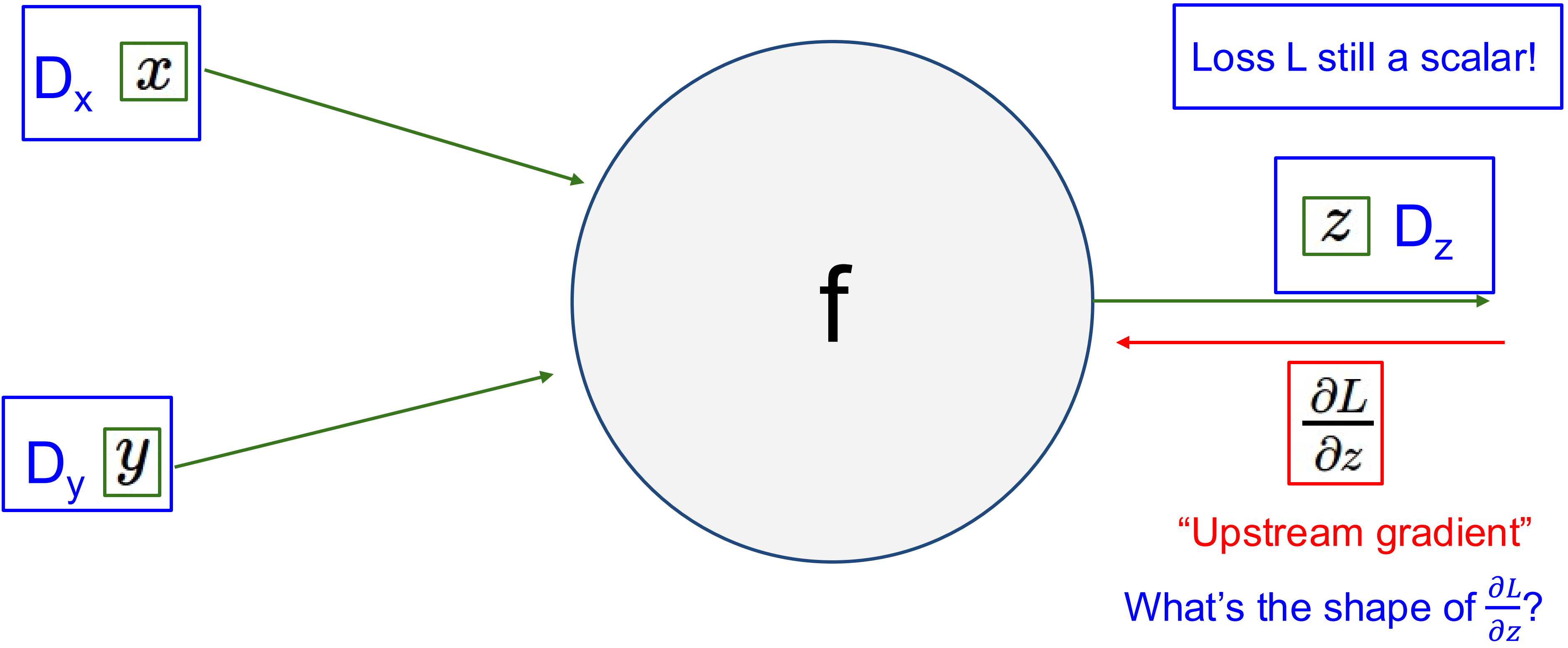
Backprop with Vectors



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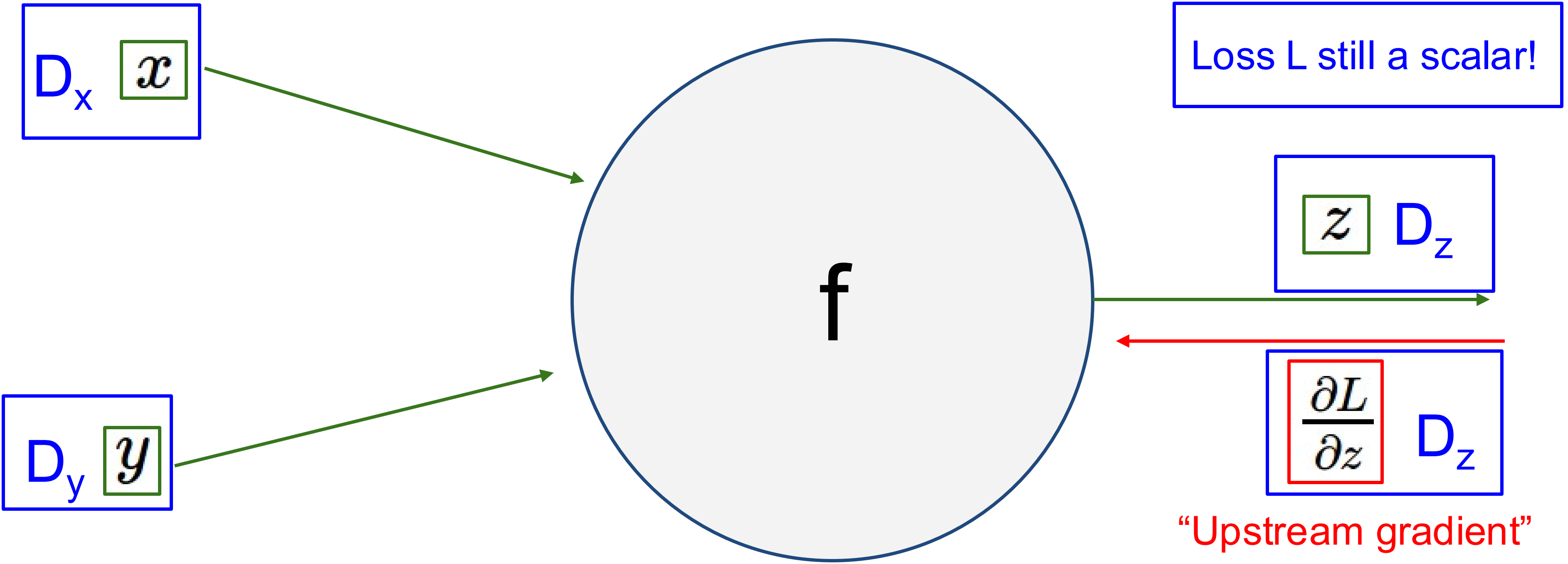
Backprop with Vectors



"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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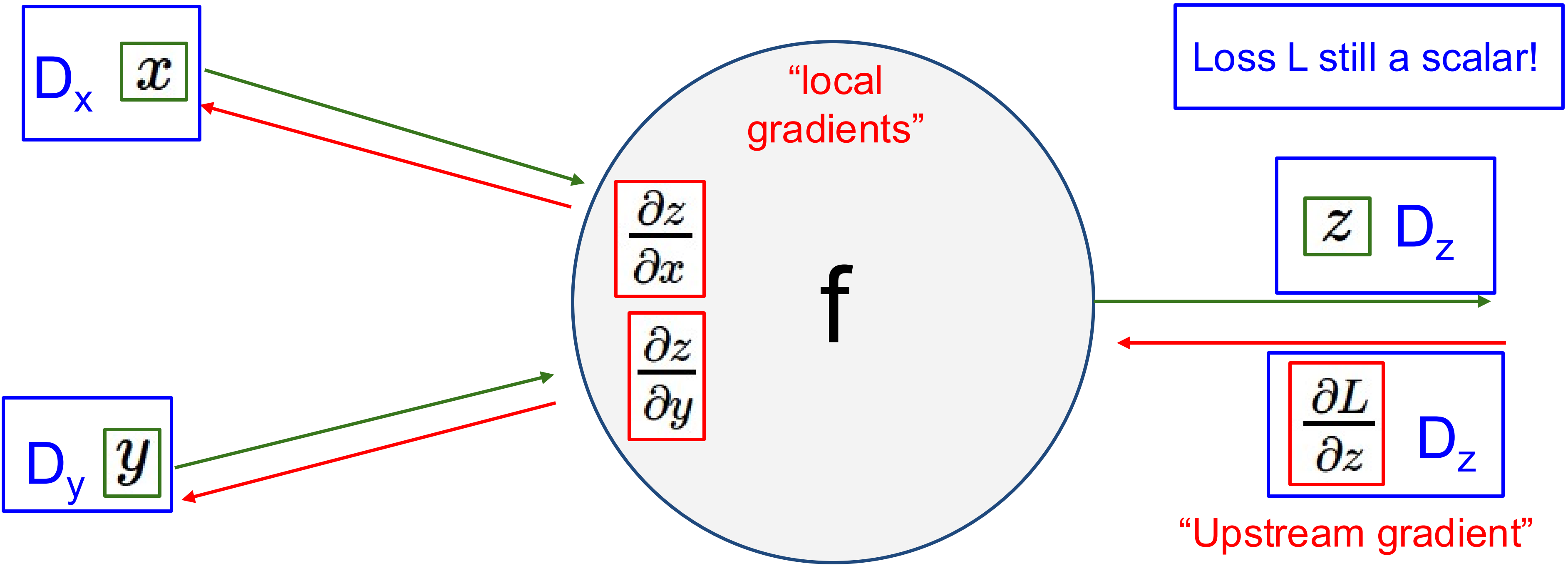
Backprop with Vectors



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

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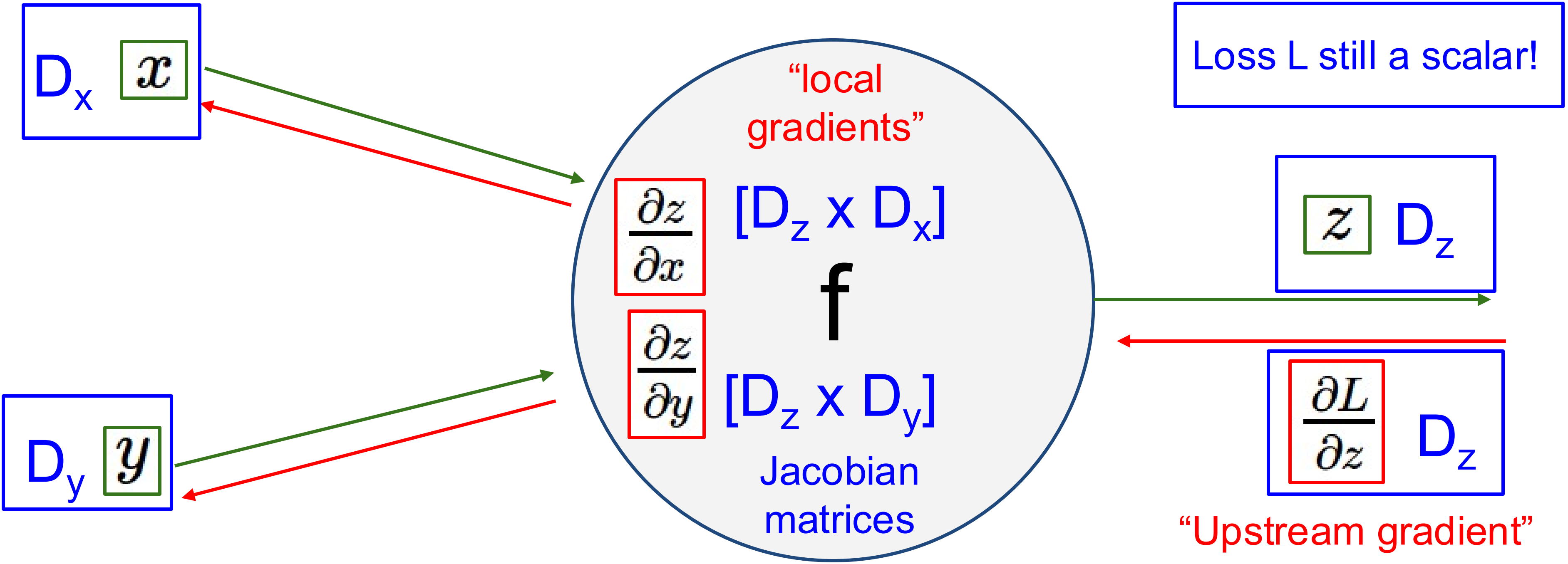
Backprop with Vectors



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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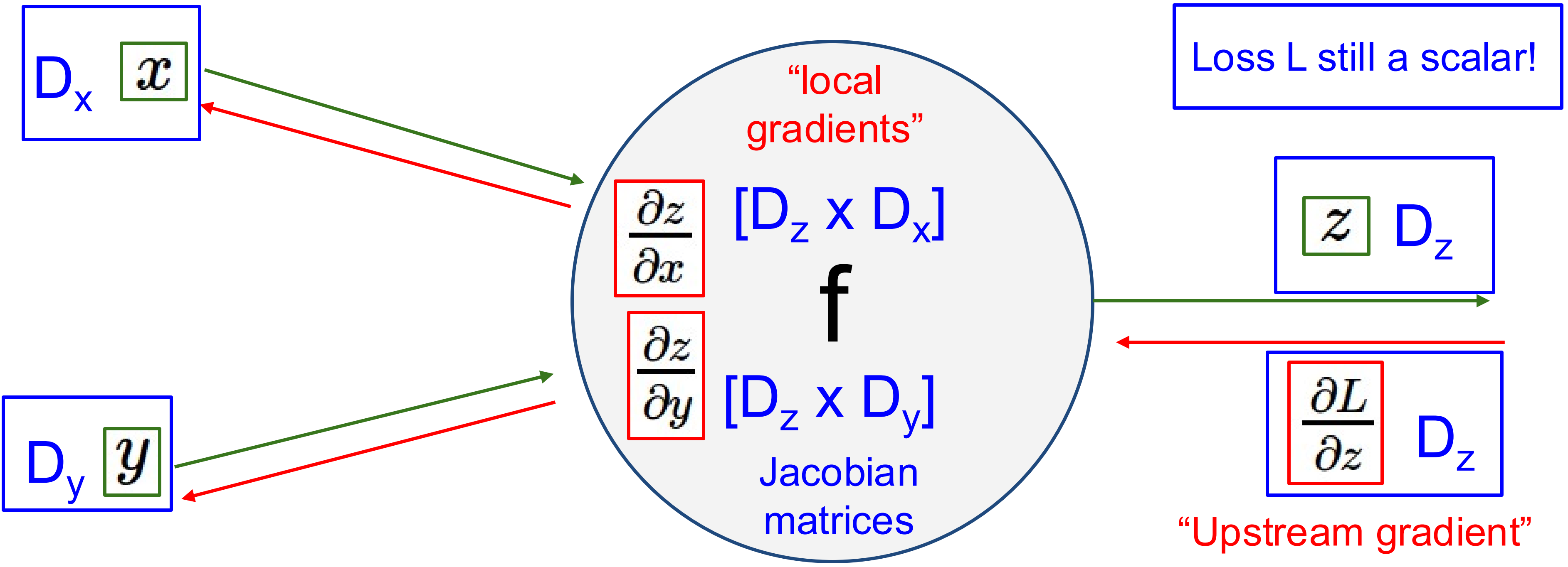
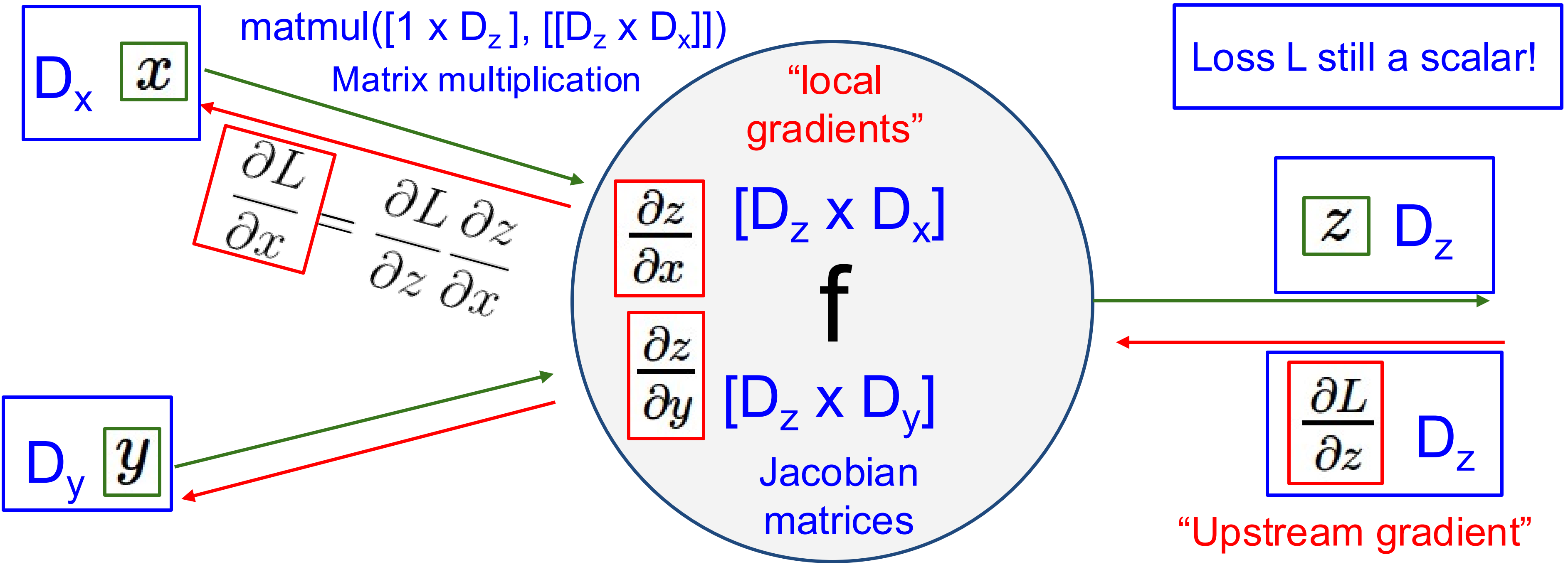
Backprop with Vectors



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

Slide credit: Stanford CS231n Instructors

Backprop with Vectors



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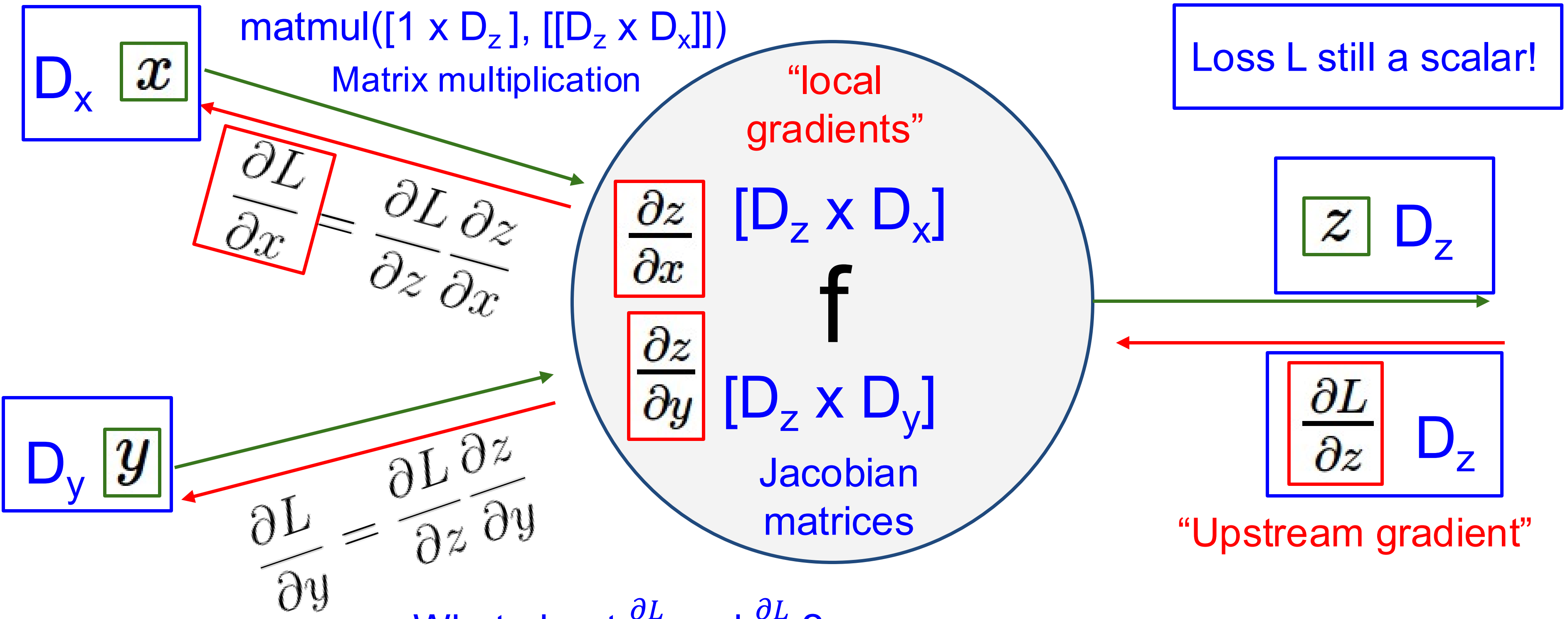
Backprop with Vectors



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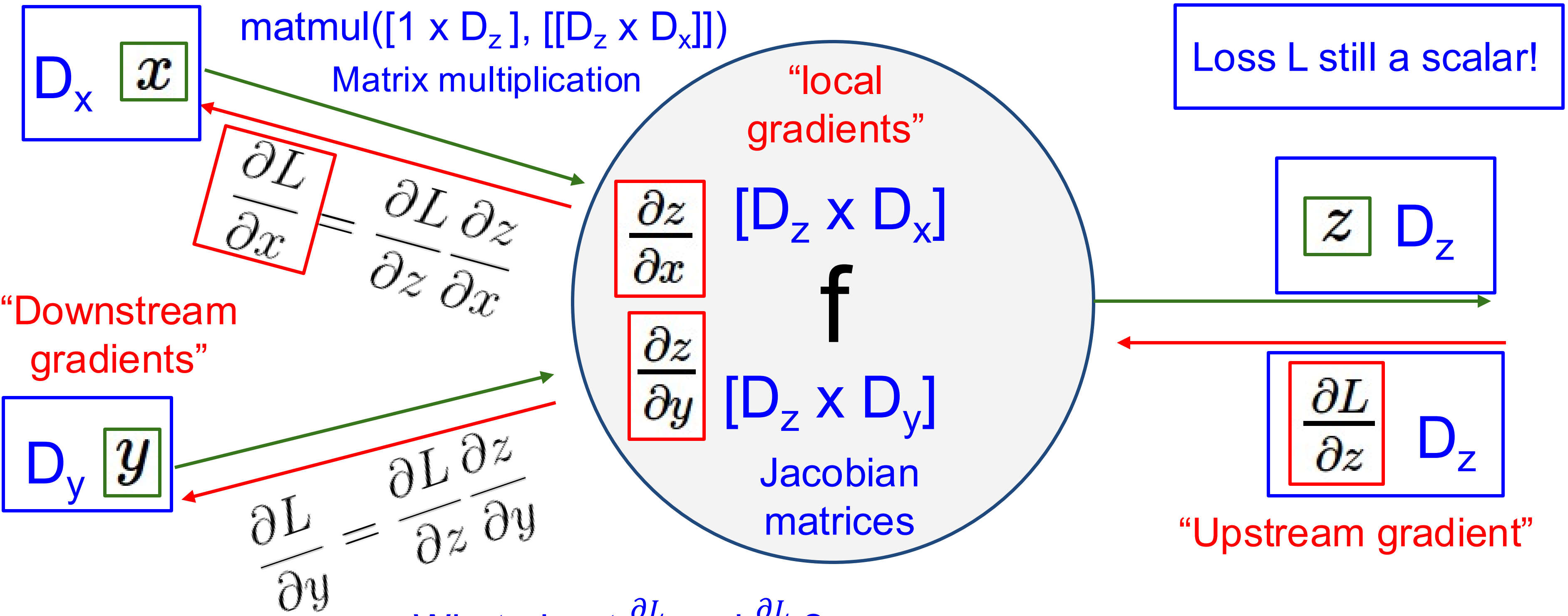
Backprop with Vectors



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

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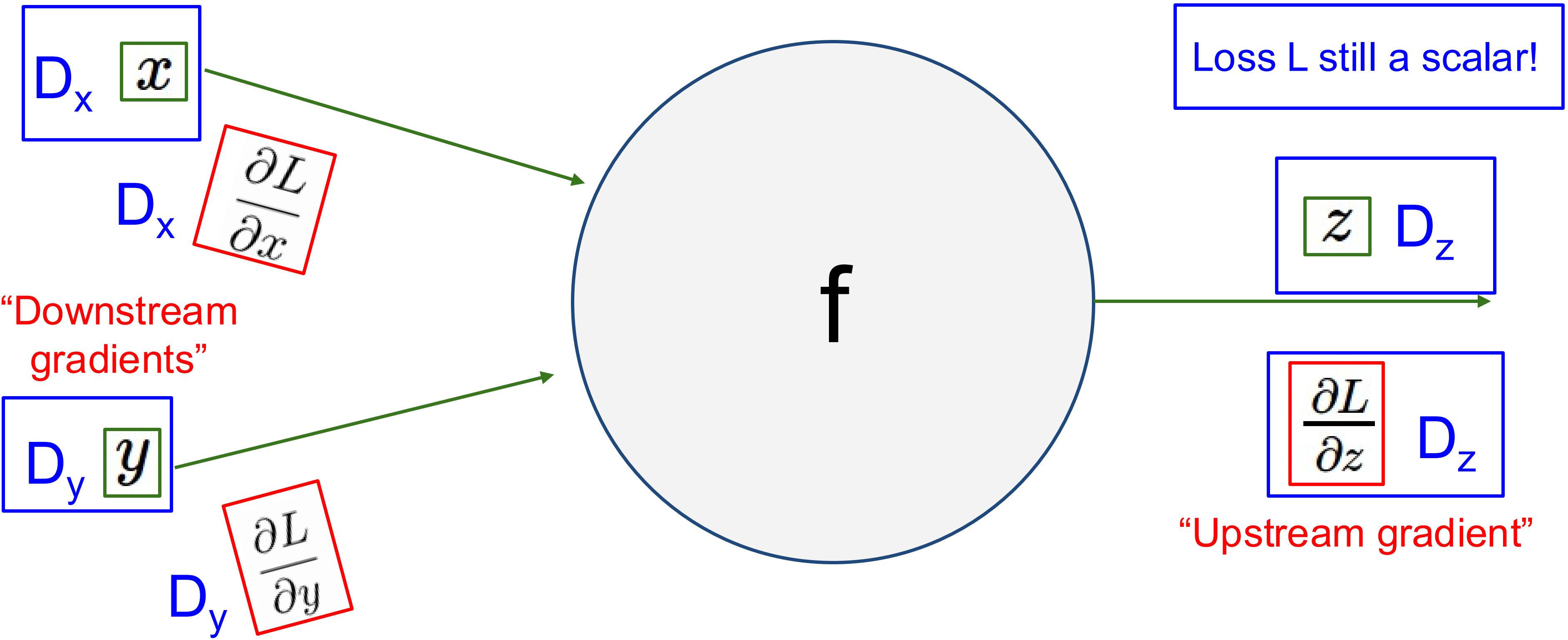
Gradients loss of wrt a variable have same dims as the original variable



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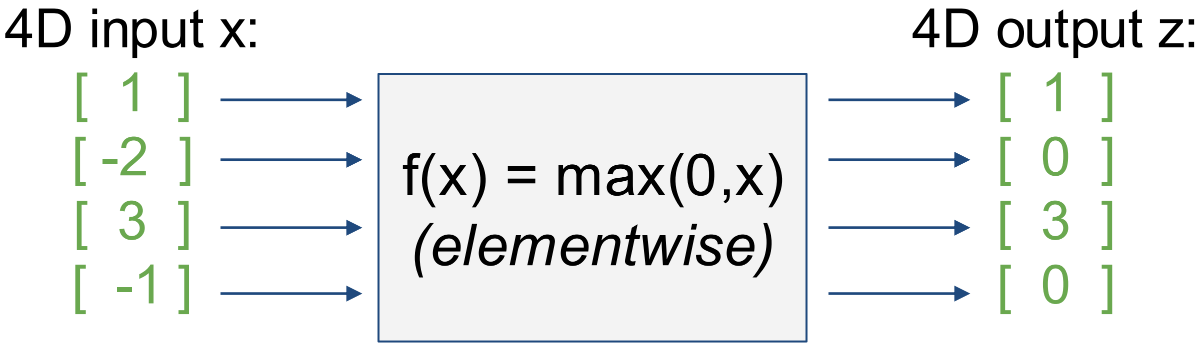
Backprop with Vectors



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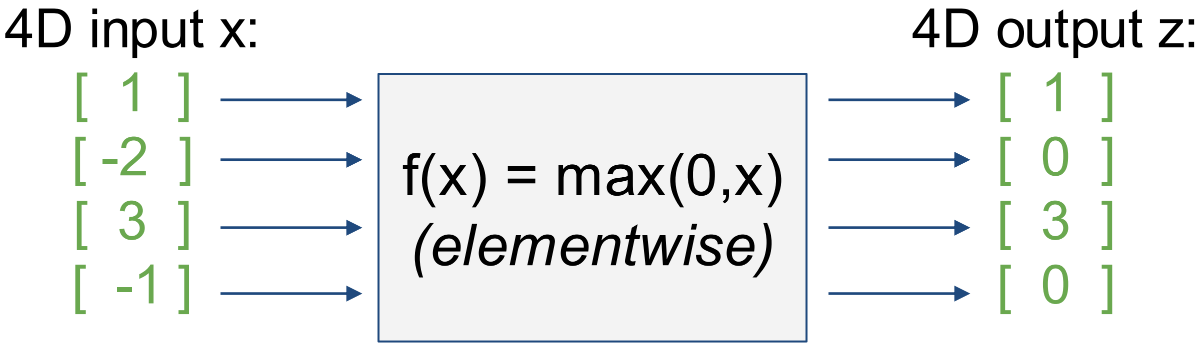
Backprop with Vectors



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

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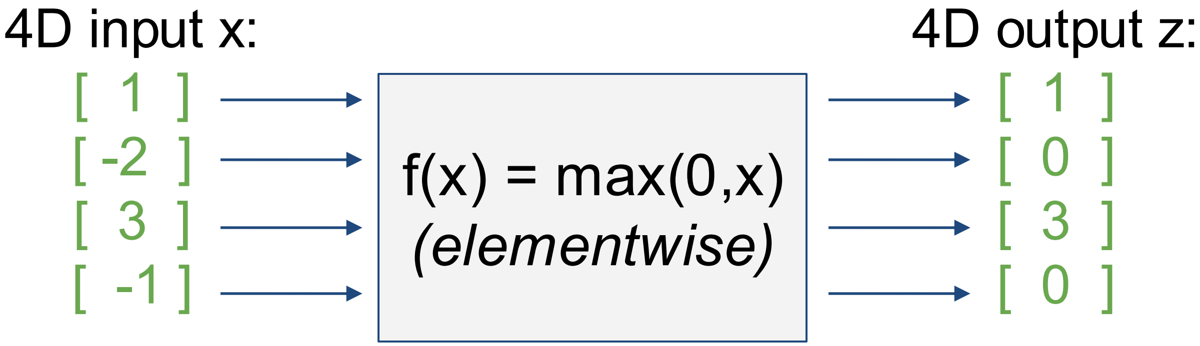
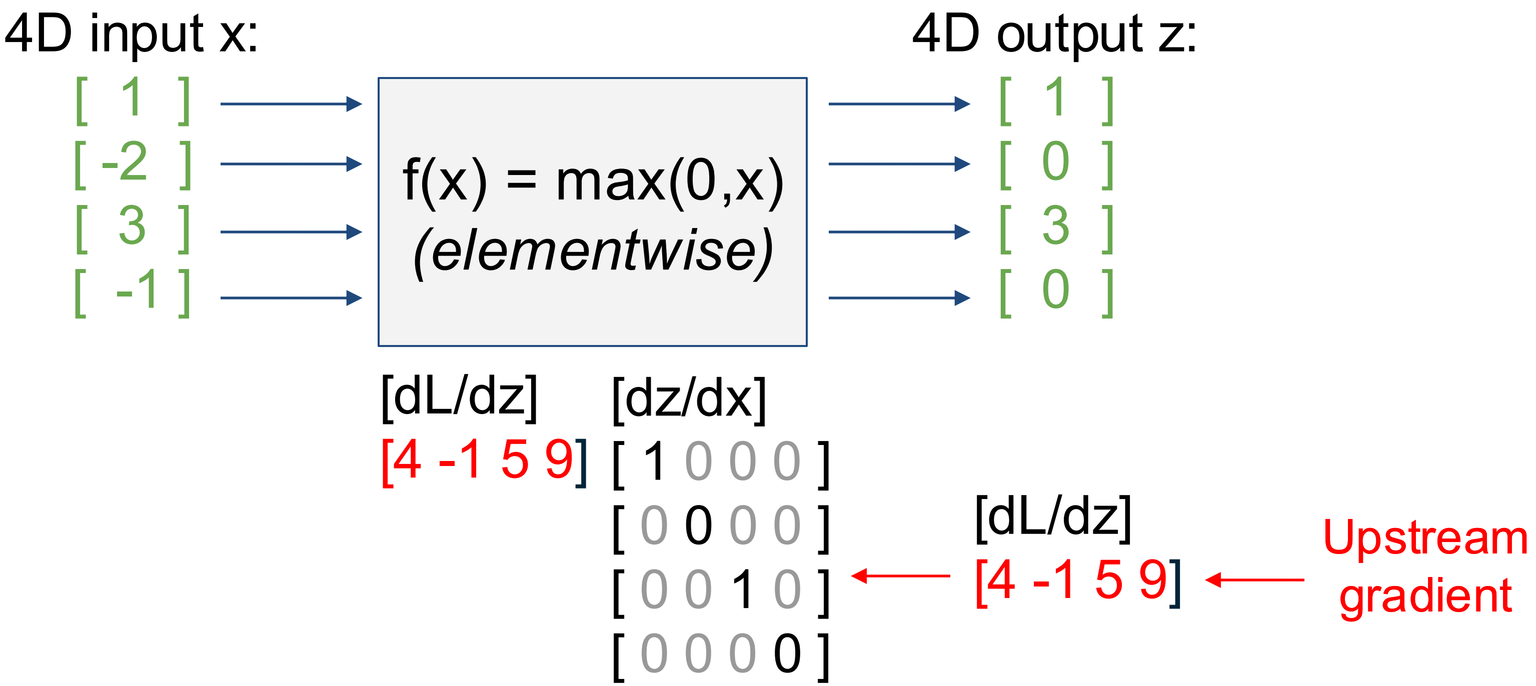
Backprop with Vectors



[dz/dx]

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

Backprop with Vectors



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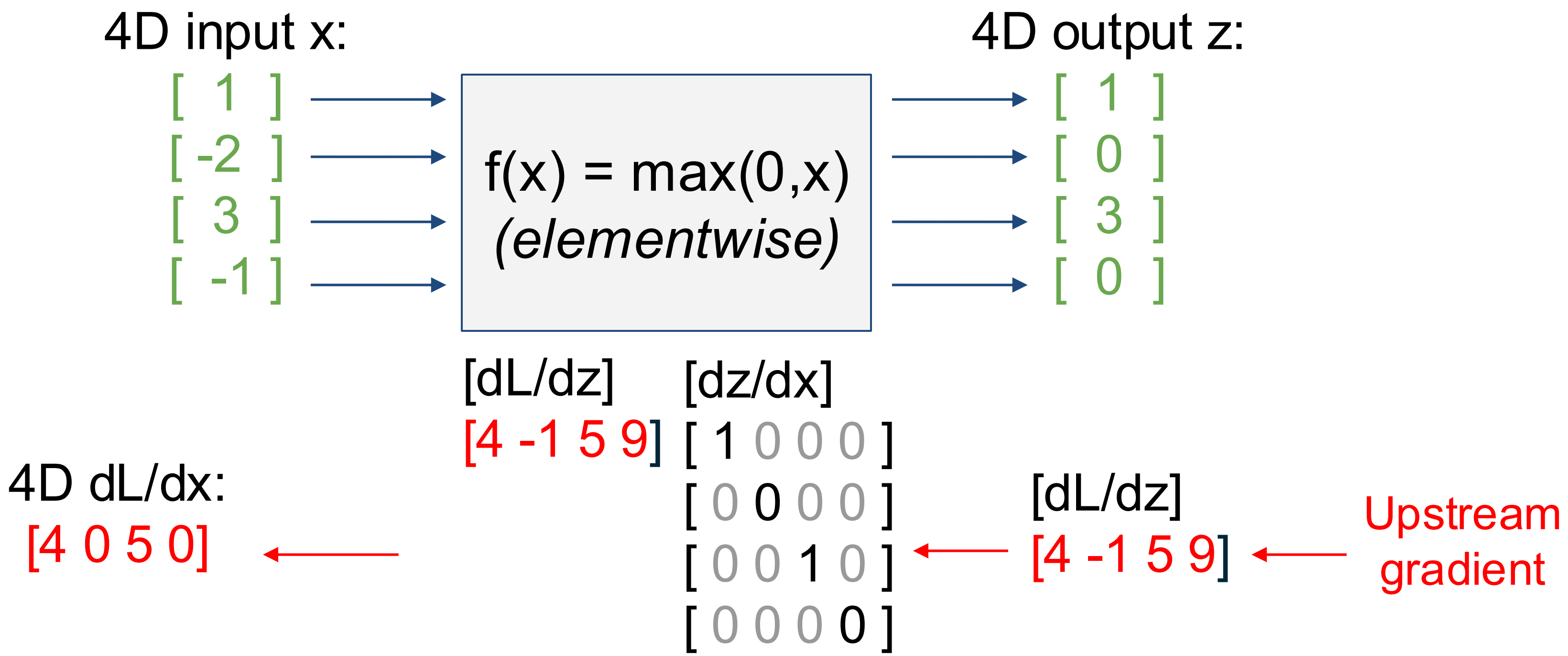
Backprop with Vectors



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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 **element-wise multiplication**

4D input x:

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

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

4D output z:

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

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

[dz/dx]
[1 0 0 0]
[0 0 0 0]
[0 0 1 0]
[0 0 0 0]

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

Upstream gradient

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

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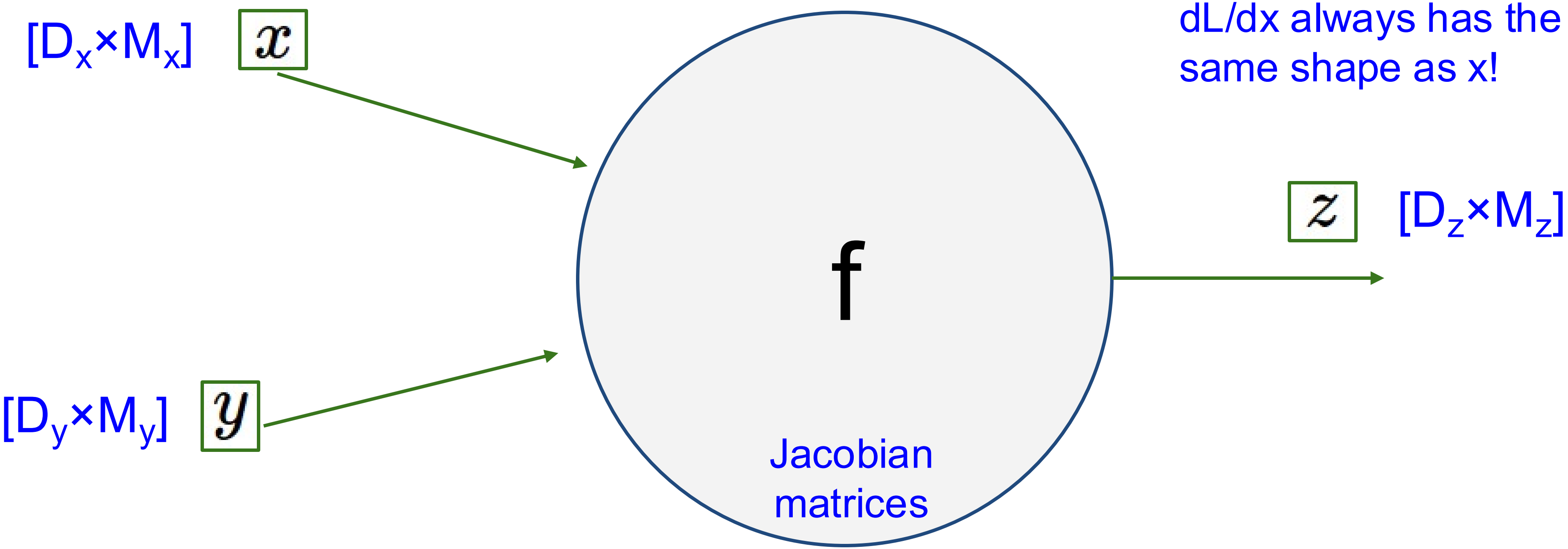
Backprop with Matrices (or Tensors)

Loss L still a scalar!

dL/dx always has the same shape as x!



Slide credit: Stanford CS231n Instructors

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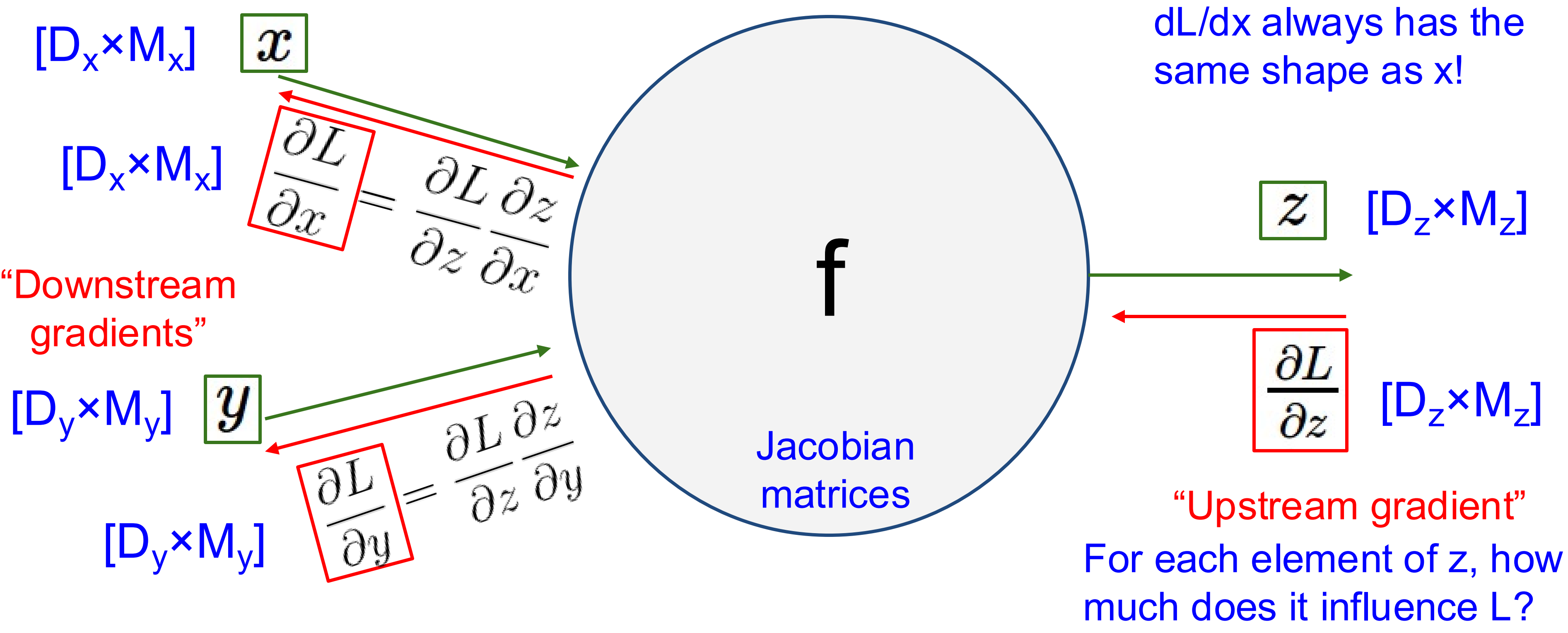

Slide credit: Stanford CS231n Instructors

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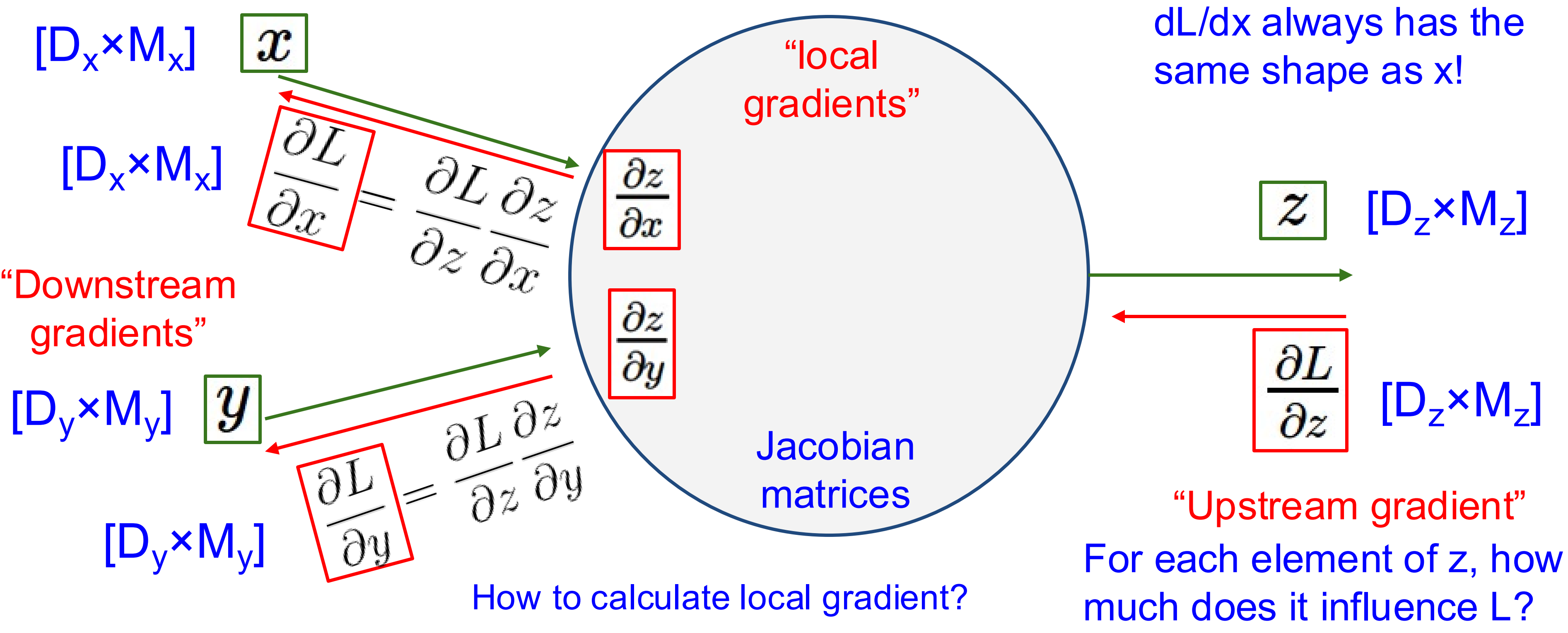

How to calculate local gradient?

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Backprop with Matrices (or Tensors)

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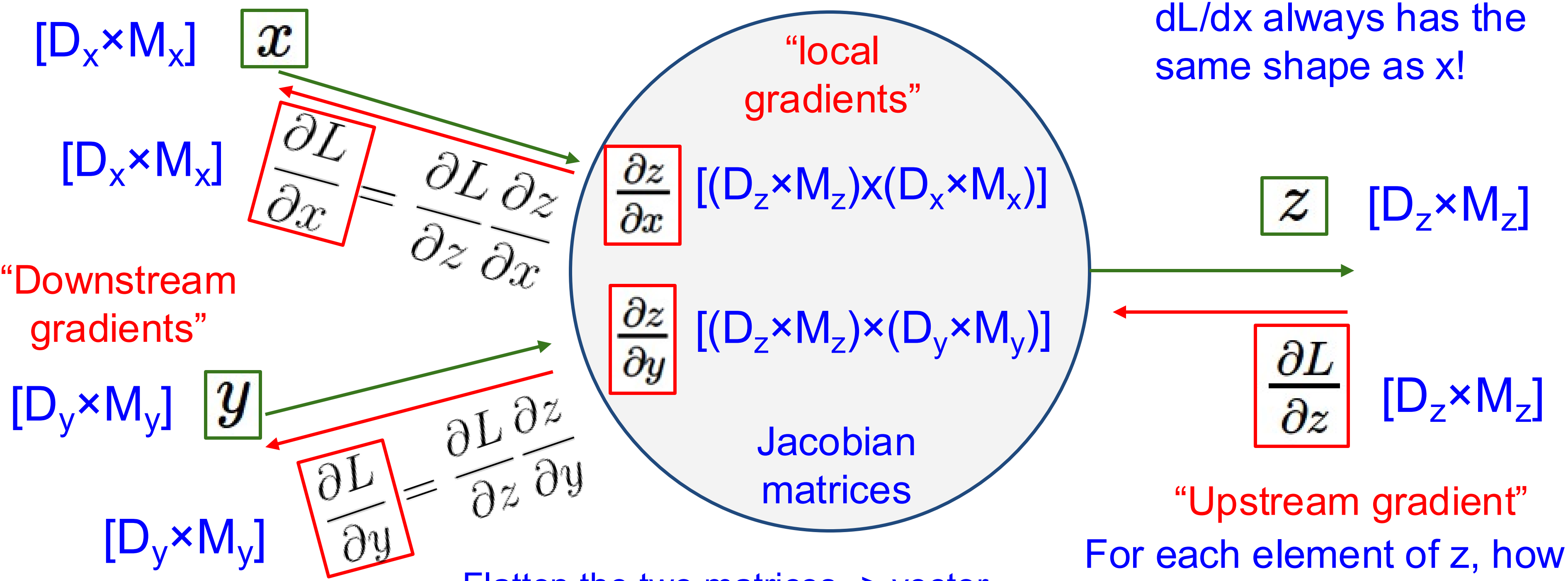

Flatten the two matrices -> vector-vector gradients -> jacobian matrices!

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

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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]

Slide credit: Stanford CS231n Instructors

Backprop with Matrices

x: [N×D]
[2 1 -3]
[-3 4 2]

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[3 2 1 -1]
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$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]
[13 9 -2 -6]
[5 2 17 1]

dL/dy: [N×M]
[2 3 -3 9]
[-8 1 4 6]

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

What do the jacobian matrices look like?

Slide credit: Stanford CS231n Instructors

Backprop with Matrices

x: [N×D]

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

w: [D×M]

[3 2 1 -1]
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$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

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[2 3 -3 9]
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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

Slide credit: Stanford CS231n Instructors

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]

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
~68 billion numbers!
Each Jacobian takes 256 GB of memory!
Must exploit its sparsity!

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial y} \frac{\partial y}{\partial x}$$

Should not have to compute this!

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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

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

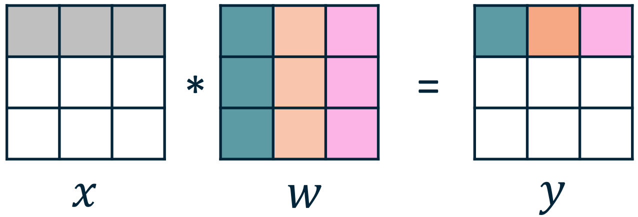
y: [N×M]

[13 9 -2 -6]
[5 2 17 1]

dL/dy: [N×M]

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

Q: Which part of y does a single element in x contribute to?



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

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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]

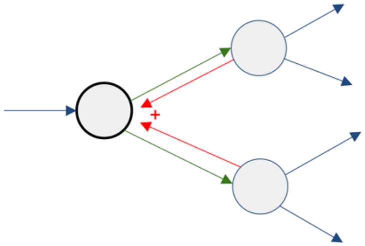
dL/dy: [N×M]

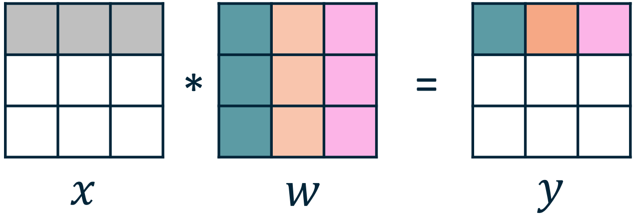
[2 3 -3 9]
[-8 1 4 6]

Q: Which part of y does a single element in x contribute to?

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

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





Recall the branching gradient rule!

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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

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

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dL/dy: [N×M]

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

Q: Which part of y does a single element in x contribute to?

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

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

Upstream gradient

local gradient

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]

Q: Which part of y does a single element in x contribute to?

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

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

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

How do we calculate this?

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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]

Q: Which part of y does a single element in x contribute to?

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

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

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

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

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

How do we calculate this?

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Backprop with Matrices

x: [N×D]
[2 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]
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A: $x_{n,d}$ affects the whole row $y_{n,\cdot}$

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

A: $w_{d,m}$

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

$w_{d,m}$

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

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

A: $w_{d,m}$

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

Just a dot product!

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Backprop with Matrices

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]

Q: Which part of y does a single element in x contribute to?

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

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

A: $w_{d,m}$

[N×D] [N×M] [M×D]

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

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

Just a matrix multiplication
No jacobian matrix needed!

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Backprop with Matrices

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]

By similar logic:

[N×D] [N×M] [M×D]

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

[D×M] [D×N] [N×M]

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

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]

By similar logic:

[N×D] [N×M] [M×D]

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

[D×M] [D×N] [N×M]

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

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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Backprop with Matrices: Summary

- Most neural network layers are tensor-in & tensor-out, with large Jacobian matrices
- When calculating $\frac{\partial L}{\partial x} = \frac{\partial L}{\partial f}\frac{\partial f}{\partial x}$, we almost never compute the Jacobian matrix $\frac{\partial f}{\partial x}$.
- Instead, we exploit the **sparsity** of the Jacobian to derive **simplified analytical gradient** of loss w.r.t to the input / weights.

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

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial f} \odot (x > 0)$$

Matmul: $f(x) = xw$

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

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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!