Neural Networks and Backpropagation

Deep Learning
26 September 2024
Profs. Luigi Cinque, Fabio Galasso and Marco Raoul Marini

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Backpropagation and Gradient Descent

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Backpropagation: a simple example

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

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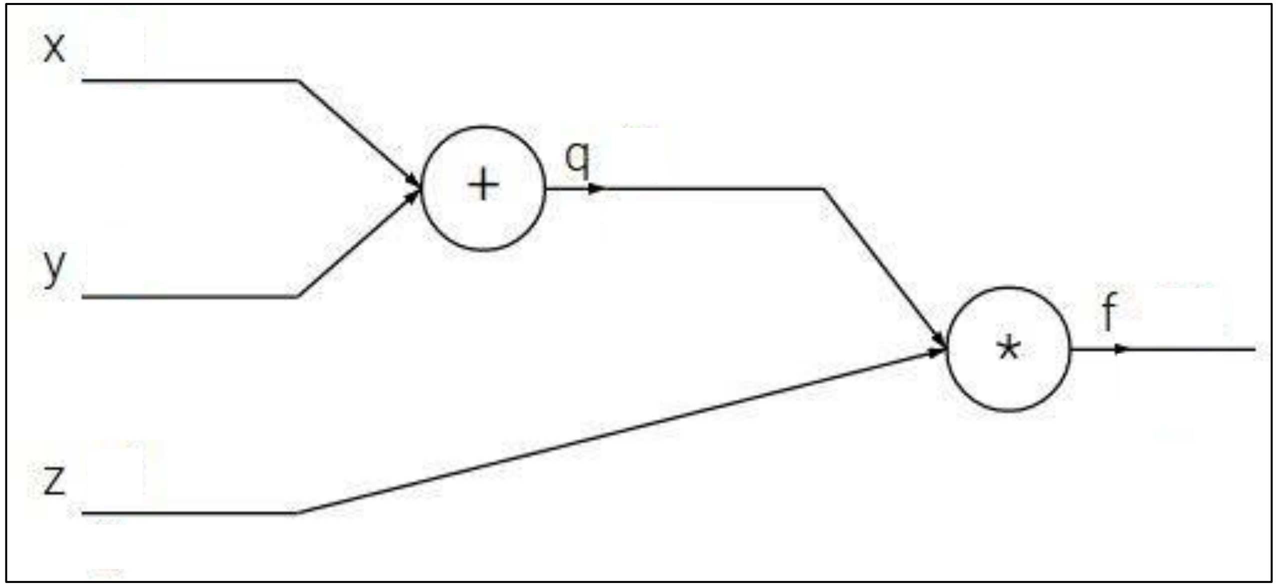

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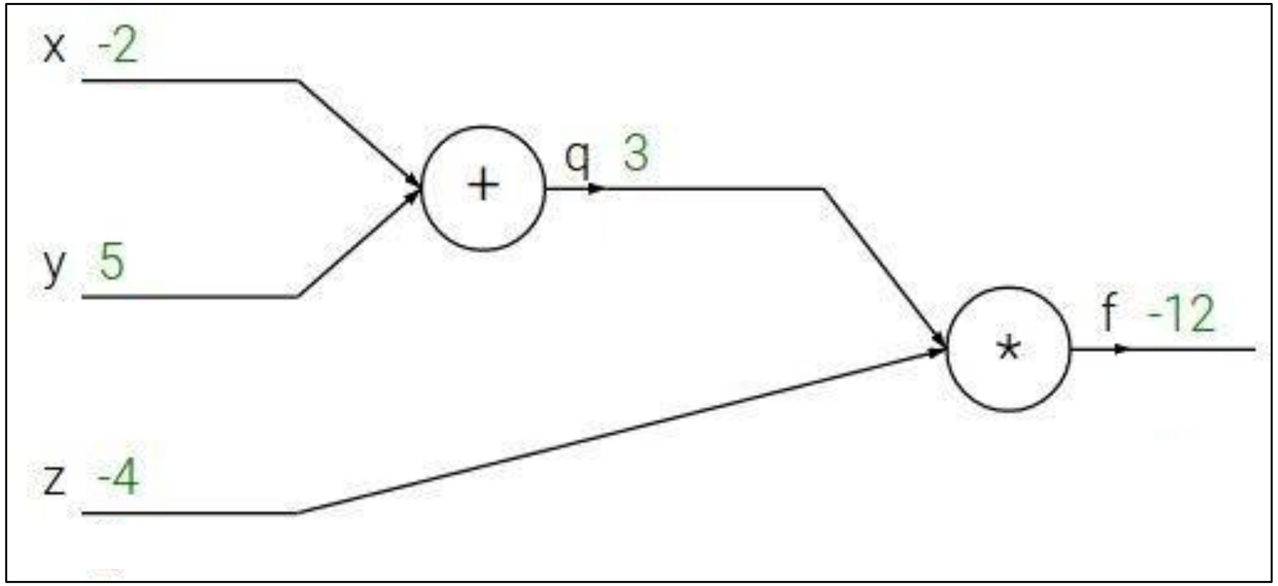
e.g. x = -2, y = 5, z = -4



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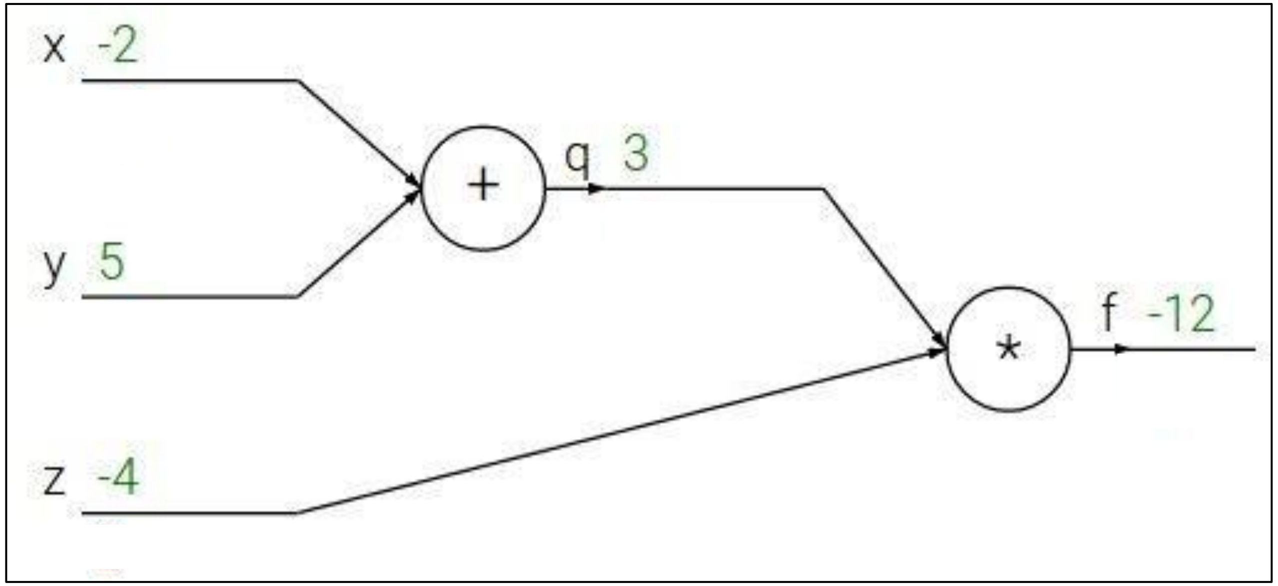
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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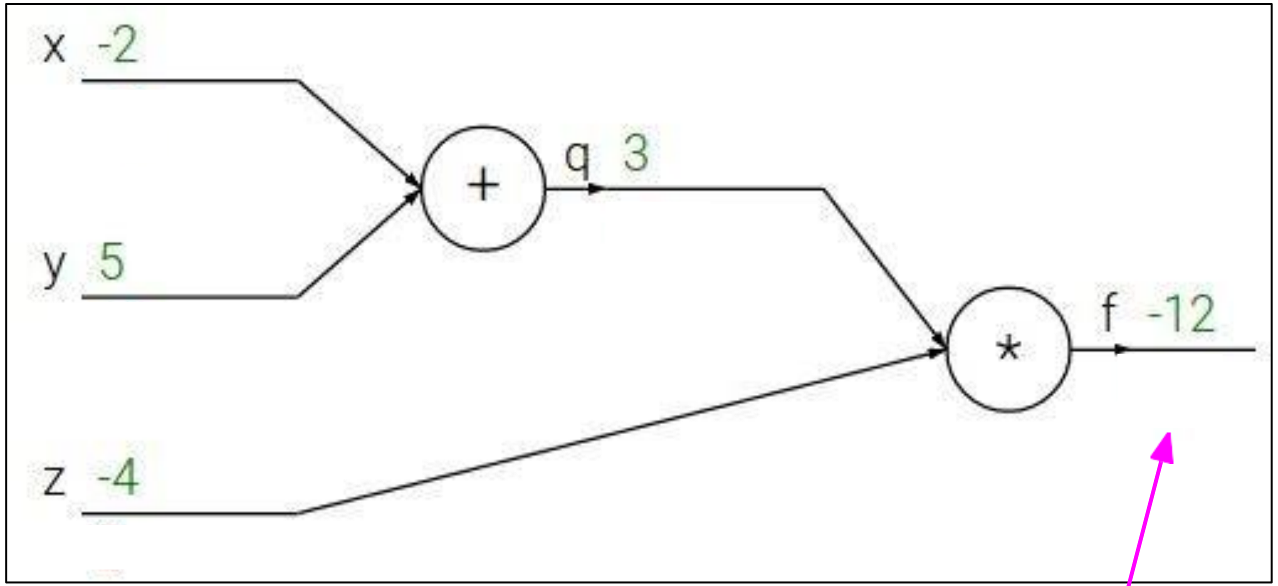

$$\frac{\partial f}{\partial f}$$

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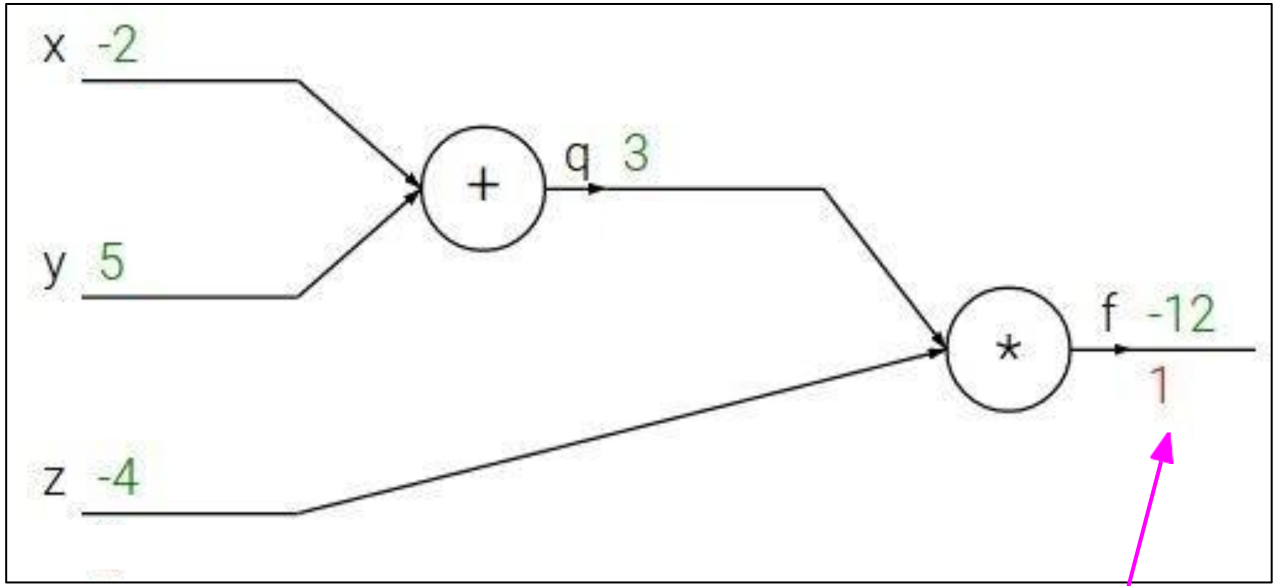

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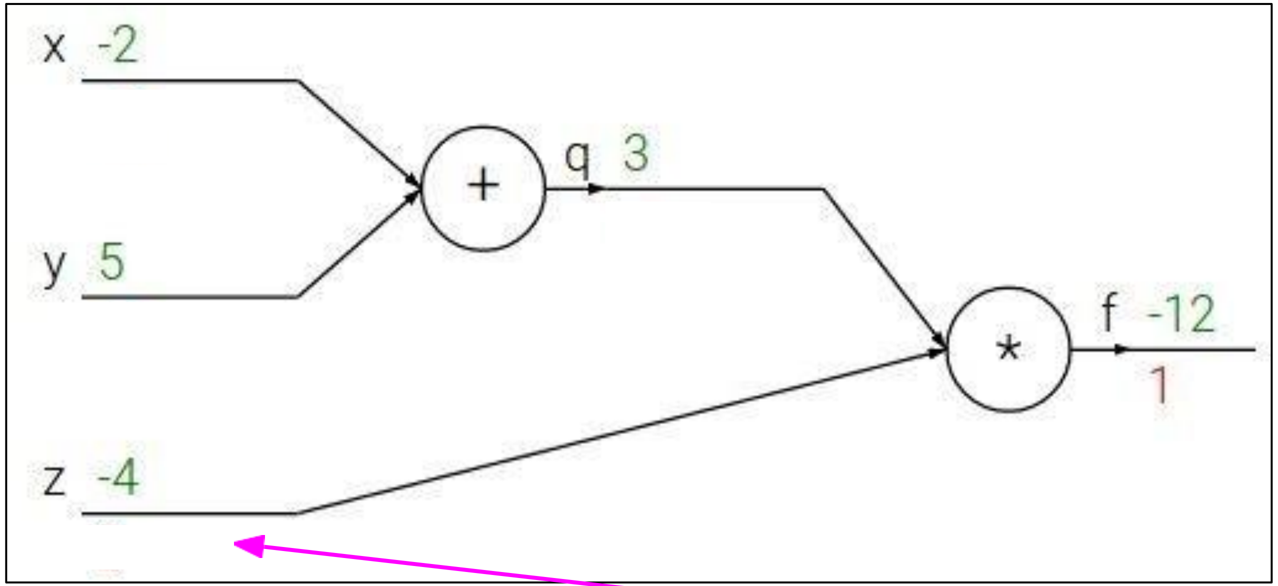

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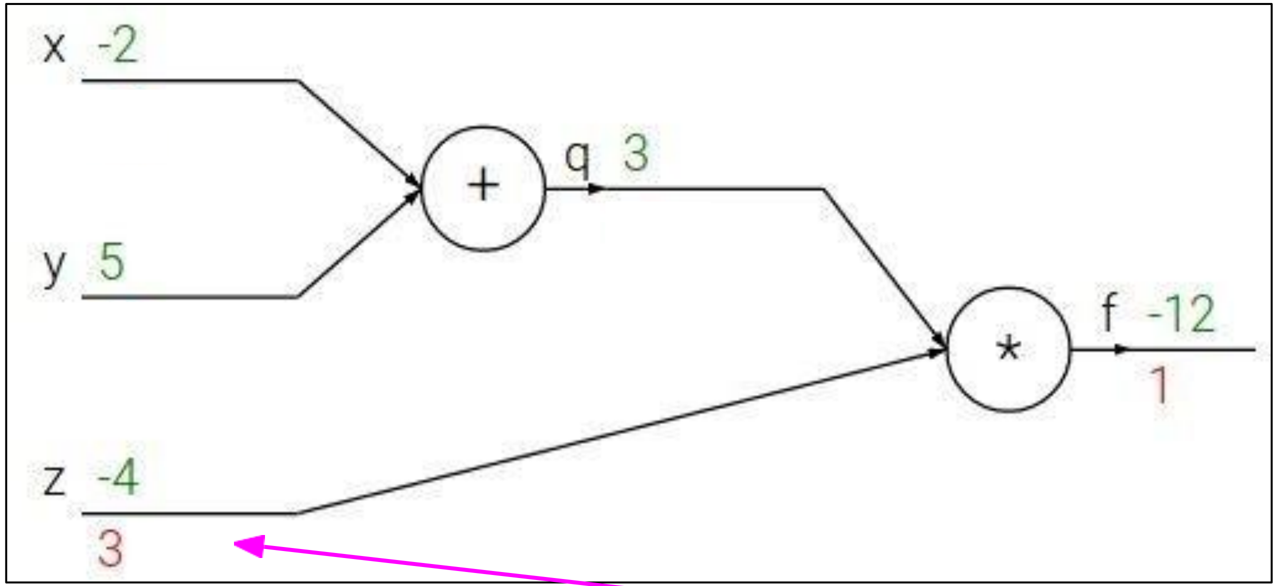

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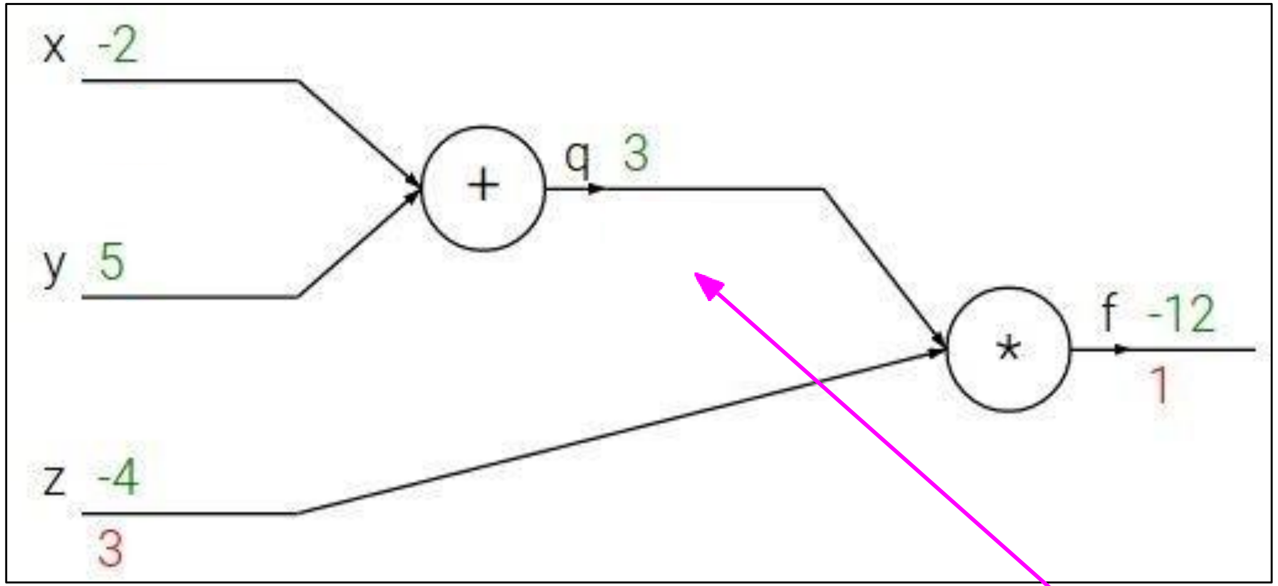

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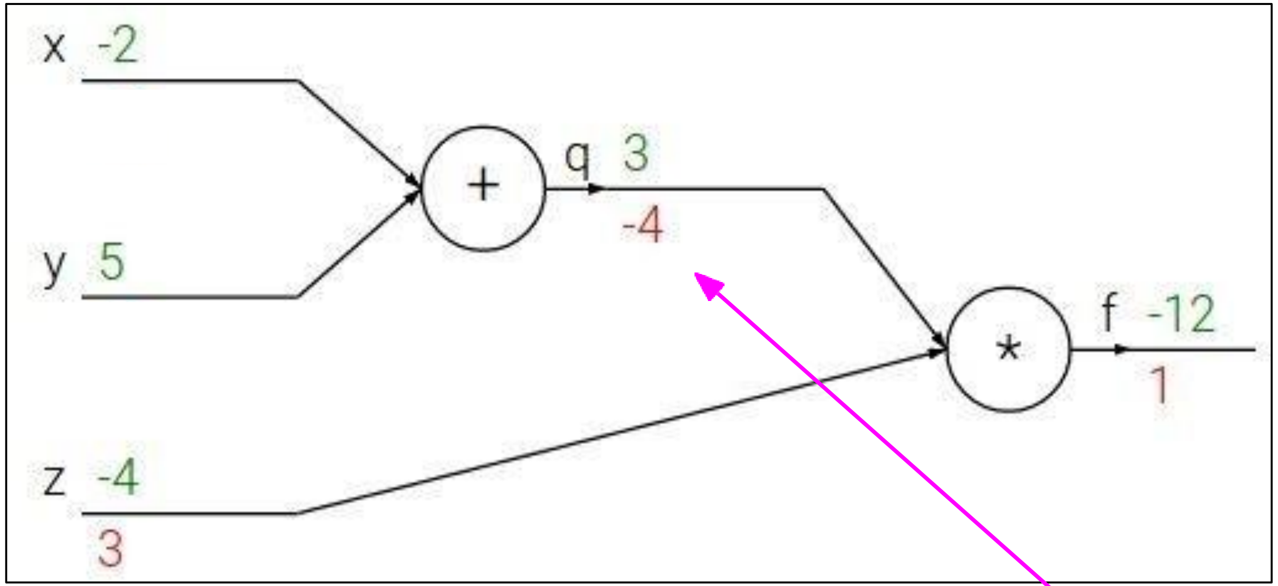

$\frac{\partial f}{\partial q}$

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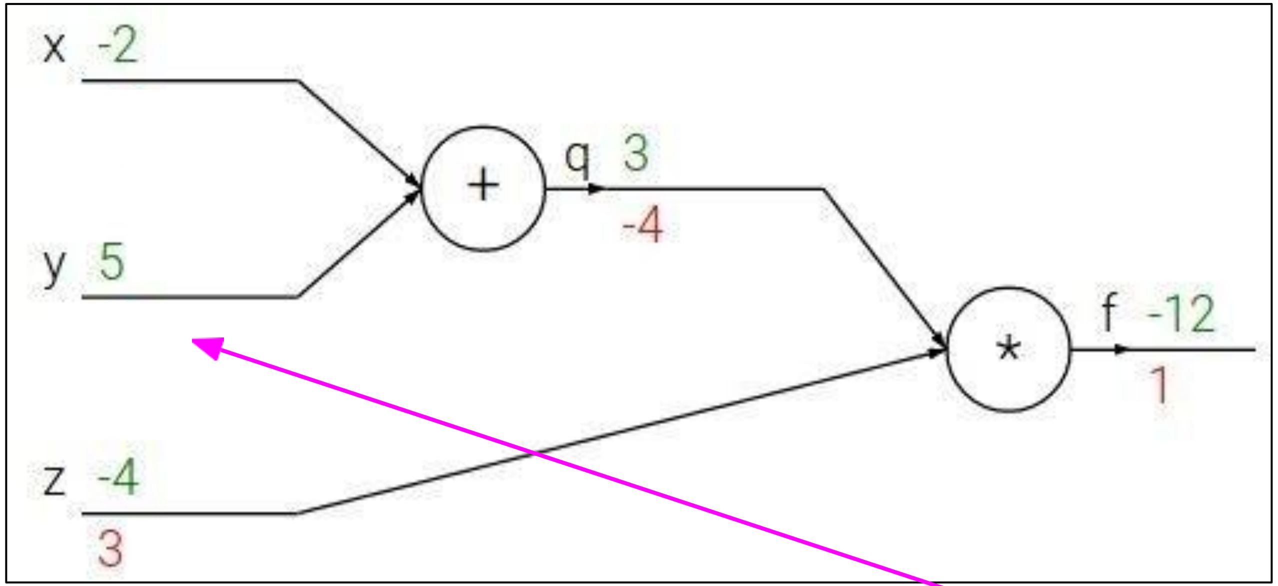

$$\frac{\partial f}{\partial y}$$

Chain rule:

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

Upstream gradient

Local gradient

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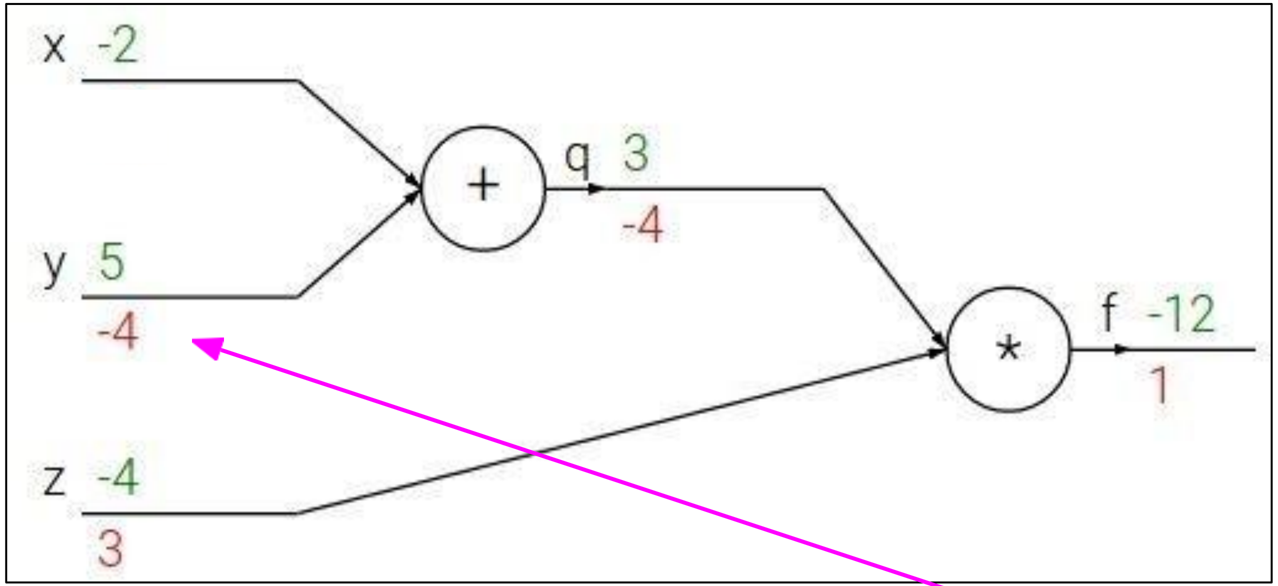

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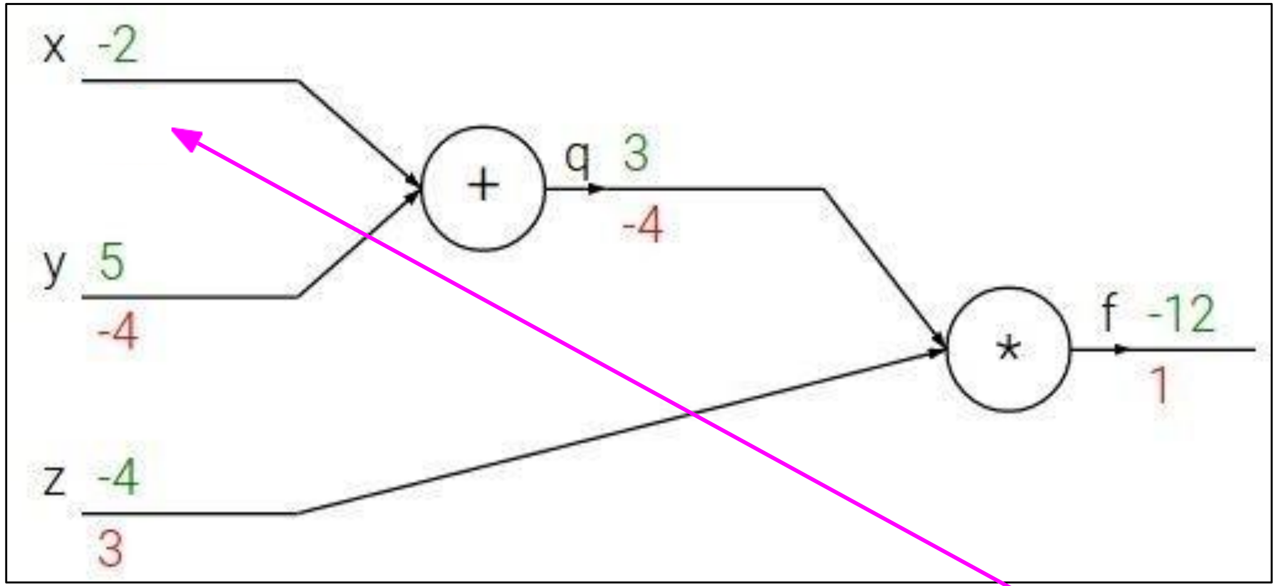

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Chain rule:

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

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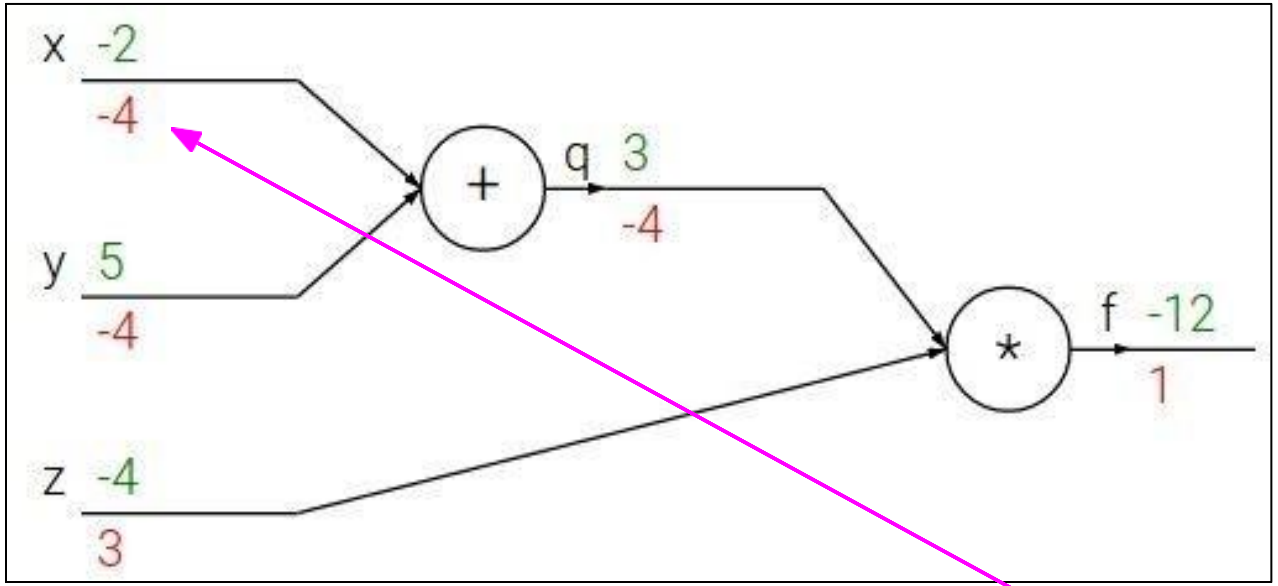

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Upstream gradient

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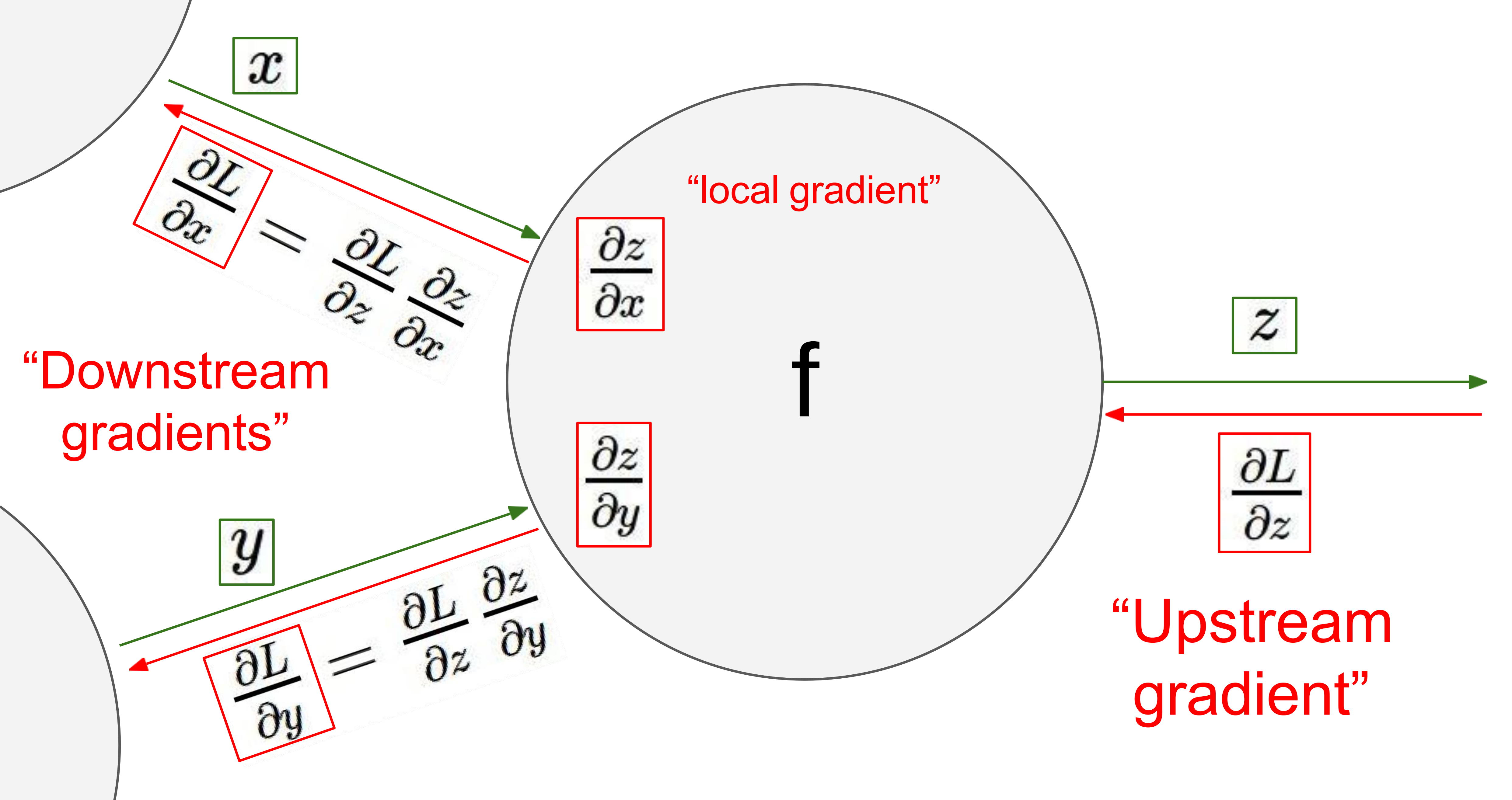
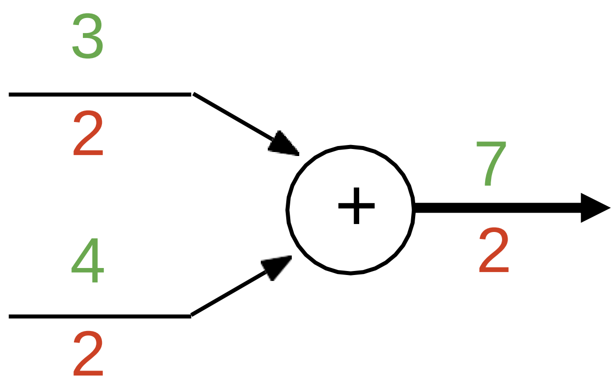
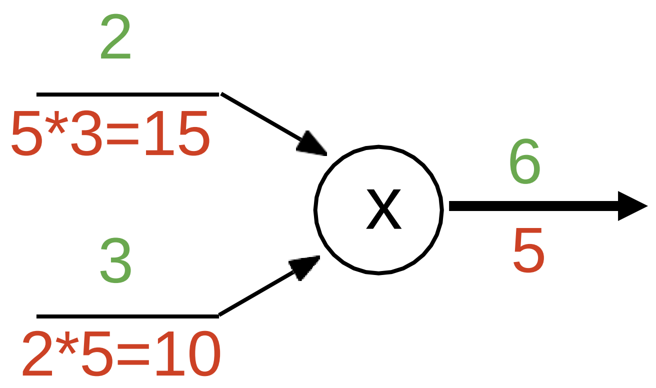

x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"Downstream gradients"
"local gradient"
$\frac{\partial z}{\partial x}$
f
$\frac{\partial z}{\partial y}$
z
$\frac{\partial L}{\partial z}$
"Upstream gradient"
y
$\frac{\partial L}{\partial y} = \frac{\partial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

Patterns in gradient flow

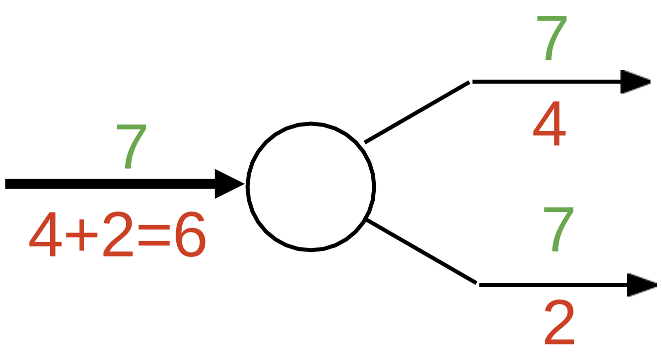
add gate: gradient distributor



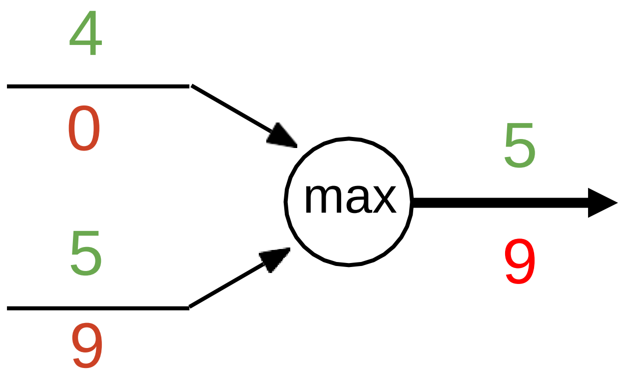
mul gate: “swap multiplier”



copy gate: gradient adder



max gate: gradient router



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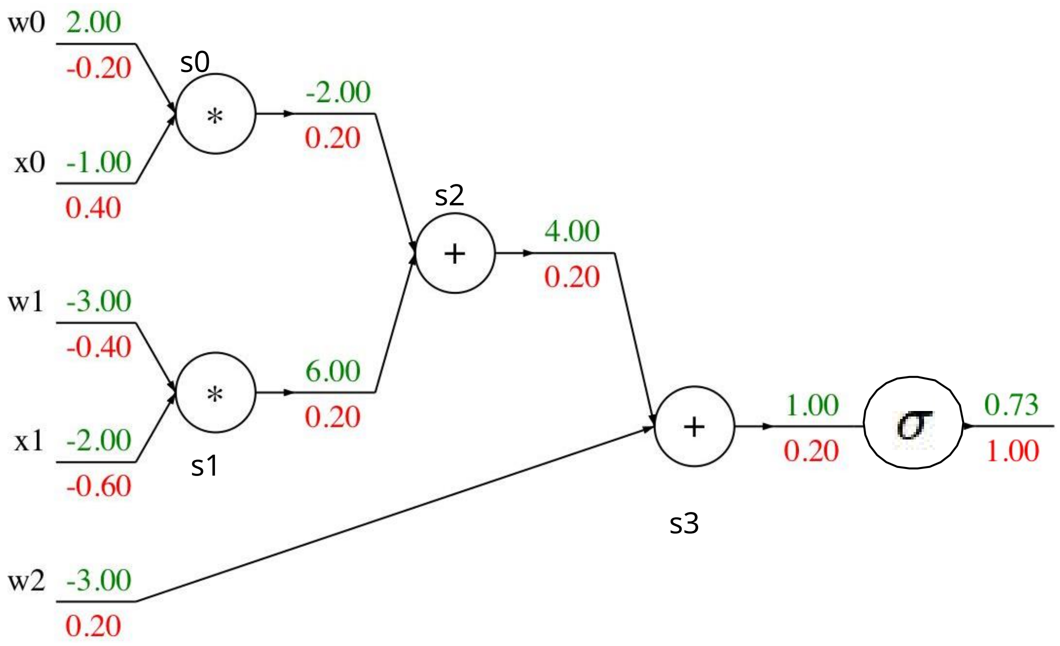
Backprop Implementation: “Flat” code



Forward pass: Compute output

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

Backward pass: Compute grads

```
    grad_L = 1.0
    grad_s3 = grad_L * (1 - L) * L
    grad_w2 = grad_s3
    grad_s2 = grad_s3
    grad_s0 = grad_s2
    grad_s1 = grad_s2
    grad_w1 = grad_s1 * x1
    grad_x1 = grad_s1 * w1
    grad_w0 = grad_s0 * x0
    grad_x0 = grad_s0 * w0
```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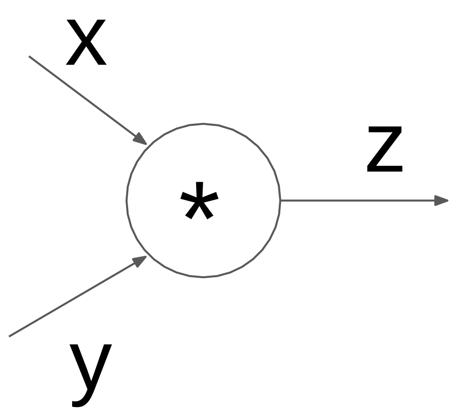
Modularized implementation: forward / backward API

Gate / Node / Function object: Actual PyTorch code



(x,y,z are scalars)

```
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 cache some values for use in backward

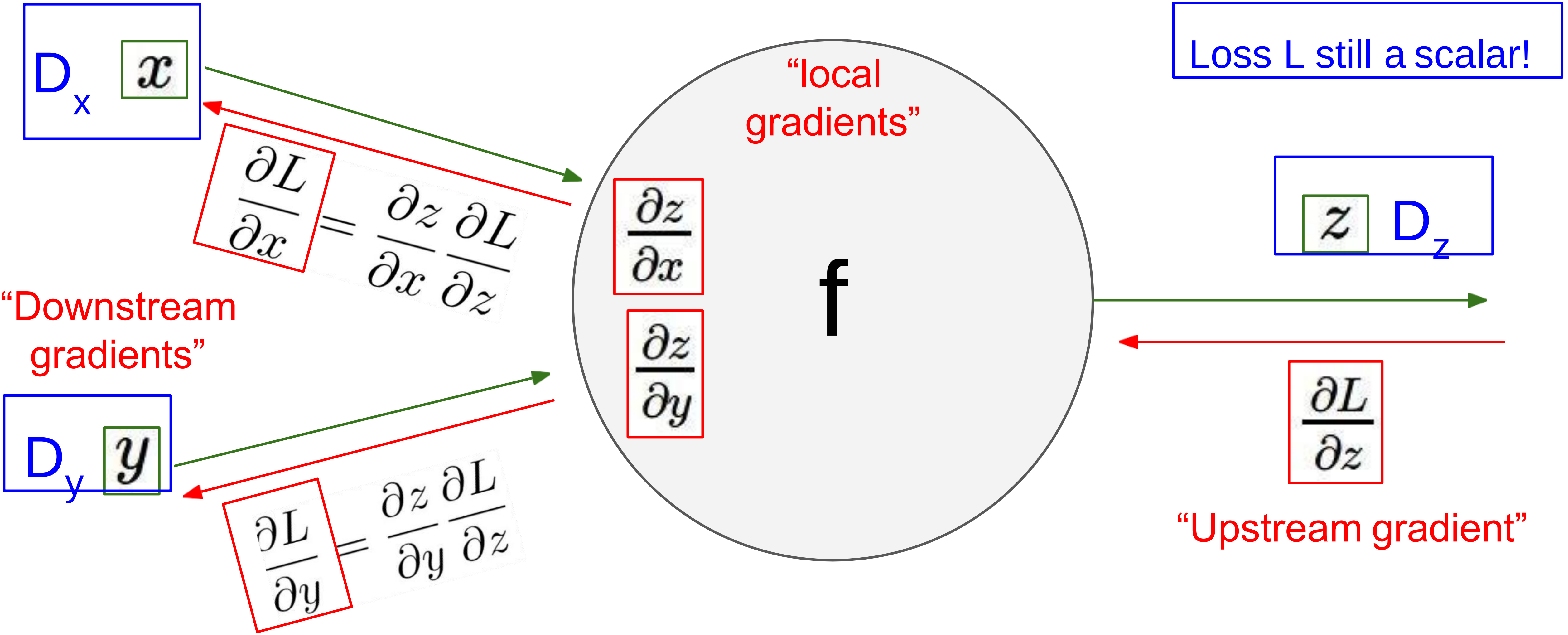
Upstream gradient

Multiply upstream and local gradients

So far: backprop with scalars

What about vector-valued functions?

Backprop with Vectors



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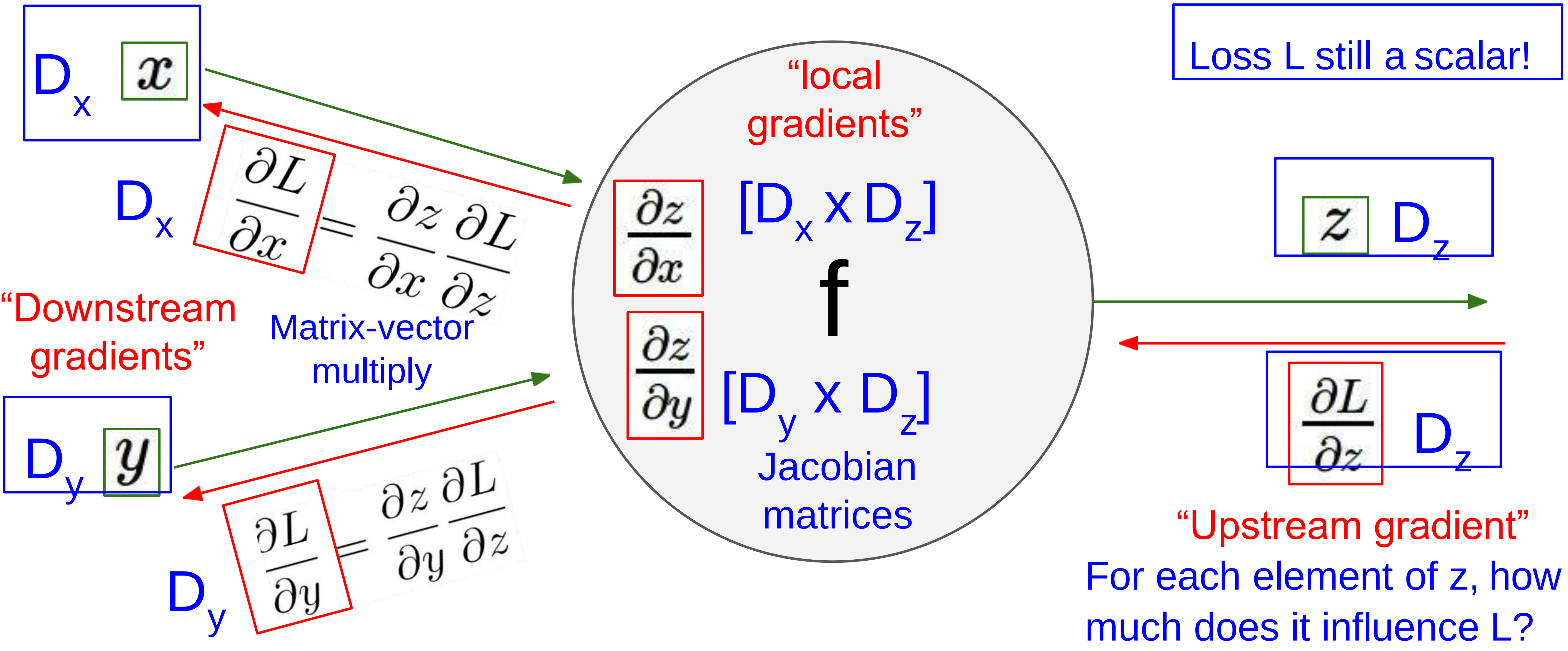
Backprop with Vectors



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Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \longrightarrow \boxed{\begin{array}{c} f(x) = \max(0,x) \\ \textit{(elementwise)} \end{array}} \longrightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D output y:

Backprop with Vectors

4D input x:

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

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

4D output y:

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

4D dL/dy:

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

Upstream gradient

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Backprop with Vectors

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[1]
[-2]
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4D output y:

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

Jacobian dy/dx

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

4D dL/dy:

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

Upstream gradient

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[dy/dx] [dL/dy]

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

4D dL/dy:

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

Upstream gradient

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4D dL/dx:

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[dy/dx] [dL/dy]

$$\begin{bmatrix}1 & 0 & 0 & 0\\0 & 0 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & 0\end{bmatrix}\begin{bmatrix}4\\-1\\5\\9\end{bmatrix}$$

4D dL/dy:

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Upstream gradient

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Backprop with Vectors

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

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

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(elementwise)

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

4D dL/dx:

$$\begin{bmatrix}4\\0\\5\\0\end{bmatrix}$$

[dy/dx] [dL/dy]

$$\begin{bmatrix}1&0&0&0\\0&0&0&0\\0&0&1&0\\0&0&0&0\end{bmatrix}\begin{bmatrix}4\\-1\\5\\9\end{bmatrix}$$

4D dL/dy:

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

Upstream gradient

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[-2]
[3]
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(elementwise)

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

4D dL/dx:

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

[dy/dx] [dL/dy]

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

4D dL/dy:

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

Upstream gradient

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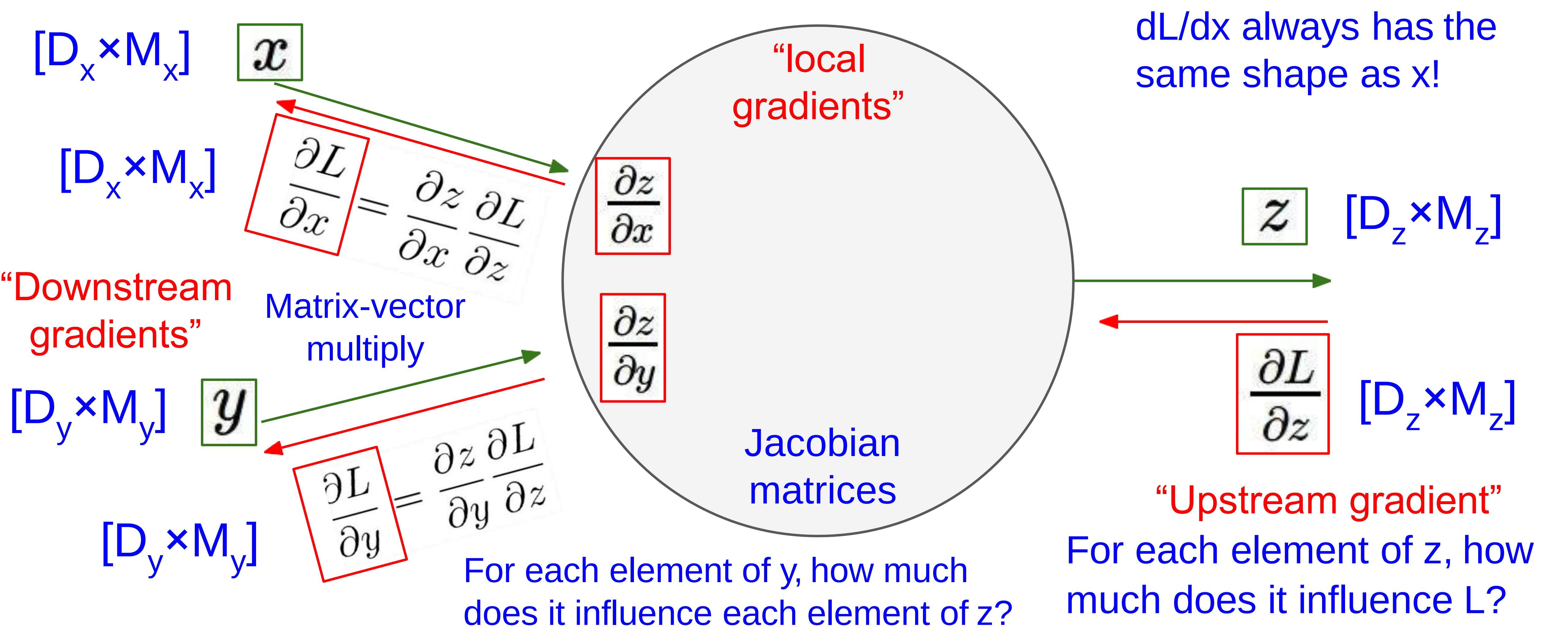
Backprop with Matrices (or Tensors)

Loss L still a scalar!



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Backprop with Matrices (or Tensors)

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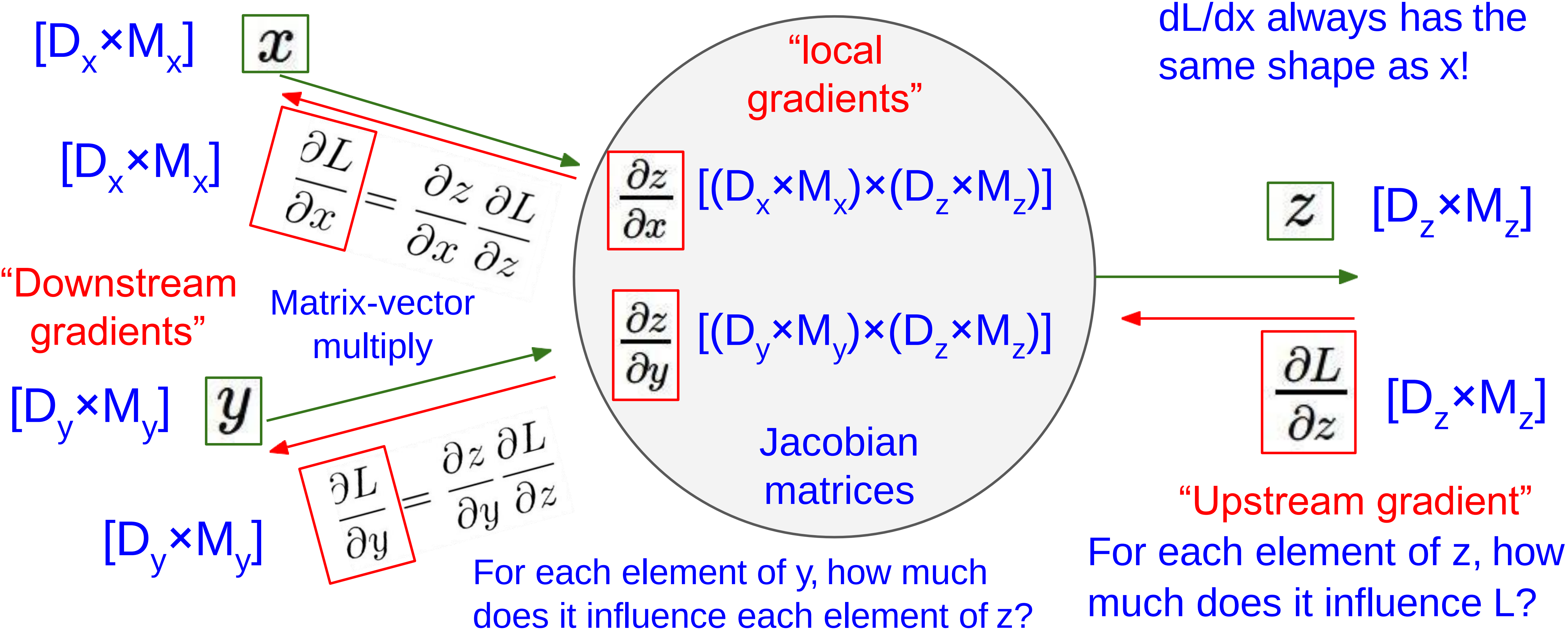

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Backprop with Matrices

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]

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

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

y: [N×M]

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

dL/dy: [N×M]

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

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

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y: [N×M]

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

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 $y_{n,\cdot}$

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

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Backprop with Matrices

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y: [N×M]

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

dL/dy: [N×M]

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

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

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

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

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

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

Matrix Multiply

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

y: [N×M]

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

dL/dy: [N×M]

[$\boxed{2 \;\; 3 \;\; -3 \;\; 9}$]
[-8 1 4 6]

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Backprop with Matrices

x: [N×D]

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

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

[N×D] [N×M] [M×D]

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

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

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Backprop with Matrices

x: [N×D]

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

w: [D×M]

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

Matrix Multiply

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

y: [N×M]

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

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]

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

[D×M] [D×N] [N×M]

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

These formulas are easy to remember: they are the only way to make shapes match up!

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Neural Networks and Deep Learning

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Università di Roma

Neural networks: deeper networks

(**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: 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: $f = W_2 \boxed{\max(0,} W_1 x)$

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!

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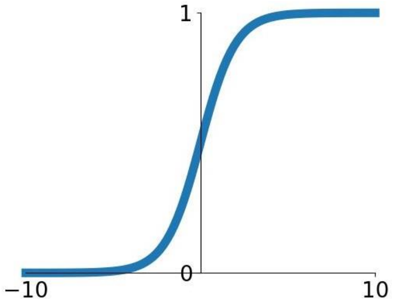
Activation functions

ReLU is a good default choice for most problems

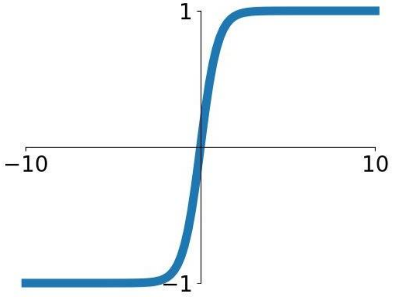
Sigmoid

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



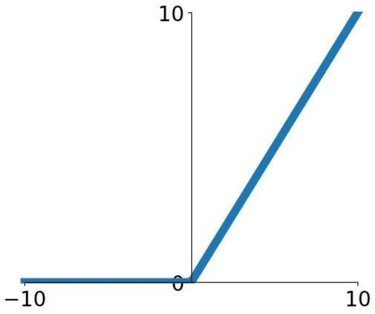
tanh

$\tanh(x)$



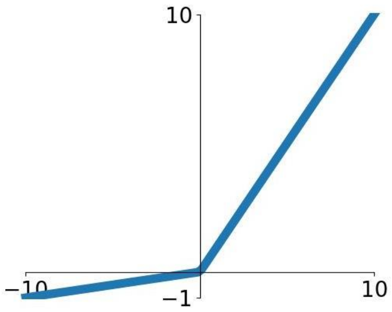
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

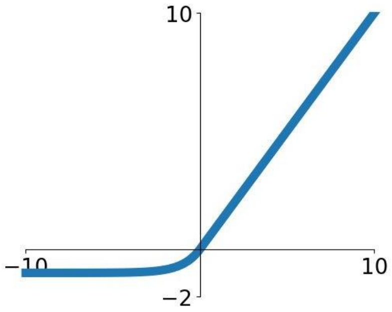


Maxout

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

ELU

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



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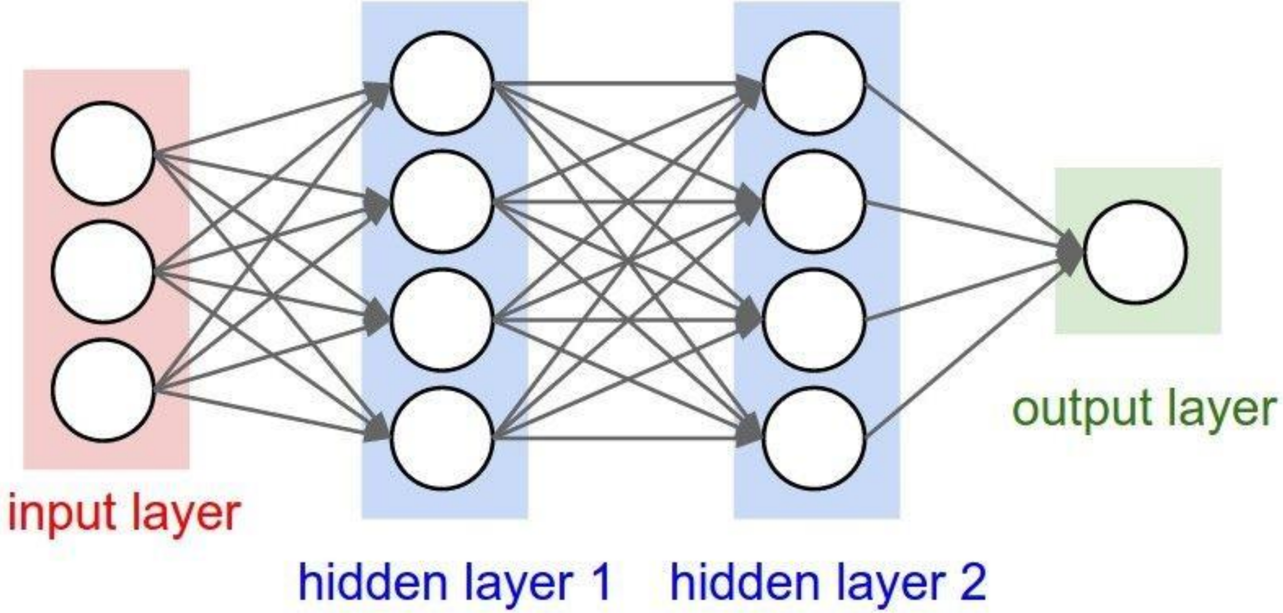
Example feed-forward computation of a neural network



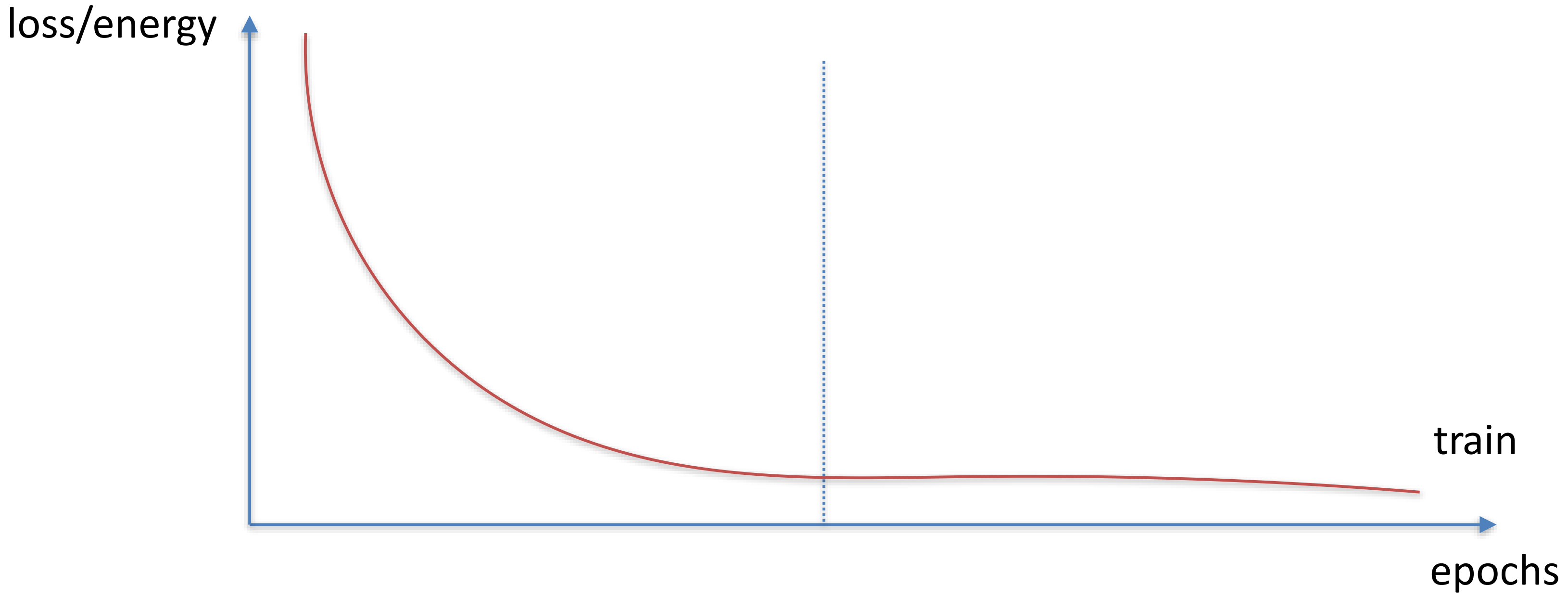

```
# forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate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

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
```

Gradient and Training

- Only two things need to be implemented to define new layer:
  - forward pass
  - error back propagation
- Watch out for overfitting



Gradient and Training

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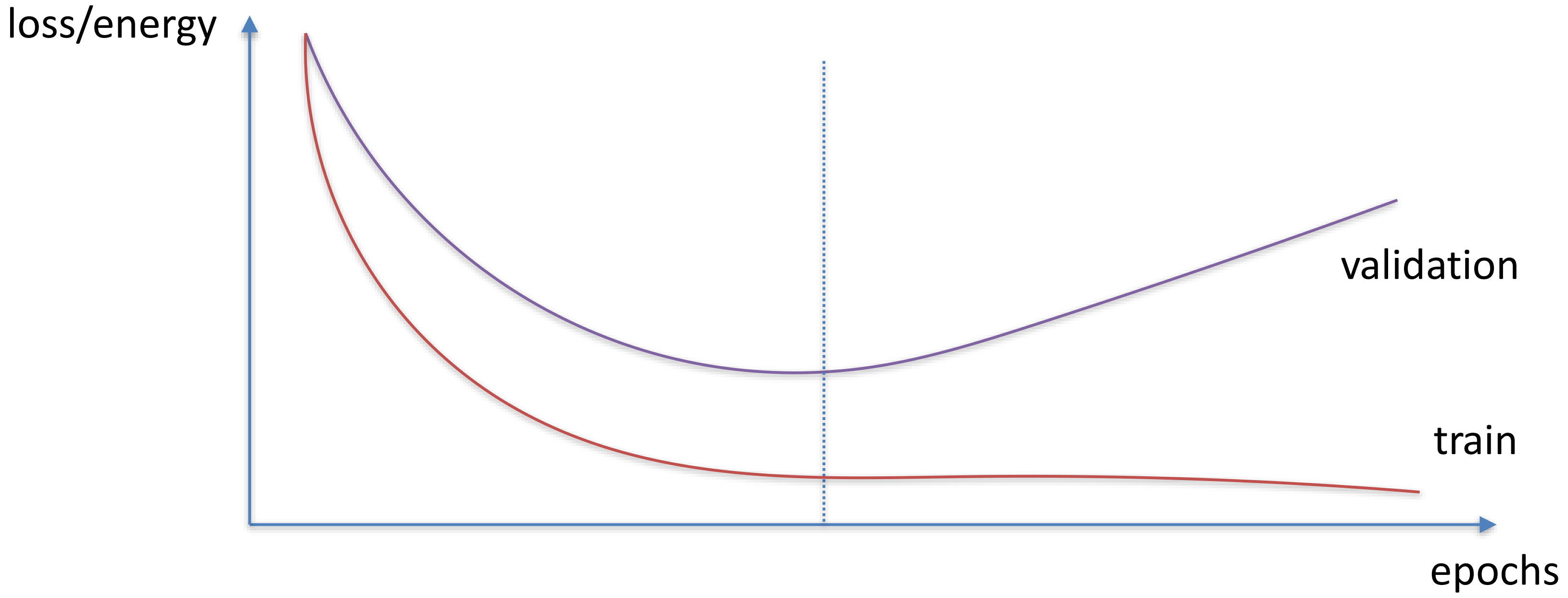

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Gradient and Training

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    - forward pass
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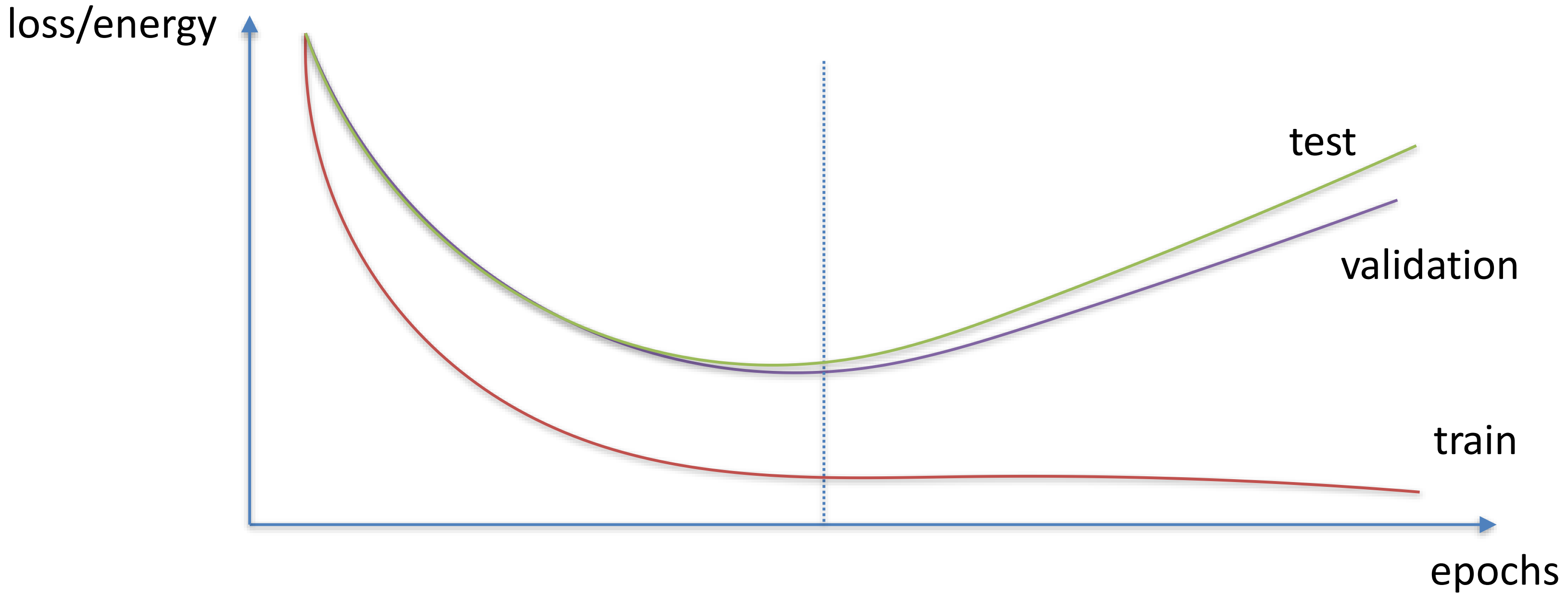

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Summary of Main Ideas in Deep Learning

- Learning of feature extraction (across many layers)
- Efficient and trainable systems by differentiable building blocks
- Composition of deep architectures via non-linear modules
- “End-to-End” training: no differentiation between feature extraction and classification

Thank you

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