

Computation Graphs, Backpropagation and Autodiff

How gradients flow through neural networks

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ES 667 · Deep Learning · IIT Gandhinagar

Backprop vocabulary

Lecture 2 built the forward map; today we reverse it

Last time, an MLP turned an input into a prediction and then one scalar loss. Today we reuse that **same graph** in reverse:

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General pattern

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Backward: compute sensitivities loss
sensitivity for every parameter θ_j

Concrete scalar example

Forward: with $(w, x, b, y) = (2, 3, 1, 10)$

$$\hat{y} = 2 \cdot 3 + 1 = 7, \quad \mathcal{L} = (7 - 10)^2 = 9$$

Backward:

$$\left(\frac{\partial \mathcal{L}}{\partial w}, \frac{\partial \mathcal{L}}{\partial b} \right) = (-18, -6)$$

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same executed graph · values flow forward, gradients flow backward

Read the notation before the algorithm

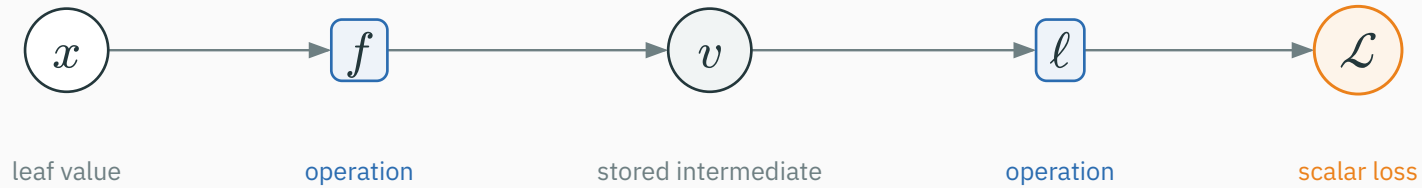
Symbol	Meaning in this lecture
u, v, z	scalars
$\mathbf{x}, \mathbf{z}, \boldsymbol{\theta}$	vectors (bold lowercase)
$\mathbf{W}, \mathbf{X}$	matrices (bold uppercase)
$\partial \mathcal{L} / \partial u$	how the loss changes when scalar u changes
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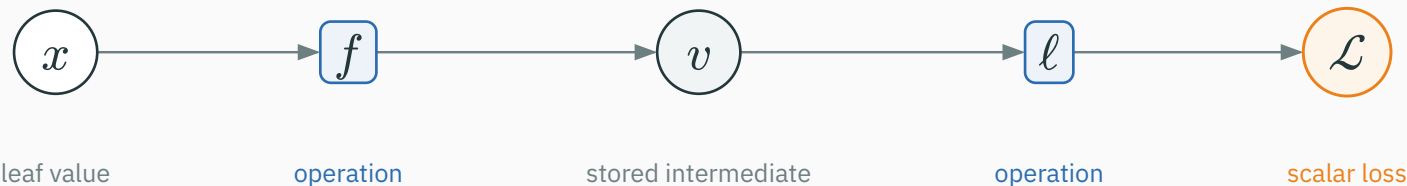
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We keep the full $\partial\mathcal{L}/\partial(\cdot)$ notation visible throughout: the numerator is always the final loss; the denominator names the stored value whose derivative we want.

Our computation-graph convention

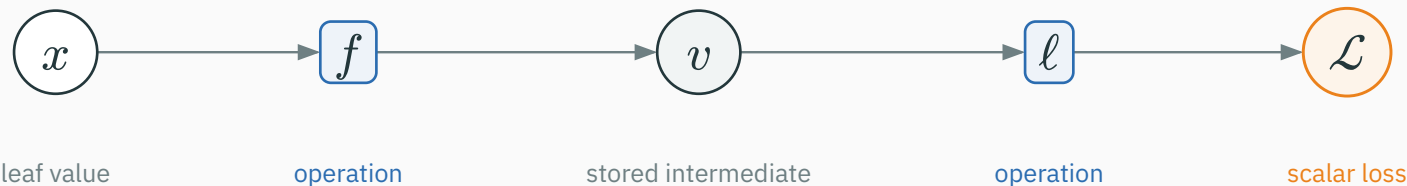


Our computation-graph convention



white circle	given value: input, parameter, or target — a graph leaf
gray circle	computed intermediate value, saved for backward when needed
blue box	operation: consumes value(s) and produces a value
gray arrow	forward dependency from a value to the operation that uses it
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circles store values • boxes transform them • arrows show dependency

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formula · approximate value · reverse sweep through the executed graph

Reverse-mode AD computes the derivative from local rules, up to floating-point arithmetic. Central difference independently approximates the same value: $g_{\text{FD}} = \frac{\mathcal{L}(\theta_j + \varepsilon) - \mathcal{L}(\theta_j - \varepsilon)}{2\varepsilon}$.

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import torch
def loss(w): return (w*3.0 + 1.0 - 10.0)**2
w, eps = 2.0, 1e-5
g_fd = (loss(w + eps) - loss(w - eps)) / (2*eps)
wt = torch.tensor(w, dtype=torch.float64, requires_grad=True)
loss(wt).backward()
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Use float64 and check only a few coordinates. Finite differences debug gradients; they do not train models because every checked coordinate needs two extra forward passes.

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Symbolic to reason • finite differences to check • reverse mode to train.

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We need all P derivatives $\partial \mathcal{L} / \partial \theta_j$. Backprop computes them together in **one reverse sweep**, without perturbing parameters one at a time.

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1 · local rule	How does one operation pass a gradient backward?

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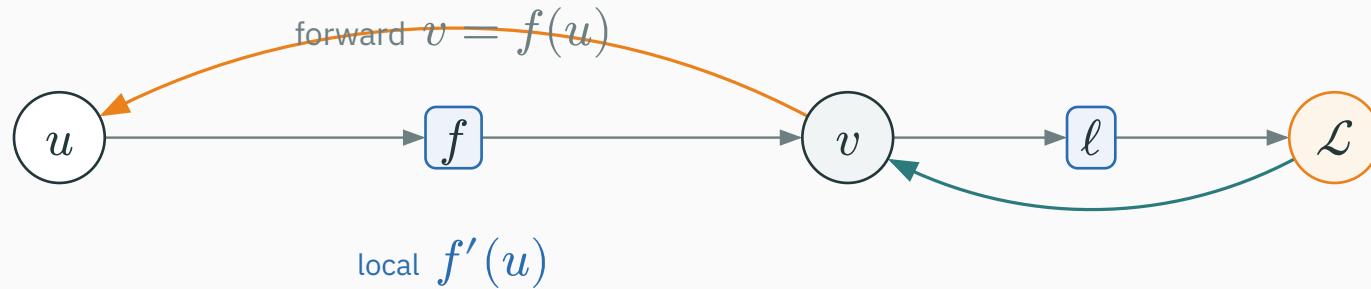
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5 · depth + gradient flow	What happens when many local gradients multiply?

One local operation

Zoom in on one operation. The value circle u enters the boxed operation f ; its output is stored in the value circle v .

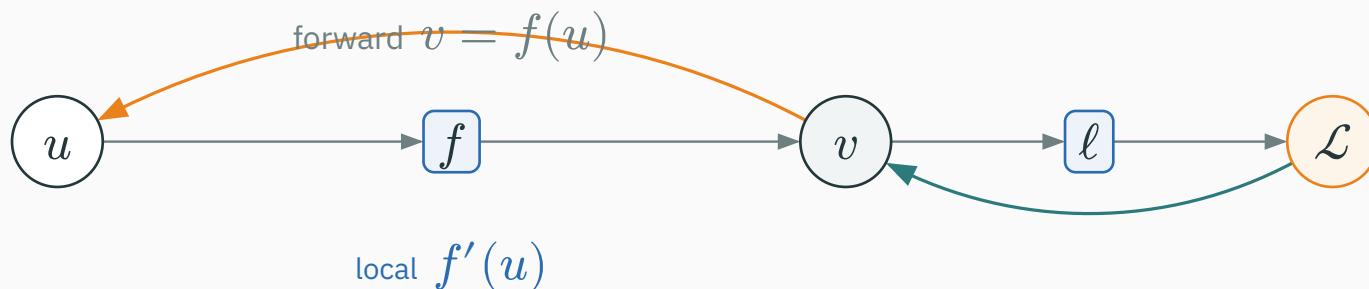
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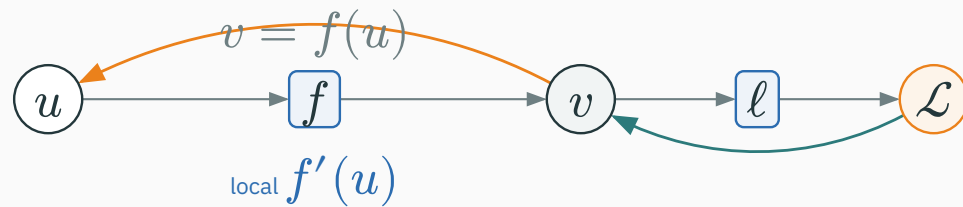


backward computes $\frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial v} \cdot f'(u)$

Every operation multiplies the arriving gradient by its local gradient

D DERIVATION

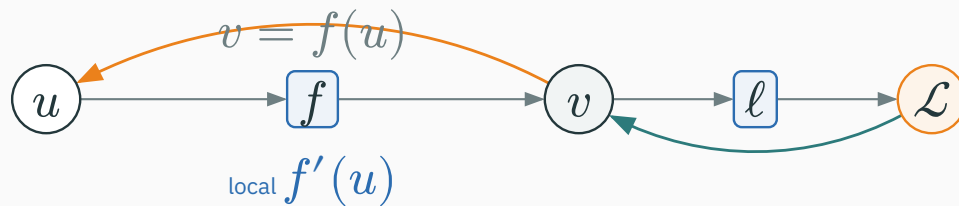
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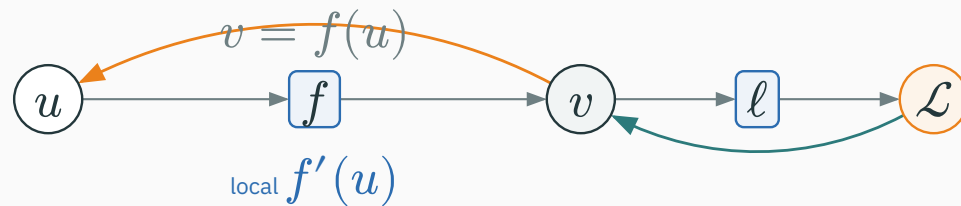


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Downstream gradient

sent back to u

$$\frac{\partial \mathcal{L}}{\partial u}$$

Upstream gradient

arriving at v

$$\frac{\partial \mathcal{L}}{\partial v}$$

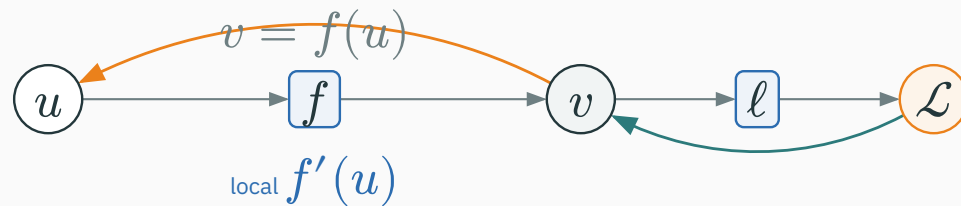
Local gradient

this operation's slope

$$f'(u) = \frac{\partial v}{\partial u}$$

The chain rule is one reusable local rule

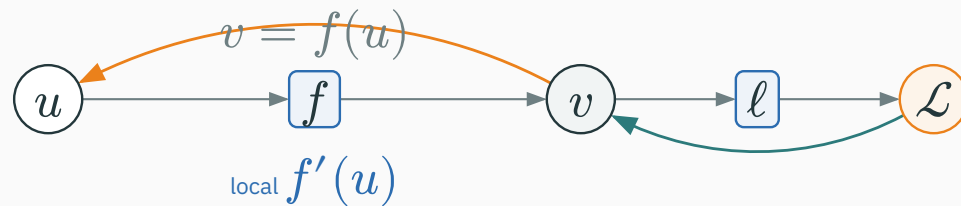
For every scalar operation $v = f(u)$:



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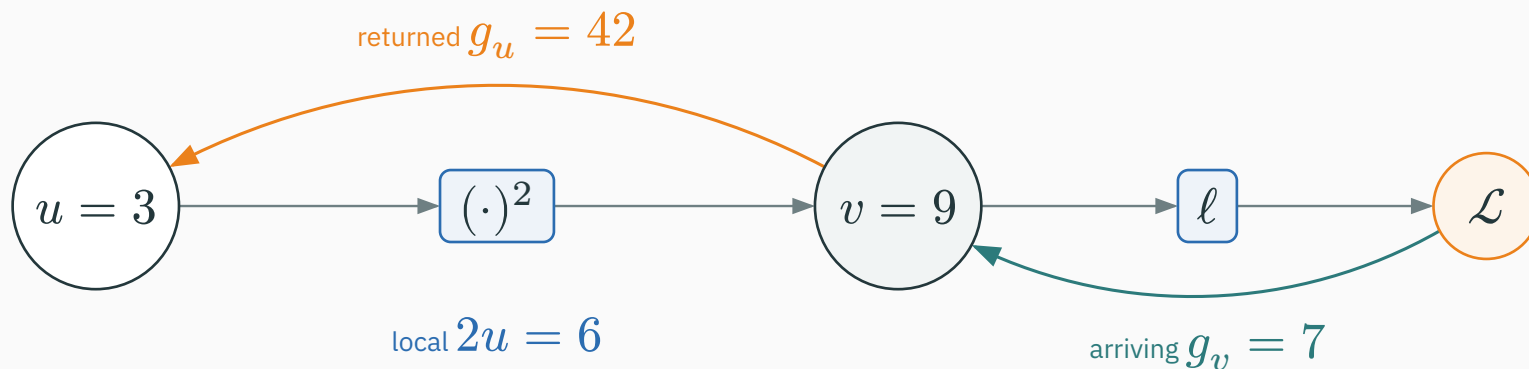
The operation multiplies its **upstream gradient** by its **local gradient** to produce the **downstream gradient**. It needs no global formula for the whole network.

Example: a square operation

For $v = u^2$ at $u = 3$, the forward value is $v = 9$ and the **local slope** is $\partial v / \partial u = 2u = 6$. Suppose the rest of the graph sends $g_v = \partial \mathcal{L} / \partial v = 7$ back to this square.

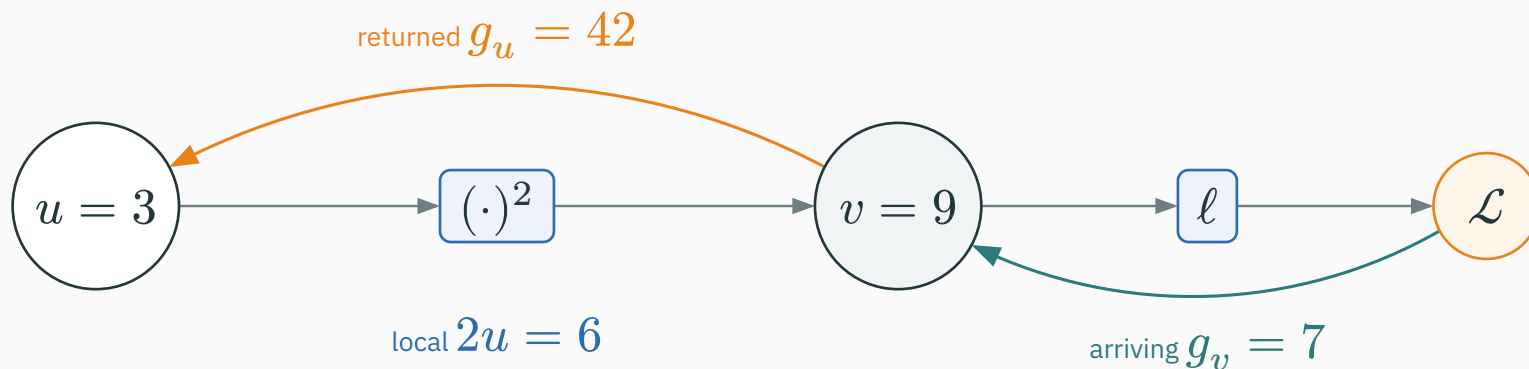
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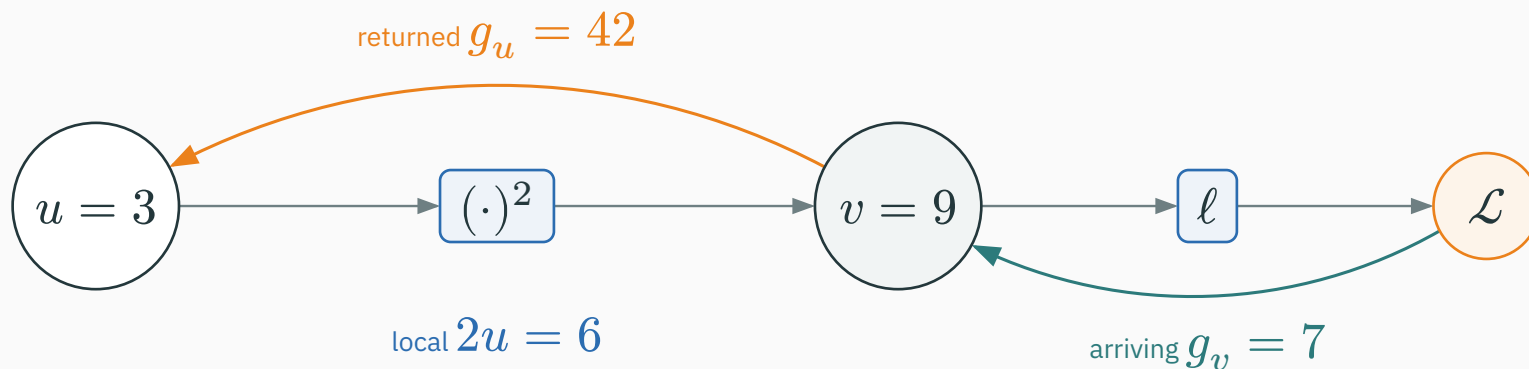
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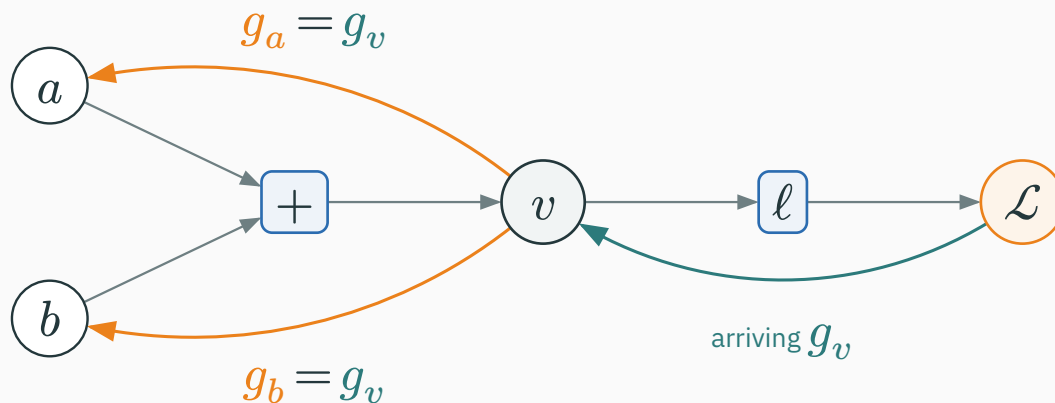
The square operation multiplies the arriving $\partial \mathcal{L} / \partial v = 7$ by its **local gradient** $2u = 6$ to produce $\partial \mathcal{L} / \partial u = 42$.

Addition copies the arriving gradient

Operation $v = a + b$. Let $g_v = \partial \mathcal{L} / \partial v$ arrive. Local derivatives: $\partial v / \partial a = 1$, $\partial v / \partial b = 1$.

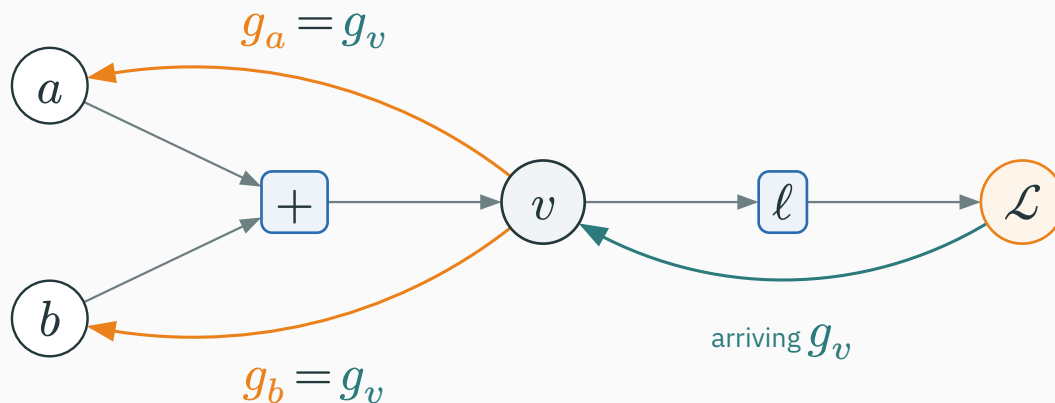
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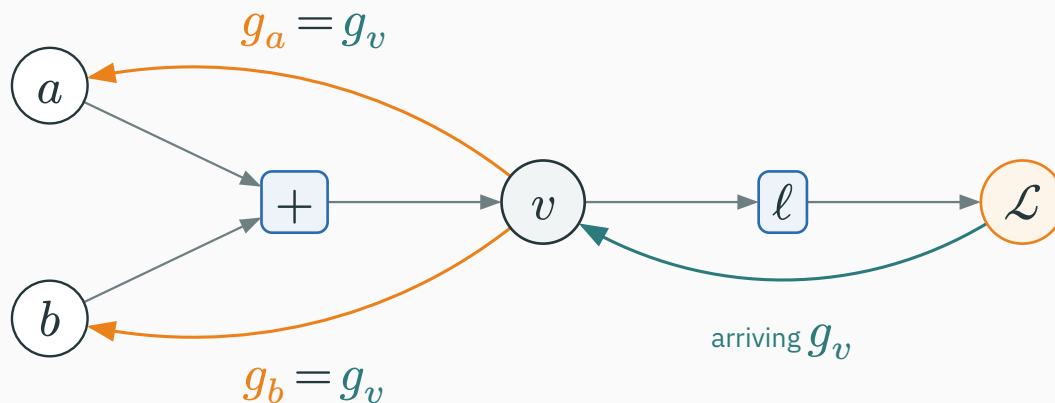
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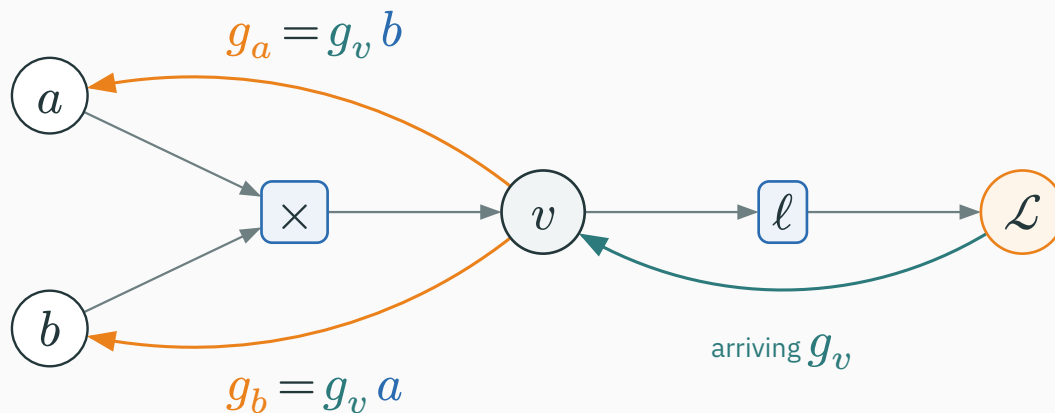
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+ copies the **arriving derivative** into a **downstream derivative** for every input.

Operation $v = ab$. Let $g_v = \partial \mathcal{L} / \partial v$ arrive. Local derivatives: $\partial v / \partial a = b$, $\partial v / \partial b = a$.

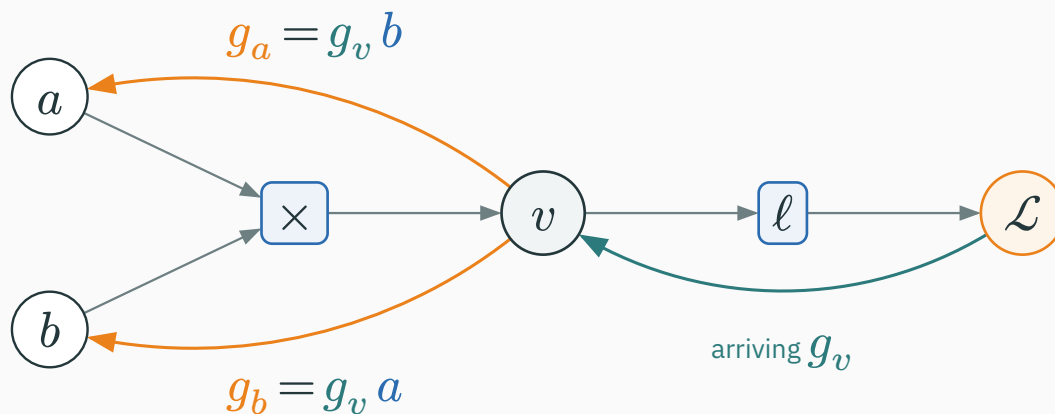
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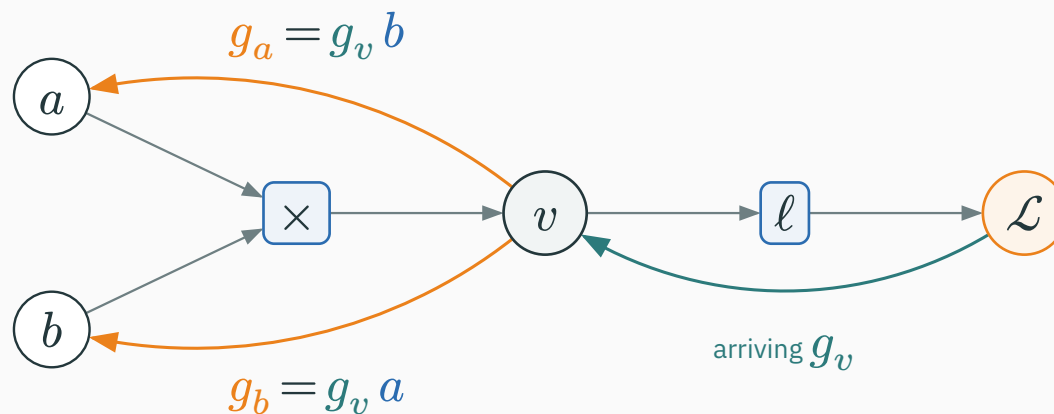
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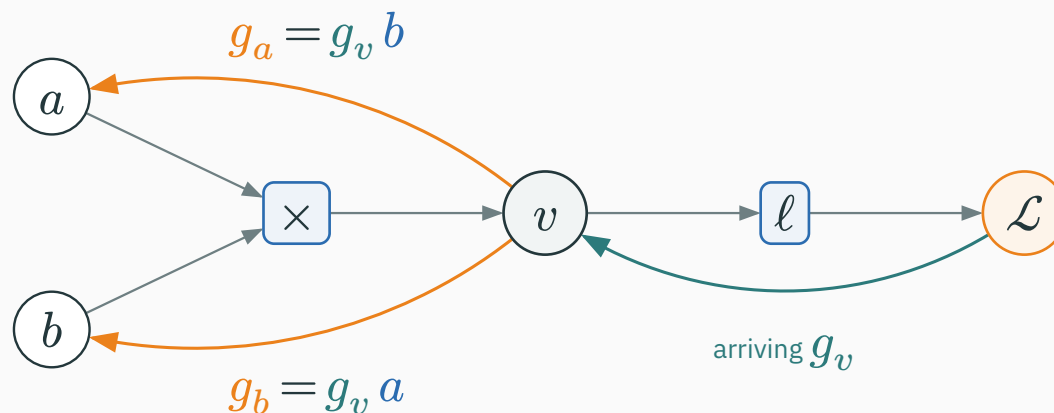


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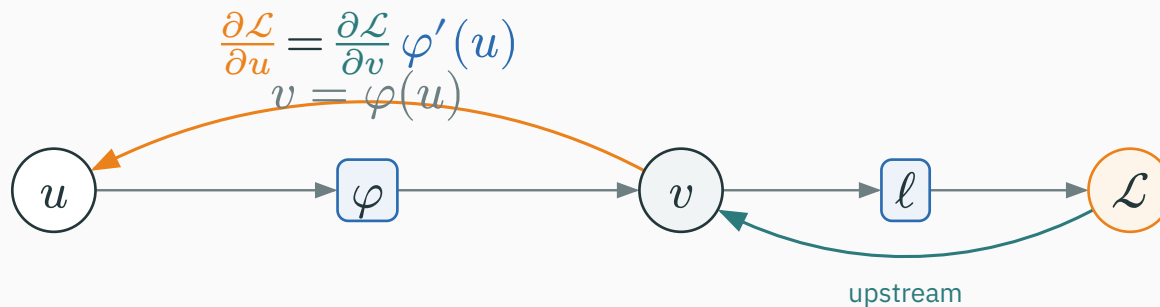
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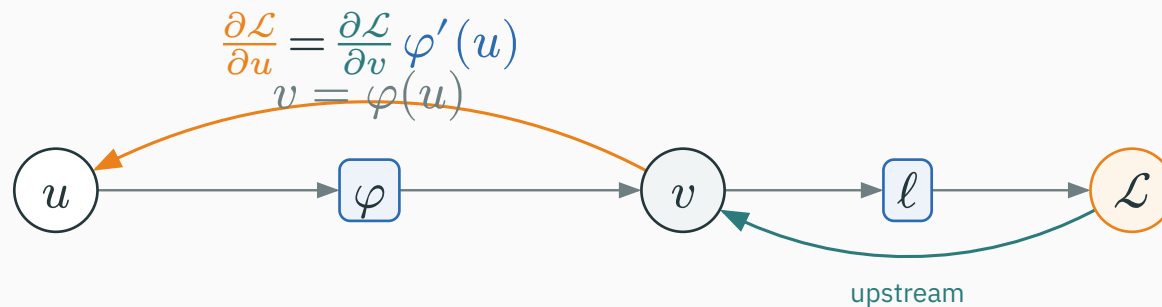
| If $a = 2$, $b = 5$, and $\partial \mathcal{L} / \partial v = 3$, then $\partial \mathcal{L} / \partial a = 15$ and $\partial \mathcal{L} / \partial b = 6$.

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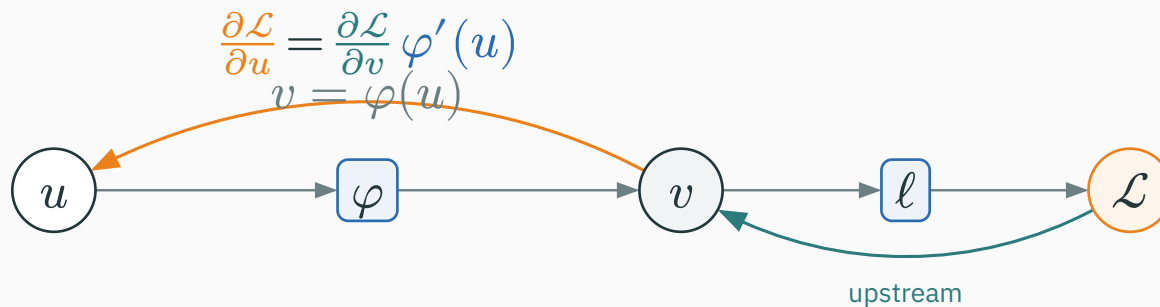


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| **sigmoid** σ : $\varphi'(u) = \sigma(u)(1 - \sigma(u))$

| **ReLU**: $\varphi'(u) = 1$ for $u > 0$, and 0 for $u < 0$

Pop quiz: what crosses an inactive ReLU?

QUESTION

Let $v = \text{ReLU}(u)$. If $u = -2$ and the upstream gradient is $\partial \mathcal{L} / \partial v = 5$, what downstream gradient $\partial \mathcal{L} / \partial u$ is sent back?

A. 5

B. -10

C. 0

D. undefined because $u < 0$

Answer: an inactive ReLU blocks the gradient

A ANSWER

Correct: C — 0

Why: For $u < 0$, the local gradient is $\partial v / \partial u = 0$. Therefore downstream = upstream $\times$ local = $5 \times 0 = 0$.

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Backward: $5 \times 0 \rightarrow \partial \mathcal{L} / \partial u = 0$

At exactly $u = 0$, ReLU's ordinary derivative is undefined. Autodiff software must choose a convention; commonly it returns 0.

The rule table — memorize this

Forward operation	Contribution sent backward
$v = a + b$	$\frac{\partial \mathcal{L}}{\partial a} += \frac{\partial \mathcal{L}}{\partial v} \cdot 1$ $\frac{\partial \mathcal{L}}{\partial b} += \frac{\partial \mathcal{L}}{\partial v} \cdot 1$
$v = ab$	$\frac{\partial \mathcal{L}}{\partial a} += \frac{\partial \mathcal{L}}{\partial v} \cdot b$ $\frac{\partial \mathcal{L}}{\partial b} += \frac{\partial \mathcal{L}}{\partial v} \cdot a$
$v = u^2$	$\frac{\partial \mathcal{L}}{\partial u} += \frac{\partial \mathcal{L}}{\partial v} \cdot 2u$
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Forward operation	Contribution sent backward
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$v = ab$	$\frac{\partial \mathcal{L}}{\partial a} += \frac{\partial \mathcal{L}}{\partial v} \cdot b$ $\frac{\partial \mathcal{L}}{\partial b} += \frac{\partial \mathcal{L}}{\partial v} \cdot a$
$v = u^2$	$\frac{\partial \mathcal{L}}{\partial u} += \frac{\partial \mathcal{L}}{\partial v} \cdot 2u$
$v = \varphi(u)$	$\frac{\partial \mathcal{L}}{\partial u} += \frac{\partial \mathcal{L}}{\partial v} \cdot \varphi'(u)$

Use +=, not = — a value consumed by several operations accumulates gradient from **all** of them.

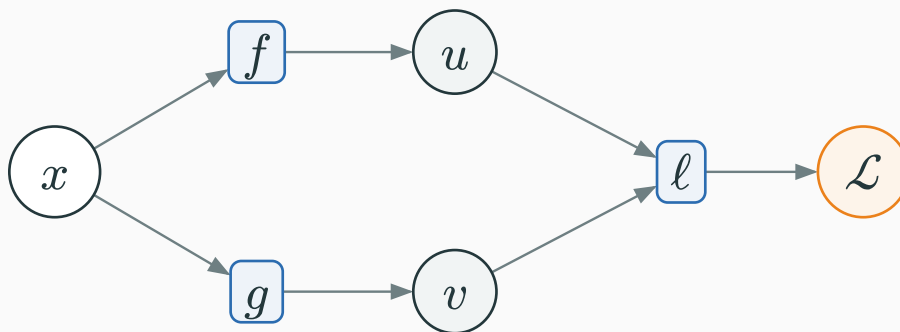
Gradients accumulate at branches

Why gradients add at a branch

Imagine nudging x from 4 to 4.01. The **same nudge** travels down both routes to the loss:

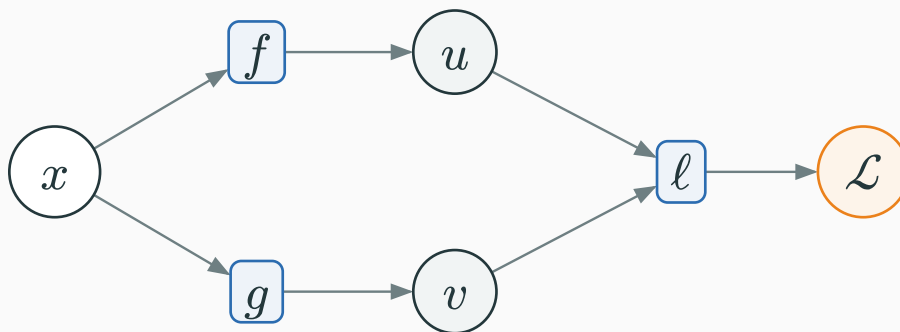
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Imagine nudging x from 4 to 4.01. The **same nudge** travels down both routes to the loss:



Via $u = x^2$: the local slope is $2x = 8$, so $\Delta x = 0.01$ changes the loss by about $8 \cdot 0.01 = 0.08$.

Via $v = 3x$: the local slope is 3, so the same nudge changes the loss by about $3 \cdot 0.01 = 0.03$.

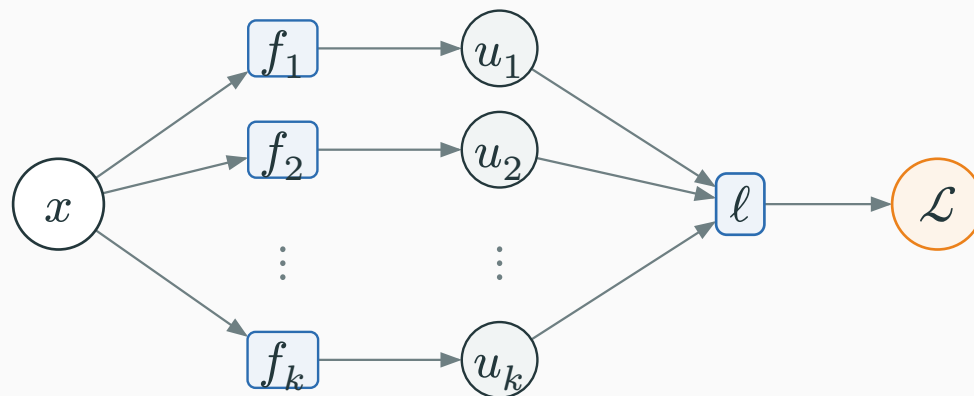
$$\text{total slope} = \text{total loss change} \div \text{nudge} = \frac{0.08+0.03}{0.01} = 8 + 3 = 11$$

The multivariable chain rule adds every path

The nudge experiment generalizes. If x influences $\mathcal{L}$ through $u_1, \dots, u_k$:

The multivariable chain rule adds every path

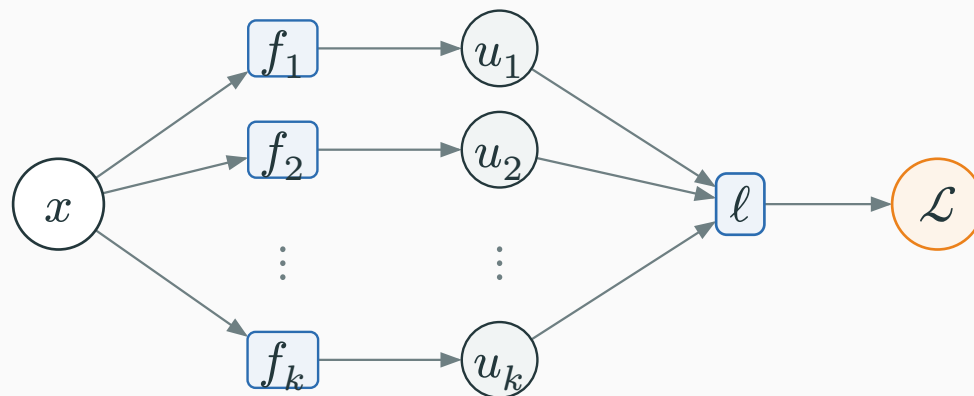
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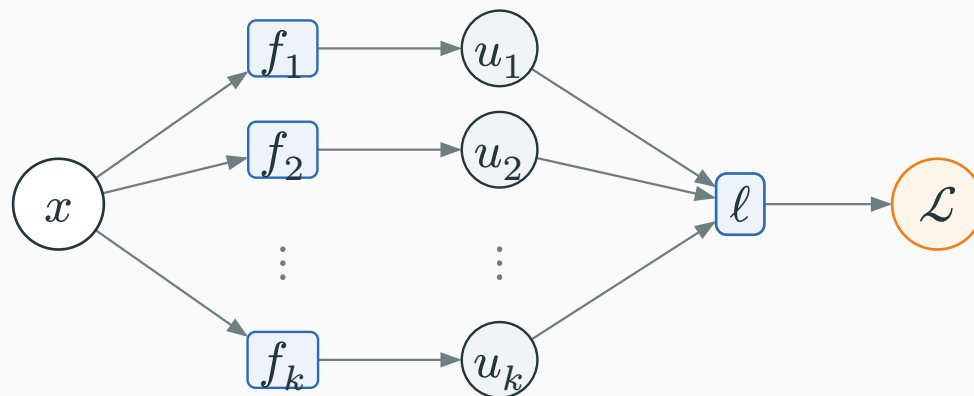


branch i contributes upstream $\partial \mathcal{L} / \partial u_i \times$ local $\partial u_i / \partial x$

$$\frac{\partial \mathcal{L}}{\partial x} = \sum_{i=1}^k \frac{\partial \mathcal{L}}{\partial u_i} \frac{\partial u_i}{\partial x}.$$

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$$\frac{\partial \mathcal{L}}{\partial x} = \sum_{i=1}^k \frac{\partial \mathcal{L}}{\partial u_i} \frac{\partial u_i}{\partial x}.$$

each path contributes one chain-rule product; the products add

Worked branch example

Let $u = x^2$, $v = 3x$, $\mathcal{L} = u + v = x^2 + 3x$.

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Now let us get the **same** answer by backprop.

Forward at $x = 4$: $u = 16$, $v = 12$, $\mathcal{L} = 28$.

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$$\frac{\partial\mathcal{L}}{\partial x} = 8 + 3 = 11. \quad \checkmark$$

PyTorch adds the same two paths

```
import torch

x = torch.tensor(4.0, requires_grad=True)
u = x**2           # path 1
v = 3*x           # path 2
L = u + v
L.backward()

print(x.grad)      # tensor(11.)
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| **via v :** $\partial \frac{v}{\partial} x = 3$

autograd accumulates both downstream contributions: $8 + 3 = 11$

The central worked example

Predict $\hat{y} = wx + b$, squared-error loss $\mathcal{L} = (\hat{y} - y)^2$.

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$$x = 3, \quad w = 2, \quad b = 1, \quad y = 10.$$

Compute $\partial\mathcal{L}/\partial w$, $\partial\mathcal{L}/\partial x$, $\partial\mathcal{L}/\partial b$, and $\partial\mathcal{L}/\partial y$ by backpropagation; verify the four values with PyTorch.

Break into primitives

Decompose the loss into elementary operations and name each stored result:

$$m = wx, \quad a = m + b, \quad e = a - y, \quad \mathcal{L} = e^2.$$

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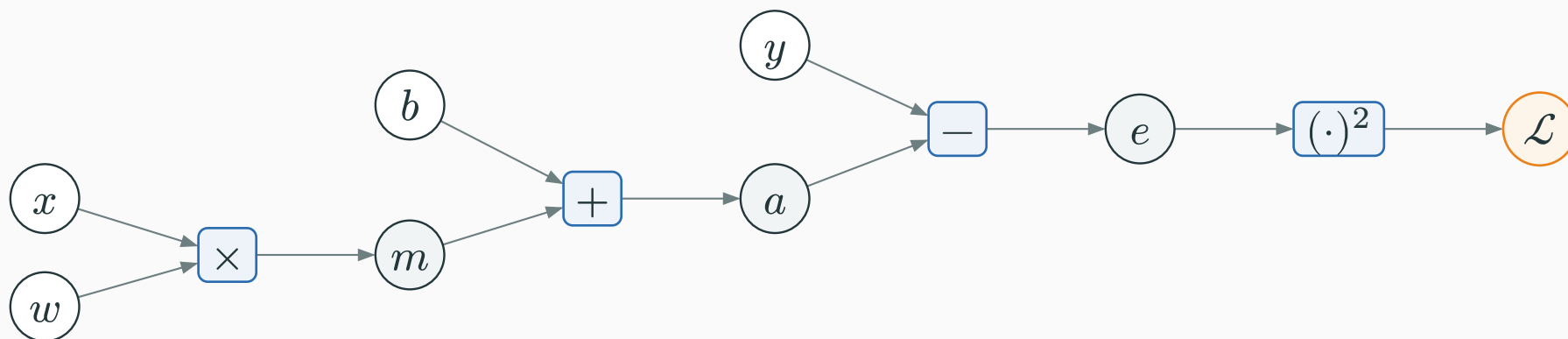
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value m after $\times$ • value a after $+$ • value e after $-$ • value $\mathcal{L}$ after $(\cdot)^2$

The symbols m , a , and e name stored intermediate values. They are circles in the graph; the four operations are boxes.

The computation graph



Given values	w, x, b, y	Stored values	m, a, e
Operations	$\times, +, -, (\cdot)^2$	Scalar loss	$\mathcal{L}$

Stored value	Operation that produces it	Numeric value
m	$w \times x$	$2 \cdot 3 = 6$
a	$m + b$	$6 + 1 = 7$
e	$a - y$	$7 - 10 = -3$
$\mathcal{L}$	e^2	$(-3)^2 = 9$

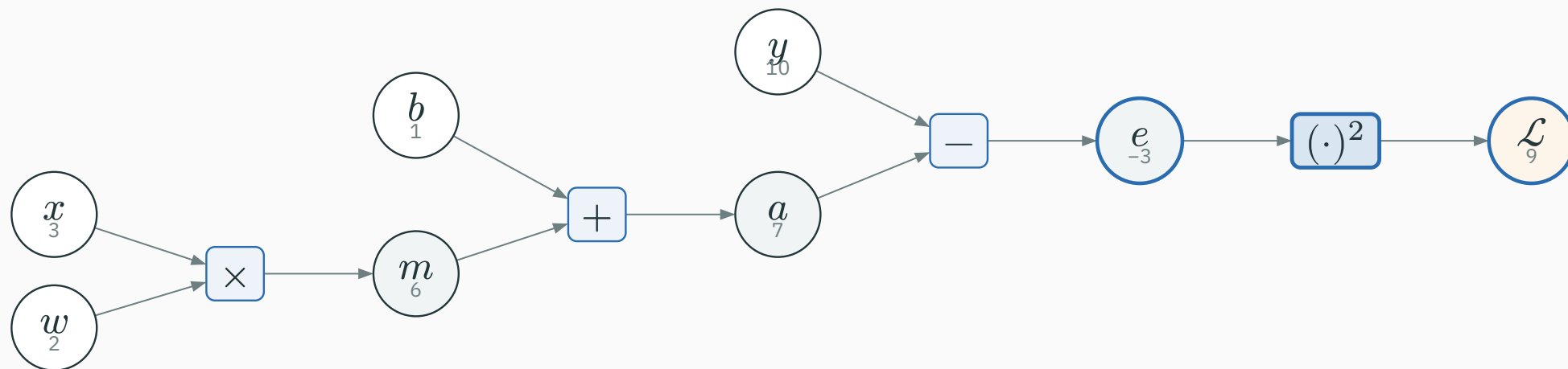
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$\mathcal{L}$	e^2	$(-3)^2 = 9$

$\mathcal{L} = 9$ — now run the graph **backward**

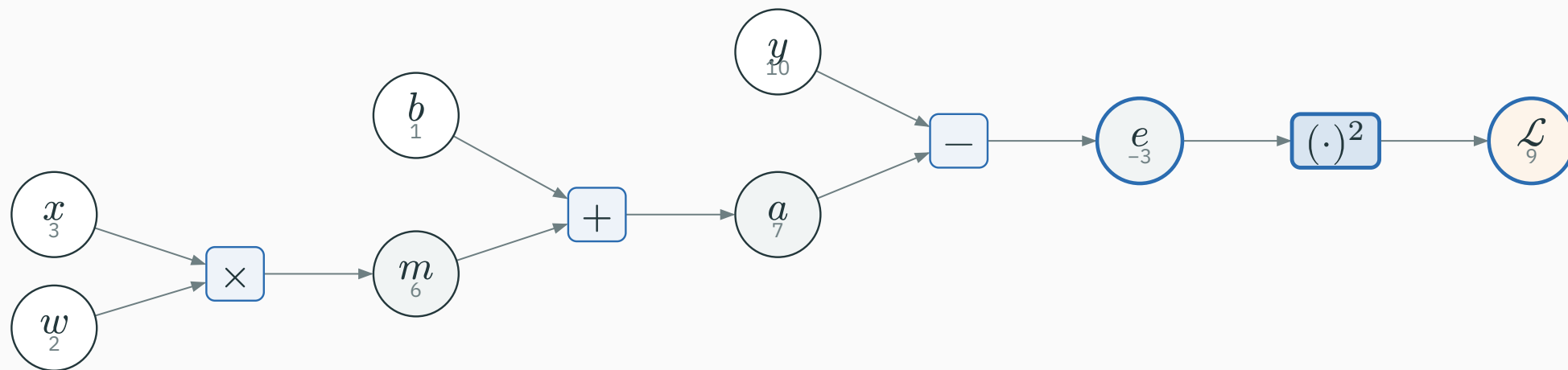
Seed the output: $\partial \mathcal{L} / \partial \mathcal{L} = 1$.

Backward: seed and the square operation

Seed the output: $\partial \mathcal{L} / \partial \mathcal{L} = 1$.



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Square operation $\mathcal{L} = e^2$, local $\partial \mathcal{L} / \partial e = 2e$:

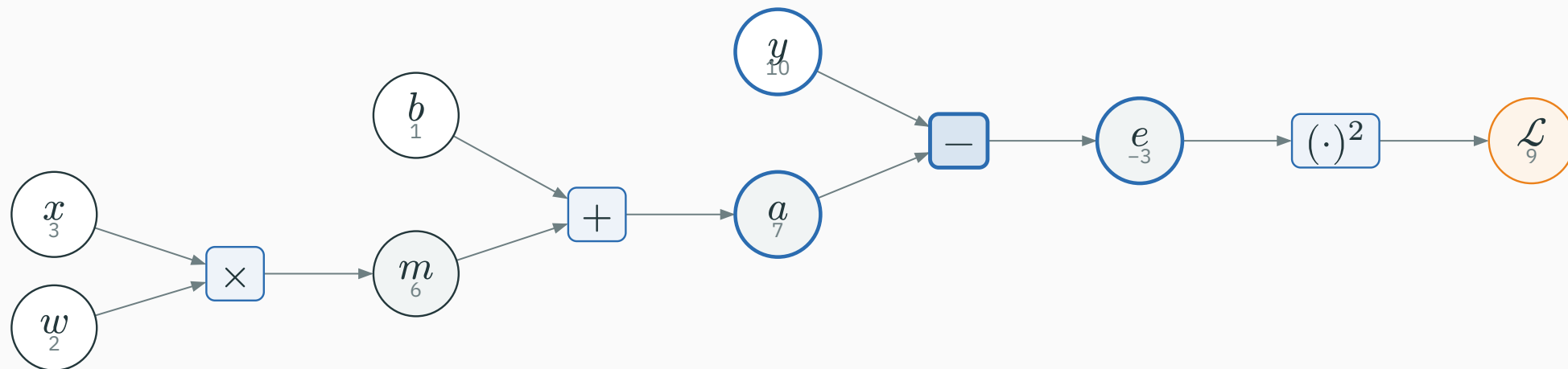
$$\frac{\partial \mathcal{L}}{\partial e} = 1 \cdot 2e = 1 \cdot 2(-3) = -6.$$

Backward: the subtraction operation

Subtraction operation $e = a - y$, locals $\partial e / \partial a = 1$, $\partial e / \partial y = -1$:

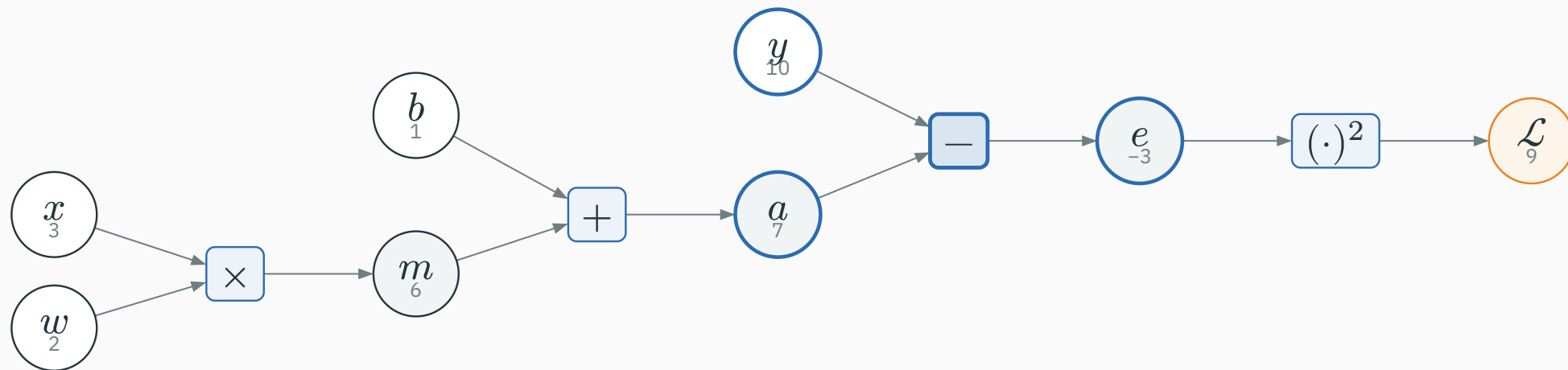
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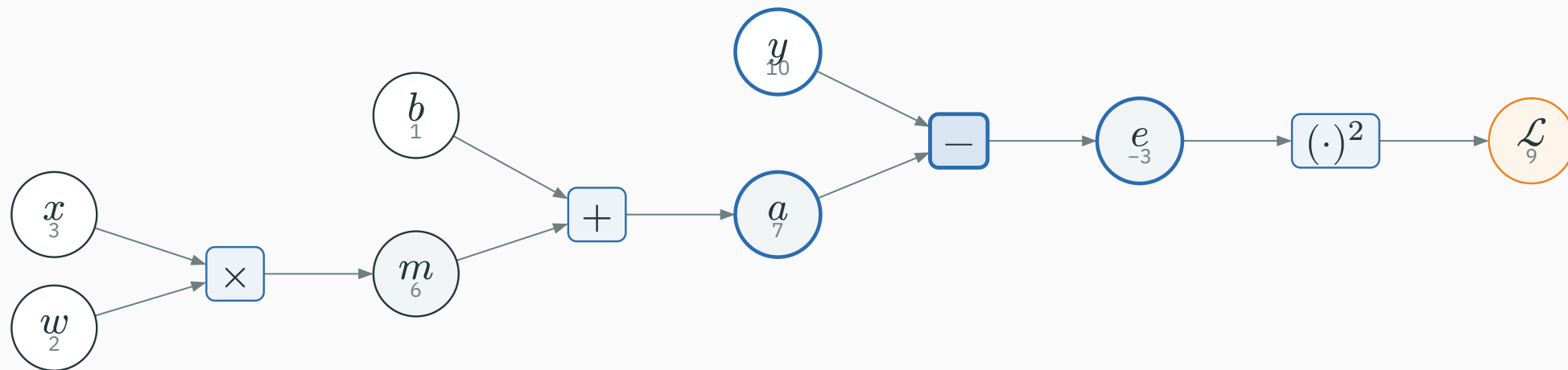
Subtraction operation $e = a - y$, locals $\partial e / \partial a = 1$, $\partial e / \partial y = -1$:



$$\frac{\partial \mathcal{L}}{\partial a} = \frac{\partial \mathcal{L}}{\partial e} \cdot 1 = -6$$

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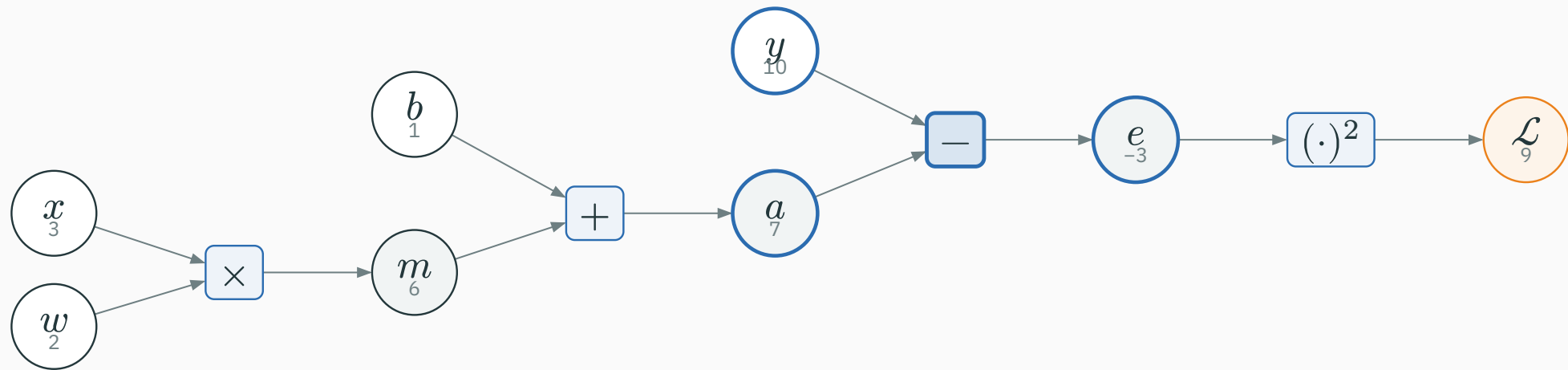
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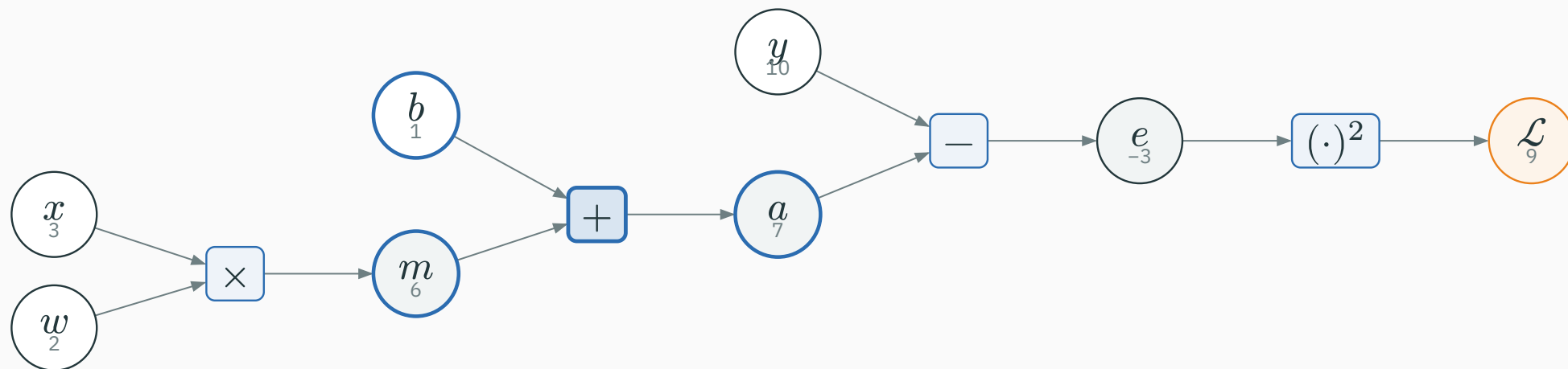
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The target y also receives a derivative. We would use $\partial \mathcal{L} / \partial y$ if y were itself a learned quantity.

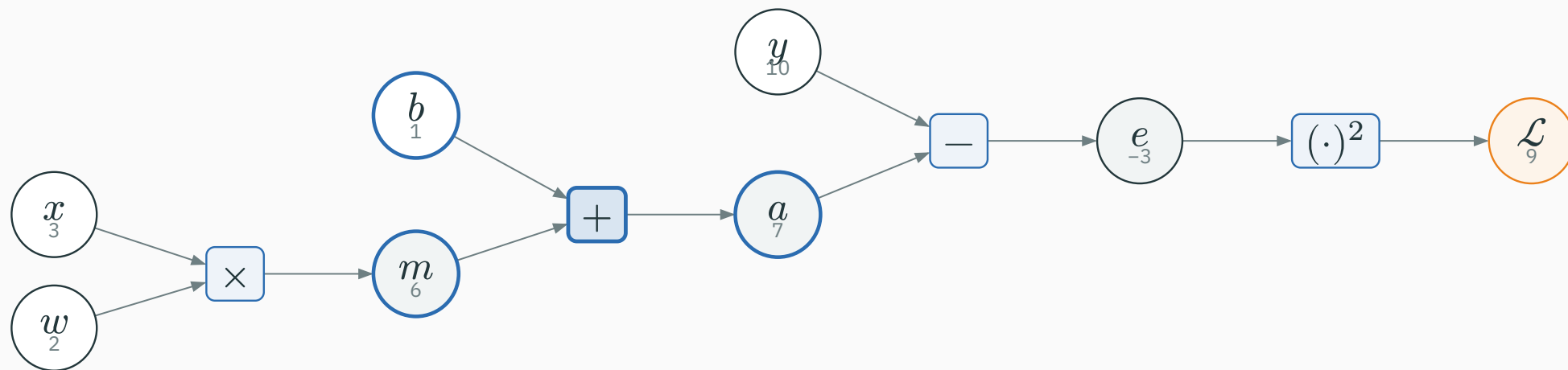
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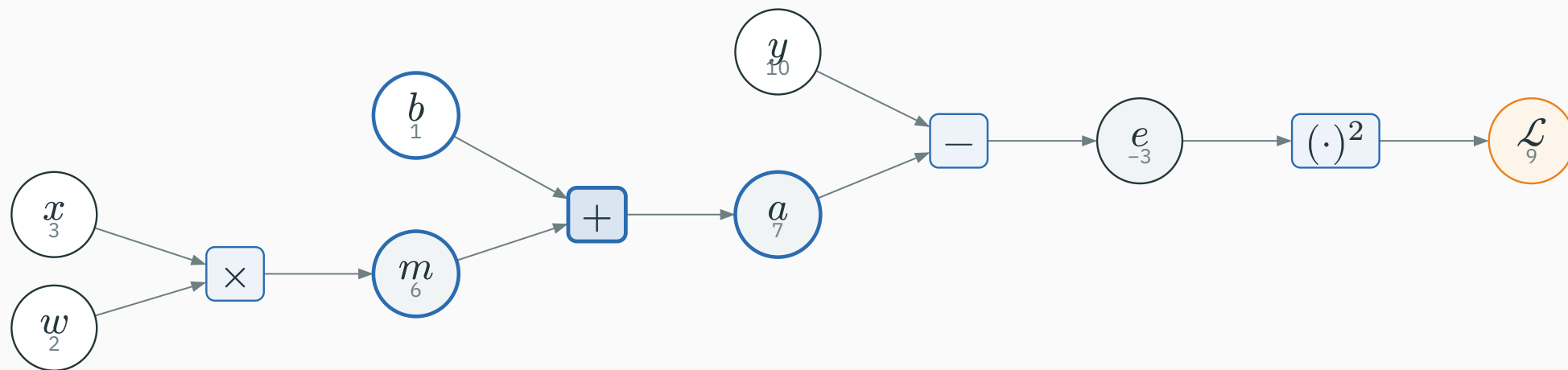


Addition operation $a = m + b$ **copies** its gradient:



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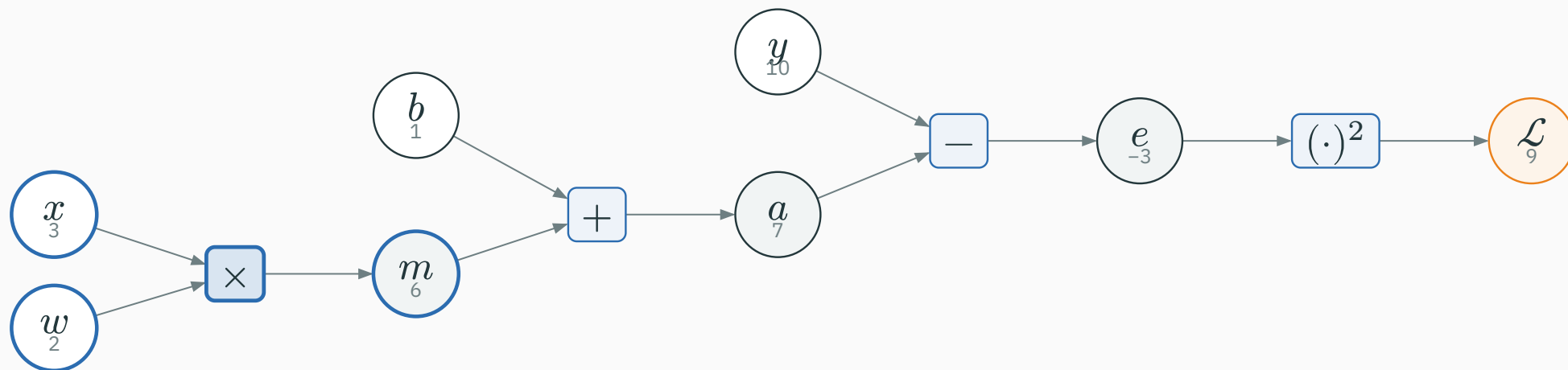
$$\frac{\partial \mathcal{L}}{\partial m} = \frac{\partial \mathcal{L}}{\partial a} = -6, \quad \frac{\partial \mathcal{L}}{\partial b} = -6.$$

So $\partial \mathcal{L} / \partial b = -6$ is one of our final answers.

Multiplication operation $m = wx$ **sends the other input:**

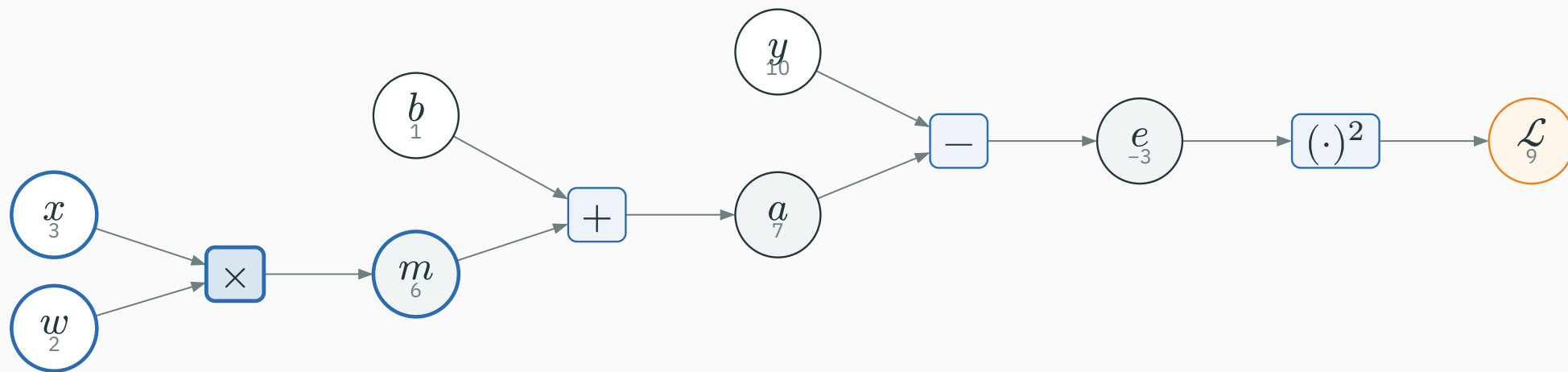
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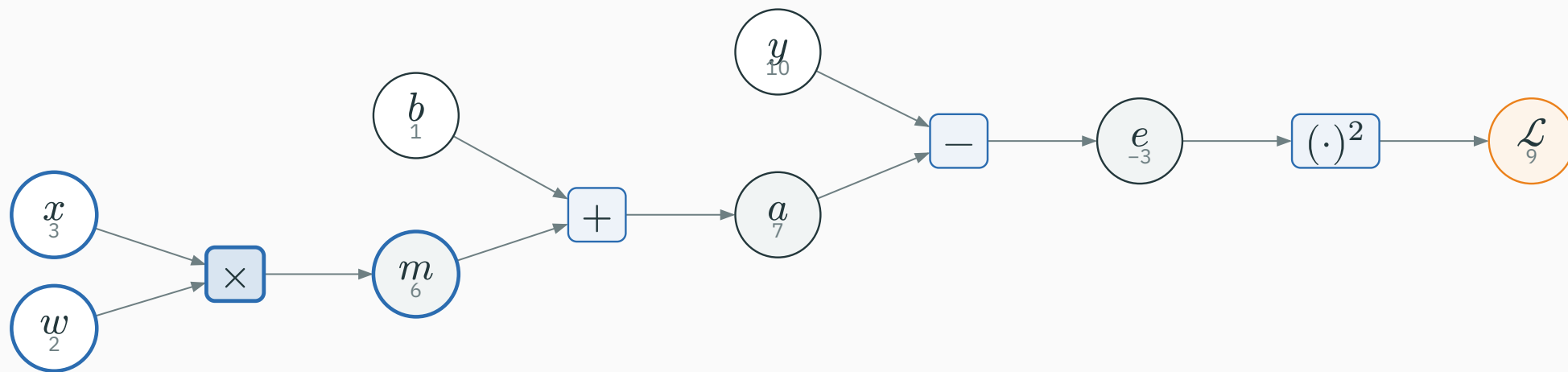
Multiplication operation $m = wx$ **sends the other input:**



$$\frac{\partial \mathcal{L}}{\partial w} = \frac{\partial \mathcal{L}}{\partial m} \cdot x = -6 \cdot 3 = -18$$

Backward: the multiplication operation

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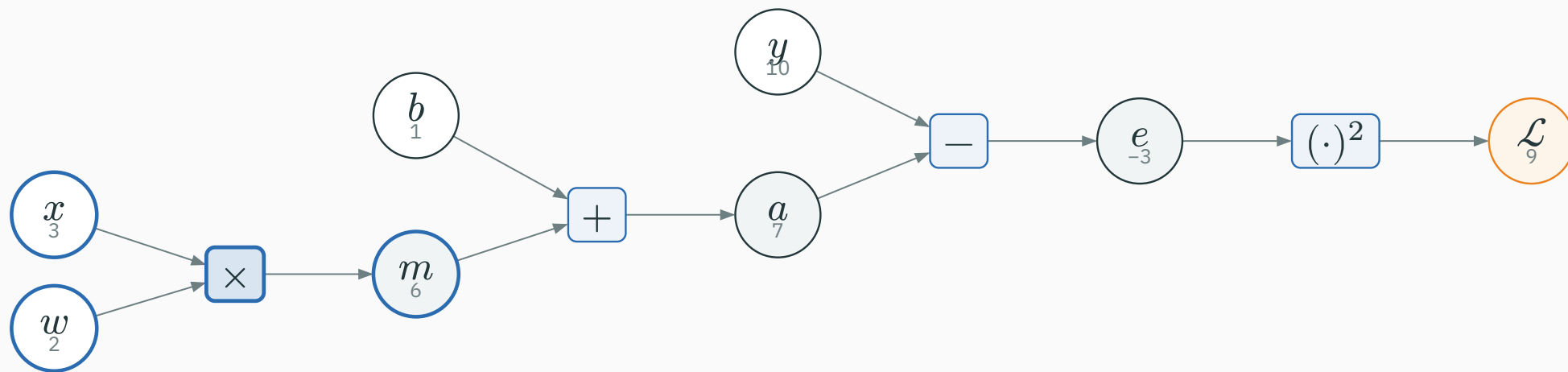


$$\frac{\partial \mathcal{L}}{\partial w} = \frac{\partial \mathcal{L}}{\partial m} \cdot x = -6 \cdot 3 = -18$$

$$\frac{\partial \mathcal{L}}{\partial x} = \frac{\partial \mathcal{L}}{\partial m} \cdot w = -6 \cdot 2 = -12$$

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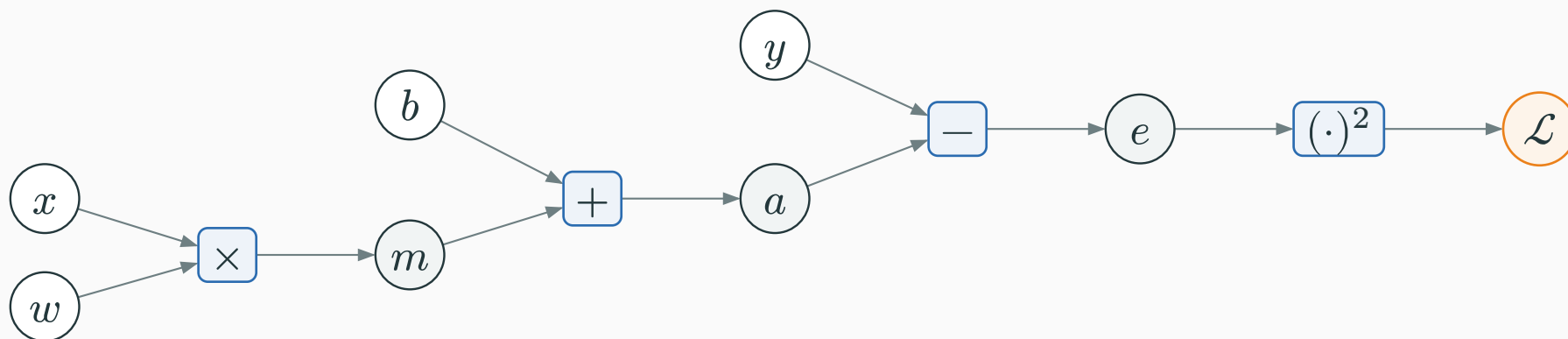
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$\partial \mathcal{L} / \partial w$	$\partial \mathcal{L} / \partial b$	$\partial \mathcal{L} / \partial x$	$\partial \mathcal{L} / \partial y$
-18	-6	-12	6

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-18	-6	-12	6

One backward sweep produced **all four** partial derivatives — no formula re-derivation per parameter.

All stored values and their gradients



first half	w	x	m	b
forward value	2	3	6	1
gradient	$g_w = -18$	$g_x = -12$	$g_m = -6$	$g_b = -6$

second half	a	y	e	$\mathcal{L}$
forward value	7	10	-3	9
gradient	$g_a = -6$	$g_y = 6$	$g_e = -6$	$g_{\mathcal{L}} = 1$

Keep w, x, b, y symbolic, derive the formulas, and only then substitute $wx + b - y = -3$:

Keep w, x, b, y symbolic, derive the formulas, and only then substitute $wx + b - y = -3$:

$$\frac{\partial \mathcal{L}}{\partial w} = 2(wx + b - y)x = 2(-3)(3) = -18 \quad \checkmark$$

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Backprop and the symbolic formulas agree at this point.

PyTorch executes the same graph

```
import torch

w = torch.tensor(2.0, requires_grad=True)
x = torch.tensor(3.0, requires_grad=True)
b = torch.tensor(1.0, requires_grad=True)
# Targets normally do not track gradients; enable it here to inspect dL/dy.
y = torch.tensor(10.0, requires_grad=True)

m = w * x
a = m + b
e = a - y
L = e**2
for value in (m, a, e, L):
    value.retain_grad()      # keep intermediate grads for inspection

L.backward()
print([t.item() for t in (m, a, e, L)])
# [6.0, 7.0, -3.0, 9.0]
print([t.grad.item() for t in (L, e, a, m, w, x, b, y)])
# [1.0, -6.0, -6.0, -6.0, -18.0, -12.0, -6.0, 6.0]
```

In our graph	In PyTorch	Meaning
stored scalar value	Tensor	one stored forward value
local backward rule	grad_fn	operation that produced a non-leaf tensor
saved forward value	saved by the operation	operand needed by a local derivative
reverse sweep	L.backward()	seed at $\mathcal{L}$; visit operations in reverse order
leaf derivative	p.grad	$\partial \mathcal{L} / \partial p$, accumulated with +=
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reverse mode = direction · backprop = algorithm · autograd = engine: record → save → replay

We found $\partial \mathcal{L} / \partial w = -18$. For a small positive learning rate, which way does gradient descent move w ?

A. Decrease w

B. Increase w

C. Leave w unchanged

D. The sign tells us nothing

Answer: a negative gradient means increase the parameter

A ANSWER

Correct: B — Increase w

Why: Gradient descent subtracts the gradient: $w \leftarrow w - \eta(-18) = w + 18\eta$.

A small gradient step reduces this loss

Take $\eta = 0.01$ and update:

$$w \leftarrow 2 - 0.01(-18) = 2.18, \quad b \leftarrow 1 - 0.01(-6) = 1.06.$$

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loss falls from 9 to $(7.60 - 10)^2 = 5.76$

Backprop supplied the direction. The learning rate controls how far we move; a later optimization lecture studies that choice.

INTERACTIVE

↗ nipunbatra.github.io/interactive-articles/autograd

Build a scalar computation graph, run the forward pass, then click **backward** to watch each $\partial \mathcal{L} / \partial u$ fill in — exactly the $(wx + b - y)^2$ example above.

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Build a scalar computation graph, run the forward pass, then click **backward** to watch each $\partial\mathcal{L}/\partial u$ fill in — exactly the $(wx + b - y)^2$ example above.

Trace which local rule changes when the final squared-error operation is replaced with $|e|$.

See it move

Step through values and loss derivatives in the interactive graph ↗.

Run one complete Colab

Open the lecture notebook ↓: manual graph, PyTorch, dense layer, batch, and MLP.

Follow the checkpoints

Predict first; then execute one checkpoint and compare. The same numbers recur throughout the lecture.

Practice the scalar graph three ways

I INTERACTIVE

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Follow the checkpoints

Predict first; then execute one checkpoint and compare. The same numbers recur throughout the lecture.

Easy	change one input and recompute the forward pass
Medium	derive all four gradients before calling <code>backward()</code>
Hard	replace the square by $ e $; state what happens at $e = 0$

From scalars to vectors

We store gradients as column vectors. The name of the local object depends on the input and output shapes:

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Operation shape	Local object	Name
$u \in \mathbb{R} \rightarrow v \in \mathbb{R}$	$\partial v / \partial u \in \mathbb{R}$	derivative
$\mathbf{x} \in \mathbb{R}^d \rightarrow z \in \mathbb{R}$	$\partial z / \partial \mathbf{x} \in \mathbb{R}^d$	gradient
$\mathbf{x} \in \mathbb{R}^d \rightarrow \mathbf{z} \in \mathbb{R}^m$	$J_{ij} = \partial z_i / \partial x_j$	Jacobian $\mathbf{J} \in \mathbb{R}^{m \times d}$

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a Jacobian contains one local derivative for every output–input pair

A 2×2 Jacobian is four familiar derivatives

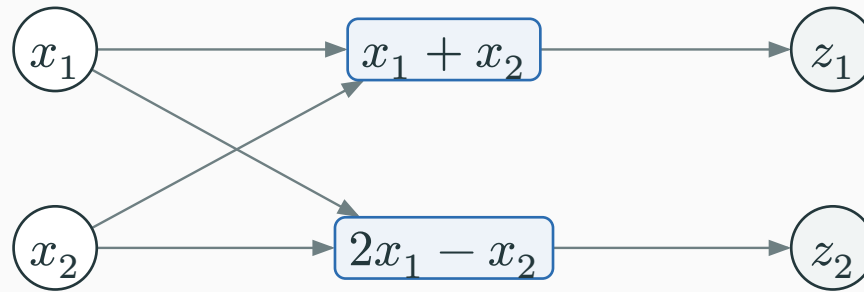
Take a vector operation with two inputs and two outputs:

$$z_1 = x_1 + x_2, \quad z_2 = 2x_1 - x_2.$$

A 2×2 Jacobian is four familiar derivatives

Take a vector operation with two inputs and two outputs:

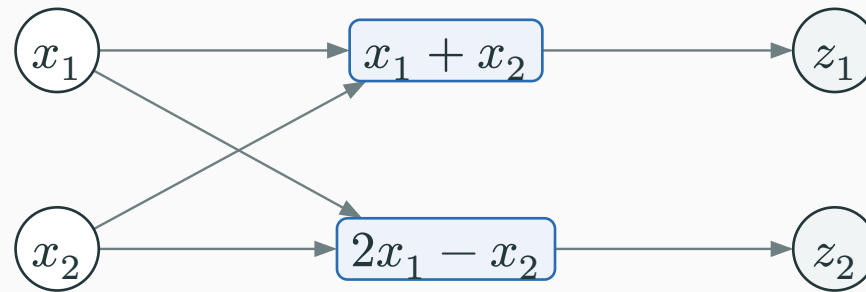
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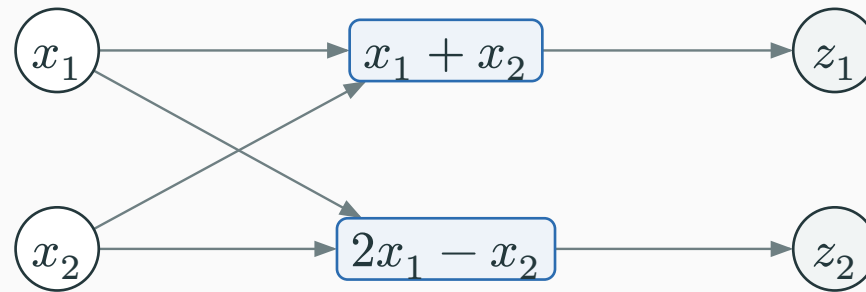


Output	Input x_1	Input x_2
z_1	$\partial z_1 / \partial x_1 = 1$	$\partial z_1 / \partial x_2 = 1$
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$$\mathbf{J} = \begin{pmatrix} 1 & 1 \\ 2 & -1 \end{pmatrix} \cdot \text{rows are outputs} \cdot \text{columns are inputs}$$

Vector chain rule: make the shapes fit

For $x \in \mathbb{R}^d \rightarrow z \in \mathbb{R}^m$, let the **local Jacobian** be

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| When $d = m = 1$, J is one number and this is the scalar chain rule from earlier.

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For the previous operation, suppose the arriving gradient is

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$\partial \mathcal{L} / \partial x_1$	$3(1) + 4(2) = 11$
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the vector rule is the scalar branch rule applied to every input

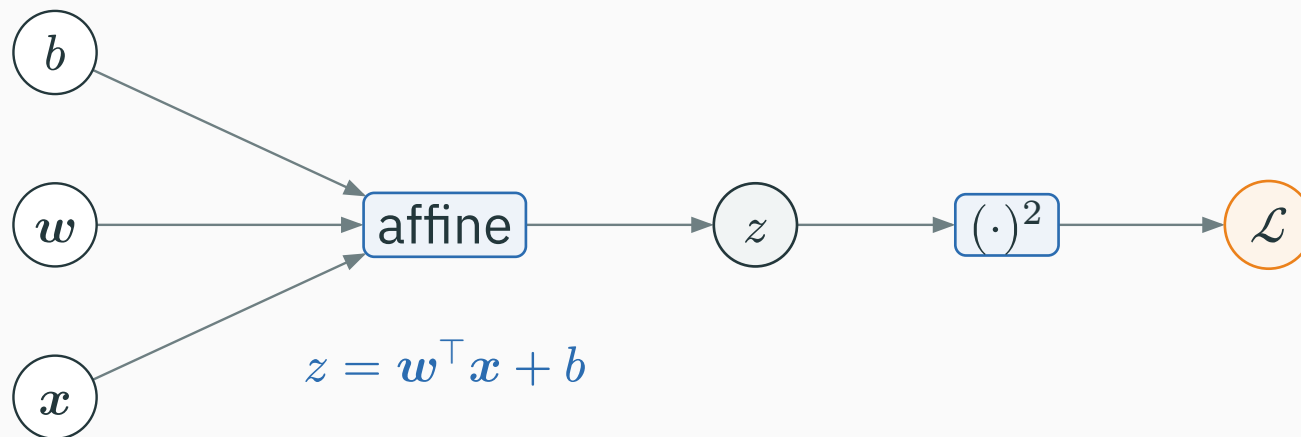
Affine means a weighted sum plus a bias:

$$z = \mathbf{w}^\top \mathbf{x} + b = \sum_{j=1}^d w_j x_j + b.$$

An affine operation adds scalar products and a bias

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$x_i \rightarrow x_i + \Delta$	$w_i(x_i + \Delta) - w_i x_i = w_i \Delta$	$\partial z / \partial x_i = w_i$
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local derivative = change in the operation's output $\div$ change in one input

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The derivatives with respect to the coordinates of a vector are stored in one column:

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the vector formulas are just the scalar coordinate derivatives stacked together

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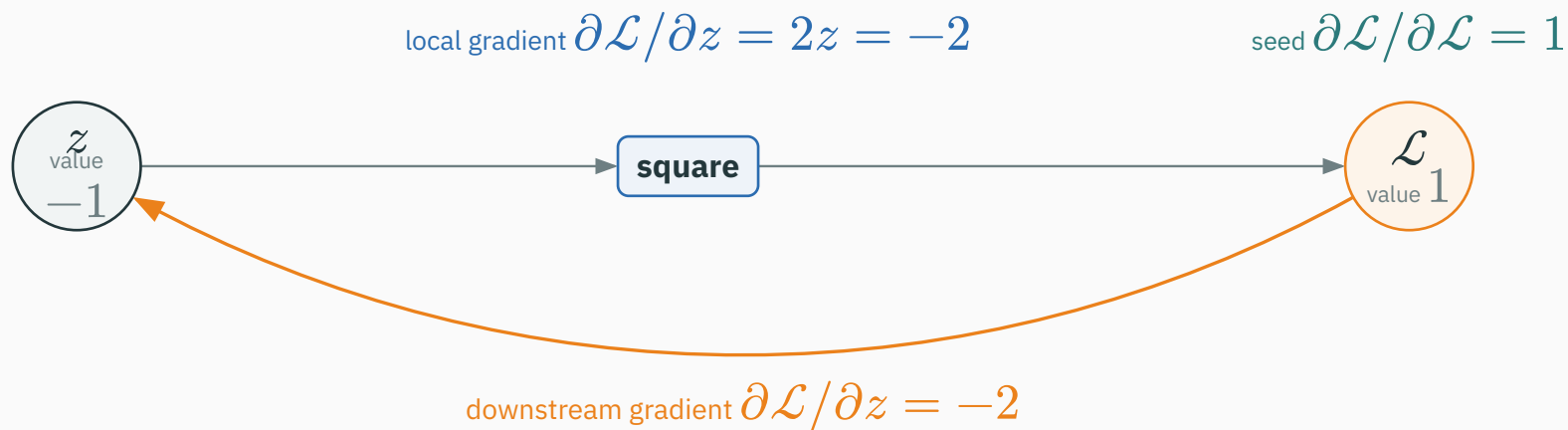
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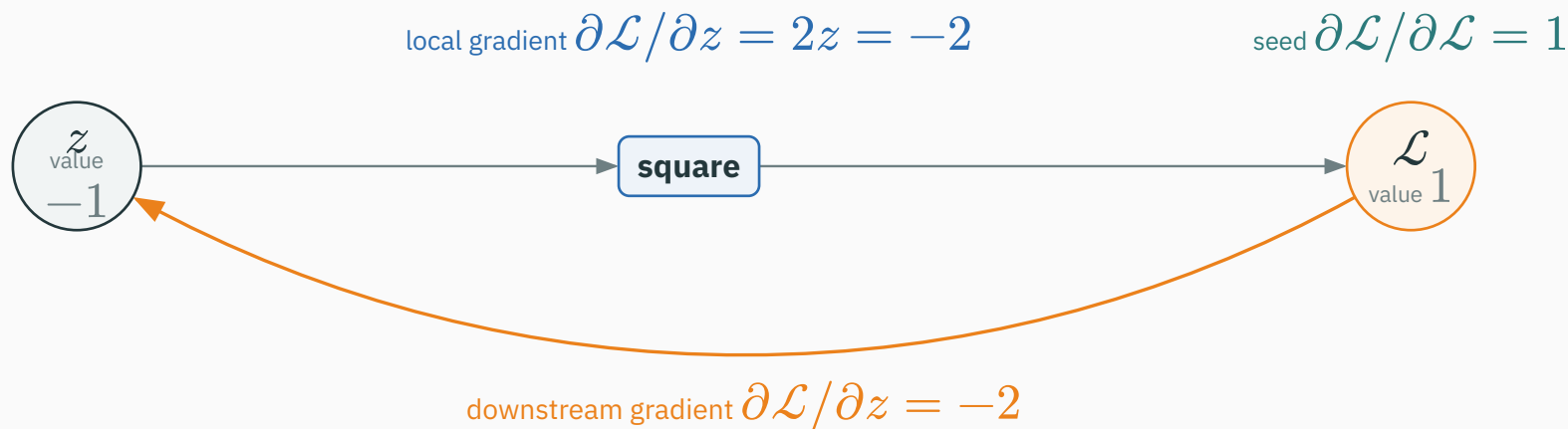
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dot product = multiply matching entries, then sum

First backward step: the square operation



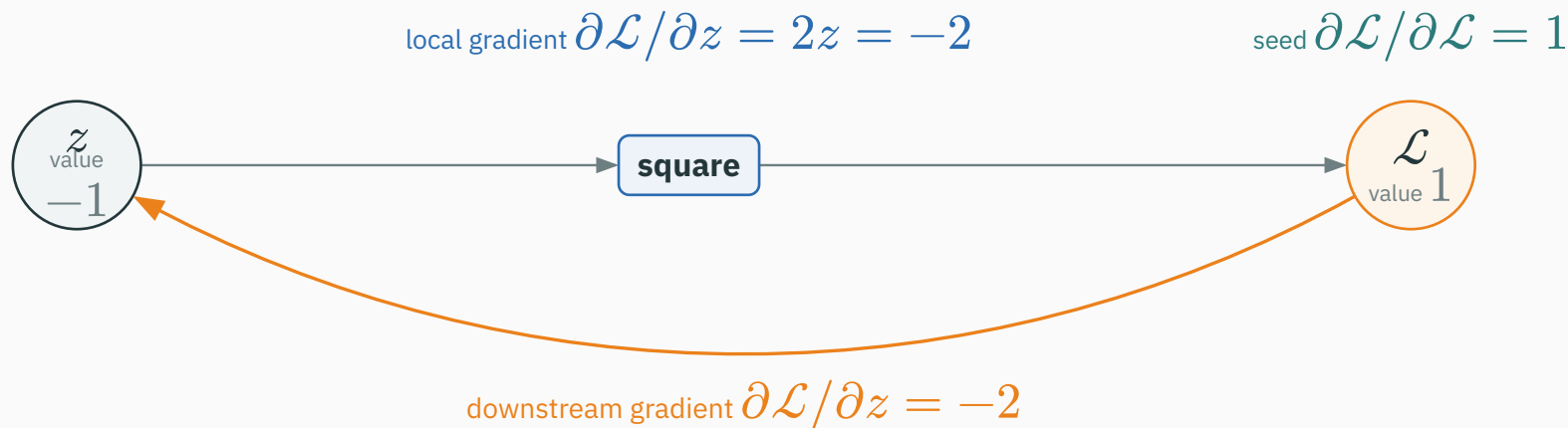
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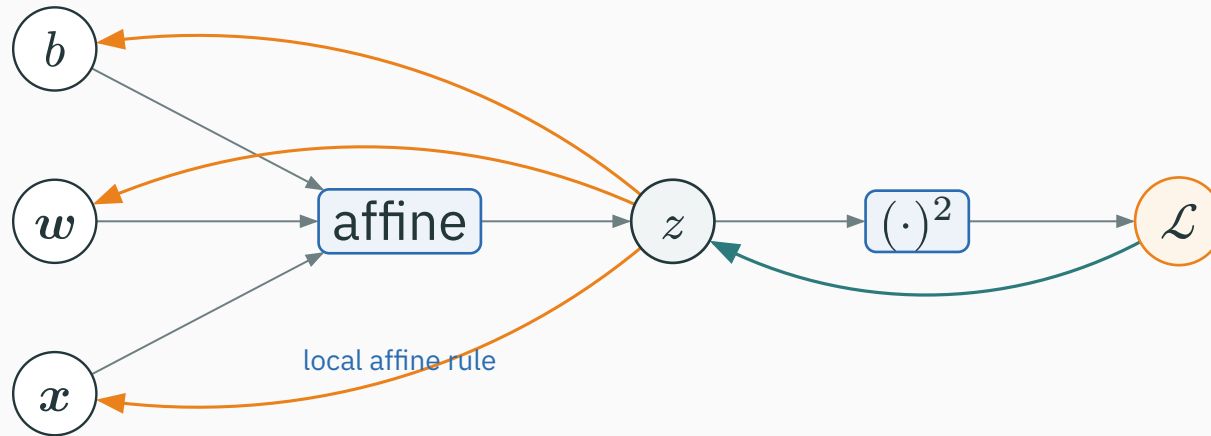


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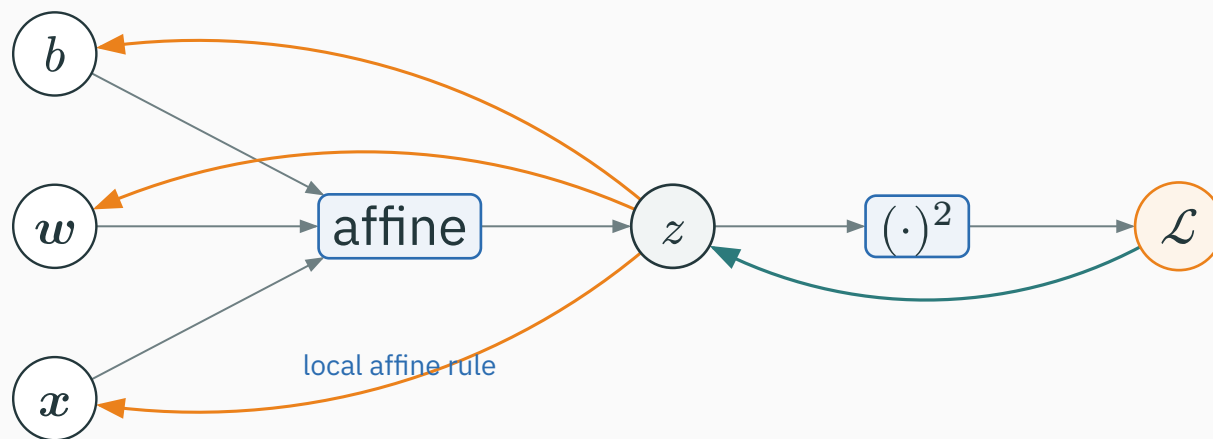
$$\frac{\partial \mathcal{L}}{\partial z} = 1 \cdot 2z = -2.$$

the square returns -2 ; it now arrives at the affine operation

Affine backward: apply the three local gradients

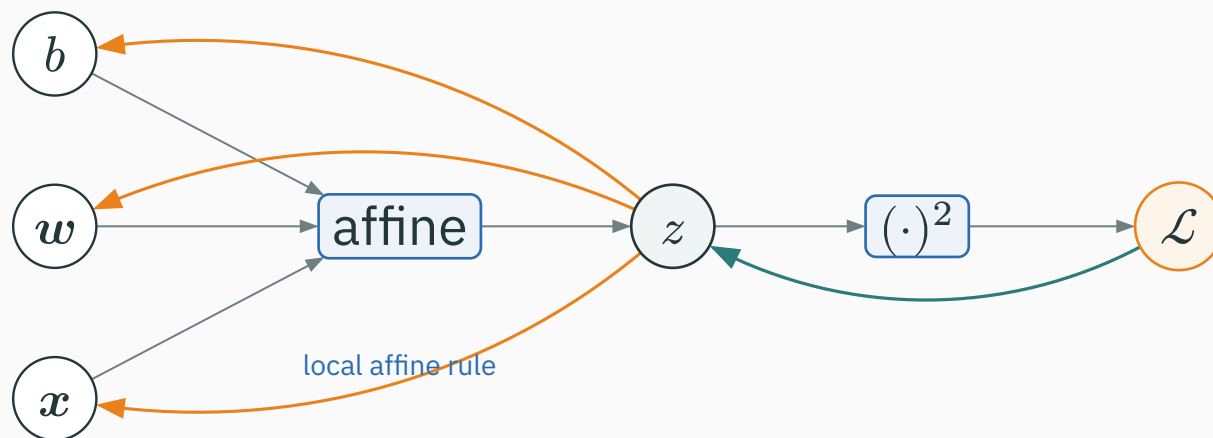


Affine backward: apply the three local gradients



Let $g_z = \partial \mathcal{L} / \partial z = -2$ arrive at the affine operation. Its **local gradients** send back:

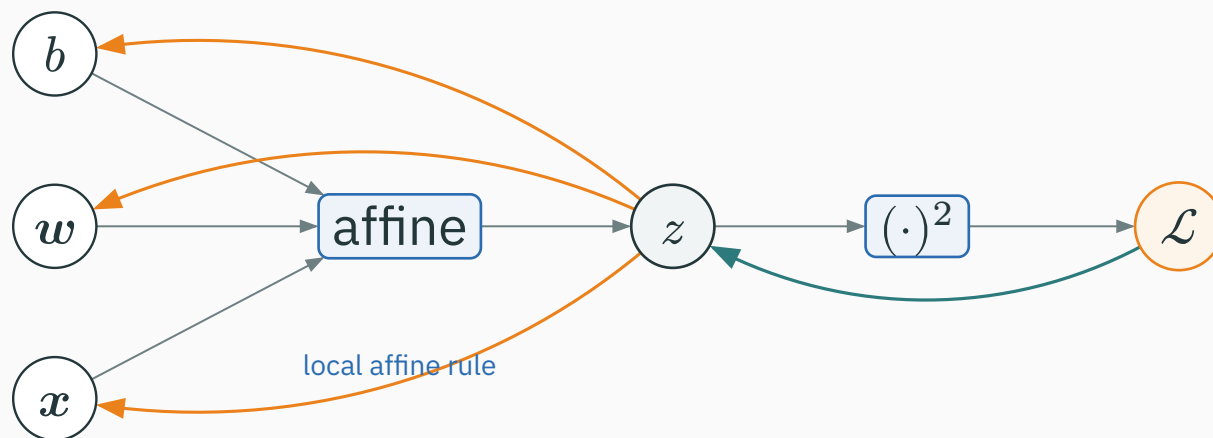
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w	$\partial z / \partial w = x$	$\partial \mathcal{L} / \partial w = (-2)x = (-4, 2)^\top$
x	$\partial z / \partial x = w$	$\partial \mathcal{L} / \partial x = (-2)w = (-2, -6)^\top$
b	$\partial z / \partial b = 1$	$\partial \mathcal{L} / \partial b = -2$

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one arriving gradient g_z produces three separate downstream gradients

PyTorch gives the same vector gradients

```
import torch

x = torch.tensor([2., -1.], requires_grad=True)
w = torch.tensor([1., 3.], requires_grad=True)
b = torch.tensor(0., requires_grad=True)

z = w @ x + b
L = z**2
L.backward()

print(z.item(), L.item())  # -1.0, 1.0
print(w.grad)              # tensor([-4.,  2.])
print(x.grad, b.grad)     # tensor([-2., -6.]), tensor(-2.)
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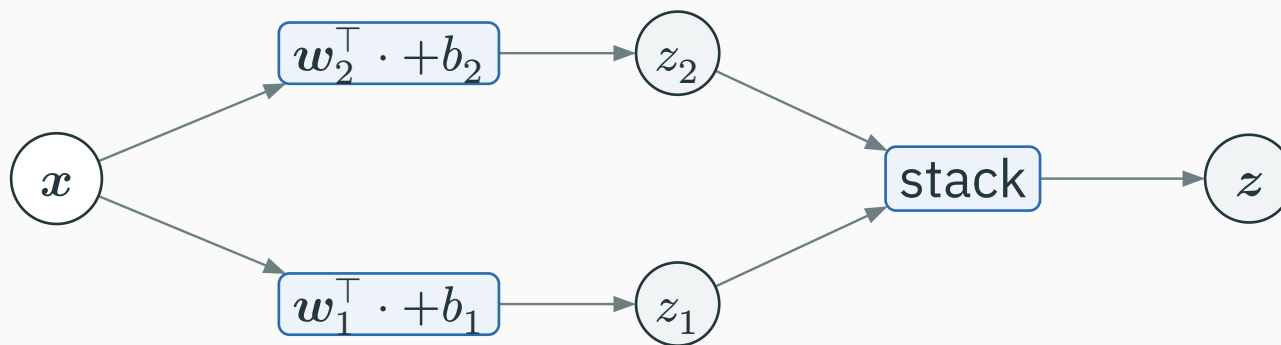
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```

@ performs the dot product; backward() still applies the same local rules

From one scalar output to a vector output

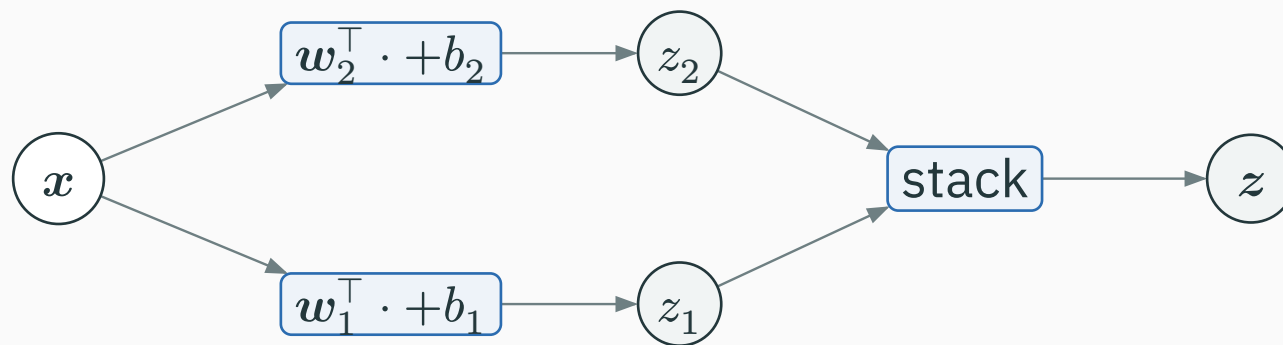
A dense layer repeats one familiar neuron

Every row of $\mathbf{W}$ is one affine neuron. All rows read the same input x .



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ROW 1 • neuron 1

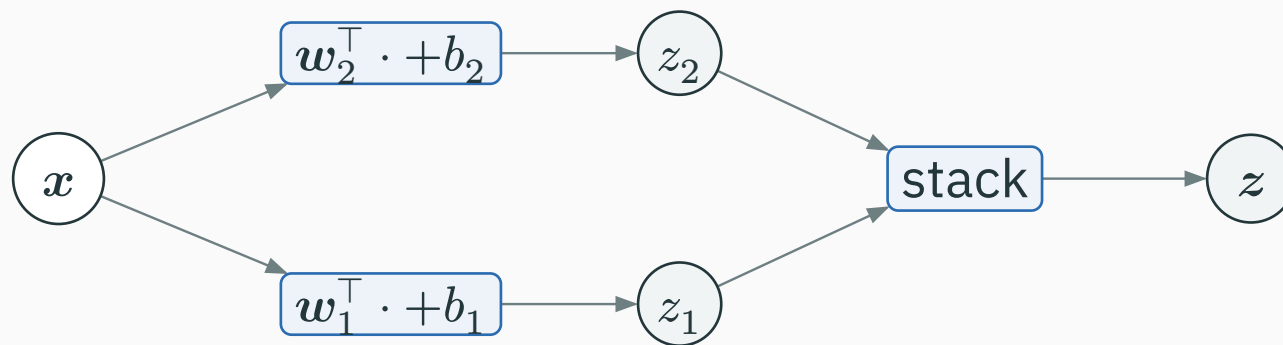
ROW 2 • neuron 2

$$z_1 = w_1^\top x + b_1$$

$$z_2 = w_2^\top x + b_2$$

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Every row of W is one affine neuron. All rows read the same input x .



ROW 1 • neuron 1

ROW 2 • neuron 2

$$z_1 = w_1^\top x + b_1$$

$$z_2 = w_2^\top x + b_2$$

stack the outputs: $z = Wx + b$

Forward, row 1: do one dot product

D DERIVATION

$$\boldsymbol{x} = \begin{pmatrix} 2 \\ -1 \end{pmatrix}, \quad \boldsymbol{w}_1^\top = (1, 3), \quad b_1 = 0$$

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| Nothing new happened: multiply matching entries, add them, then add the bias.

Forward, row 2: repeat, then stack

D DERIVATION

$$\mathbf{w}_2^\top = (-2, 1), \quad b_2 = 1$$

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$$w_2^\top = (-2, 1), \quad b_2 = 1$$

$$z_2 = (-2)(2) + 1(-1) + 1 = -4$$

$$z = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} -1 \\ -4 \end{pmatrix}$$

$$W = \begin{pmatrix} 1 & 3 \\ -2 & 1 \end{pmatrix} \text{ simply stores the two neuron rows together}$$

Backward: reuse the scalar affine rule for each row

D DERIVATION

Use column vectors: $\mathbf{x} \in \mathbb{R}^{d \times 1}$, $\mathbf{W} \in \mathbb{R}^{m \times d}$, and $\mathbf{z} \in \mathbb{R}^{m \times 1}$. Suppose the later loss sends $\mathbf{g}_z = \partial \mathcal{L} / \partial \mathbf{z} = \begin{pmatrix} 4 \\ -2 \end{pmatrix}$ back.

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$$z_i = \sum_j W_{i,j} x_j + b_i, \quad g_i := \partial \mathcal{L} / \partial z_i.$$

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TO $W_{i,j}$

TO b_i

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contribution g_i

$\mathbf{g}_z = (4, -2)^\top$ means two scalar arrivals: $g_1 = 4$ and $g_2 = -2$

The same x enters both output rows, so both rows return a contribution.

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ROW 1 RETURNS

$$g_1 w_1 = 4 \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \begin{pmatrix} 4 \\ 12 \end{pmatrix}$$

ROW 2 RETURNS

$$g_2 w_2 = (-2) \begin{pmatrix} -2 \\ 1 \end{pmatrix} = \begin{pmatrix} 4 \\ -2 \end{pmatrix}$$

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Shape check: $(d \times 1) = (d \times m)(m \times 1)$. The transpose arranges the row contributions so shared input paths add.

Weight and bias gradients: separate rows stack

D DERIVATION

Output i owns row i of W , so that gradient row is $g_i x^\top$.

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ROW 2

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Each bias has local derivative 1, so

$$\mathbf{g}_b = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} = \mathbf{g}_z = \begin{pmatrix} 4 \\ -2 \end{pmatrix}.$$

Weight and bias gradients: separate rows stack

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returns to a shared input add • returns to separate parameter rows stack

Recipient	Coordinate rule	Stacked rule	Shape check
x	$(g_x)_j = \sum_i g_i W_{i,j}$	$g_x = W^\top g_z$	$(d \times 1) = (d \times m)(m \times 1)$
W	$(g_W)_{i,j} = g_i x_j$	$g_W = g_z x^\top$	$(m \times d) = (m \times 1)(1 \times d)$
b	$(g_b)_i = g_i$	$g_b = g_z$	$(m \times 1) = (m \times 1)$

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The coordinate rules **derive** the gradients. Shape matching then verifies their orientation: $g_z x^\top$ has the same row-by-column shape as W .

From one example to a batch

One example remains a column $\boldsymbol{x}^n \in \mathbb{R}^{d \times 1}$. A framework stores their transposes as rows of

$$\boldsymbol{X} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \\ 2 & 2 \end{pmatrix} \in \mathbb{R}^{3 \times 2}.$$

A batch adds an axis—not new parameters

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SHARED PARAMETERS

$$\mathbf{W} \in \mathbb{R}^{m \times d}$$

$$\mathbf{b} \in \mathbb{R}^{m \times 1}$$

the same values serve every
row

BATCH FORWARD

$$\mathbf{Z} = \mathbf{X}\mathbf{W}^\top + \mathbf{1}_B \mathbf{b}^\top$$

$$(B \times m) = (B \times d)(d \times m)$$

PyTorch: `X @ W.T + b`

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$$(B \times m) = (B \times d)(d \times m)$$

PyTorch: `X @ W.T + b`

batching adds an example axis; every row still uses the same $\mathbf{W}, \mathbf{b}$

Three examples, three residuals

For row n , first compute z^n , then $r^n = z^n - y^n$.

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n	$\mathbf{x}^{(n)\top}$	$\mathbf{z}^{(n)\top}$	$\mathbf{y}^{(n)\top}$	$\mathbf{r}^{(n)\top}$	ℓ_n
1	$(2, -1)$	$(-1, -4)$	$(-5, -2)$	$(4, -2)$	10
2	$(-1, 2)$	$(5, 5)$	$(7, 1)$	$(-2, 4)$	10
3	$(2, 2)$	$(8, -1)$	$(7, -2)$	$(1, 1)$	1

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3	$(2, 2)$	$(8, -1)$	$(7, -2)$	$(1, 1)$	1

row 1 reproduces the earlier single example: its residual $(4, -2)^\top$ is the arriving g_z

Why the loss sends residuals backward

For one example, use half-squared error:

$$\ell_n = \frac{1}{2} \sum_k (z_k^n - y_k^n)^2.$$

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THREE LOSSES

$$\ell_1 = 10, \quad \ell_2 = 10, \quad \ell_3 = 1$$

ONE SCALAR MEAN

$$\mathcal{L} = \frac{1}{3}(10 + 10 + 1) = 7$$

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The residual is the upstream gradient from each example's loss. The mean contributes the factor $\frac{1}{B} = \frac{1}{3}$.

One example proposes one dense-layer gradient

D DERIVATION

Reuse the single-example rules on example 1, before doing any batch algebra.

One example proposes one dense-layer gradient

Reuse the single-example rules on example 1, before doing any batch algebra.

to W

$$\begin{aligned} G_W^1 &= \mathbf{r}^1 (\mathbf{x}^1)^\top \\ &= \begin{pmatrix} 8 & -4 \\ -4 & 2 \end{pmatrix} \end{aligned}$$

to b

$$\begin{aligned} g_b^1 &= \mathbf{r}^1 \\ &= \begin{pmatrix} 4 \\ -2 \end{pmatrix} \end{aligned}$$

to x^1

$$\begin{aligned} g_x^1 &= \mathbf{W}^\top \mathbf{r}^1 \\ &= \begin{pmatrix} 8 \\ 10 \end{pmatrix} \end{aligned}$$

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$$\begin{aligned} g_x^1 &= W^\top r^1 \\ &= \begin{pmatrix} 8 \\ 10 \end{pmatrix} \end{aligned}$$

these are unscaled example-1 returns; its contribution to the mean loss is each value divided by 3

Shared parameters add, then the mean scales

Each example proposes one outer product for the **same** W . Shared paths add; the mean loss scales the final sum.

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EXAMPLE 1

$$G_W^1 = \begin{pmatrix} 8 & -4 \\ -4 & 2 \end{pmatrix}$$

EXAMPLE 2

$$G_W^2 = \begin{pmatrix} 2 & -4 \\ -4 & 8 \end{pmatrix}$$

EXAMPLE 3

$$G_W^3 = \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}$$

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$$G_W^3 = \begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix}$$

$$G_W^1 + G_W^2 + G_W^3 = \begin{pmatrix} 12 & -6 \\ -6 & 12 \end{pmatrix}$$

Each example proposes one outer product for the **same** W . Shared paths add; the mean loss scales the final sum.

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$$G_W^1 + G_W^2 + G_W^3 = \begin{pmatrix} 12 & -6 \\ -6 & 12 \end{pmatrix}$$

MEAN WEIGHT GRADIENT

$$g_W = \frac{1}{3} \begin{pmatrix} 12 & -6 \\ -6 & 12 \end{pmatrix} = \begin{pmatrix} 4 & -2 \\ -2 & 4 \end{pmatrix}$$

MEAN BIAS GRADIENT

$$g_b = \frac{1}{3} \left(\begin{pmatrix} 4 \\ -2 \end{pmatrix} + \begin{pmatrix} -2 \\ 4 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right) =$$

Let $\mathbf{G}_Z = \frac{\mathbf{R}}{\mathbf{B}} \in \mathbb{R}^{B \times m}$. The formulas below package the rowwise returns; they do not replace the derivation.

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W	$g_W = G_Z^\top X$	$(m \times d) = (m \times B)(B \times d)$
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$$g_X = \frac{1}{3} \begin{pmatrix} 8 & 10 \\ -10 & -2 \\ -1 & 4 \end{pmatrix}$$

W, b are shared, so their example paths add. The three input rows are distinct, so their gradients stay in three separate rows.

Sum or mean? The reduction chooses the scale

SUM OVER EXAMPLES

$$\mathcal{L}_{\text{sum}} = \sum_n \ell_n$$

$$\mathbf{G}_Z = \mathbf{R}$$

$$\mathbf{g}_W = \mathbf{R}^\top \mathbf{X}$$

MEAN OVER EXAMPLES

$$\mathcal{L}_{\text{mean}} = \frac{1}{B} \sum_n \ell_n$$

$$\mathbf{G}_Z = \frac{\mathbf{R}}{B}$$

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```
loss = 0.5 * ((Z - Y)**2).sum(dim=1).mean()  
# sum output coordinates inside each example; mean over examples
```

Sum or mean? The reduction chooses the scale

D DERIVATION

SUM OVER EXAMPLES

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the dense local rules do not change; the scalar loss reduction chooses their final scale

PyTorch verifies the single example and the batch

```
X = torch.tensor([[ 2., -1.], [-1., 2.], [2., 2.]],
                  requires_grad=True)
Y = torch.tensor([[-5., -2.], [ 7., 1.], [7., -2.]])
W = torch.tensor([[1., 3.], [-2., 1.]], requires_grad=True)
b = torch.tensor([0., 1.], requires_grad=True)

Z = X @ W.T + b
loss = 0.5 * ((Z - Y)**2).sum(dim=1).mean()
loss.backward()

print(loss.item()) # 7.0
print(W.grad)      # [[ 4., -2.], [-2.,  4.]]
print(b.grad)      # [1., 1.]
print(X.grad)      # [[ 8/3, 10/3], [-10/3, -2/3], [-1/3, 4/3]]
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```

Continue in the complete lecture Colab ↗: checkpoints 11–16 derive the dense VJP, expose every batch contribution, verify microbatches, run one update, and finish with the tiny MLP.

The training loop now has a concrete batch

I INTERACTIVE

```
for X, Y in loader:
    optimizer.zero_grad()      # clear the previous update's buffers
    Z = model(X)               # all examples reuse the same parameters
    loss = loss_fn(Z, Y)       # reduce example losses to one scalar
    loss.backward()            # aggregate this batch's contributions
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<code>zero_grad()</code>	starts one intentional update window
<code>model(X)</code>	records one graph whose rows share the same parameters
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clear → batch forward → scalar loss → batch backward → update

One batch can arrive in pieces

Microbatches can reproduce the same mean gradient

ONE FULL BATCH

```
zero_grad()  
((e111 + e112 + e113) /  
3).backward()  
step()
```

THREE PIECES · ONE UPDATE

```
zero_grad()  
(e111 / 3).backward()  
(e112 / 3).backward()  
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Microbatches can reproduce the same mean gradient

ONE FULL BATCH

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THREE PIECES · ONE UPDATE

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$$W.\text{grad} : \frac{G_W^1}{3} \rightarrow \frac{G_W^1 + G_W^2}{3} \rightarrow \begin{pmatrix} 4 & -2 \\ -2 & 4 \end{pmatrix}$$

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Equivalence requires fixed parameters, the same overall reduction, no `step()`, and no `zero_grad()` between pieces. Batch-coupled operations such as BatchNorm need extra care.

Microbatches can reproduce the same mean gradient

D DERIVATION

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clear once before the update window · add every scaled piece · step once after it

A tiny neural network

ReLU is what prevents two dense layers from collapsing into one

Without a nonlinearity, two affine maps are still one affine map:

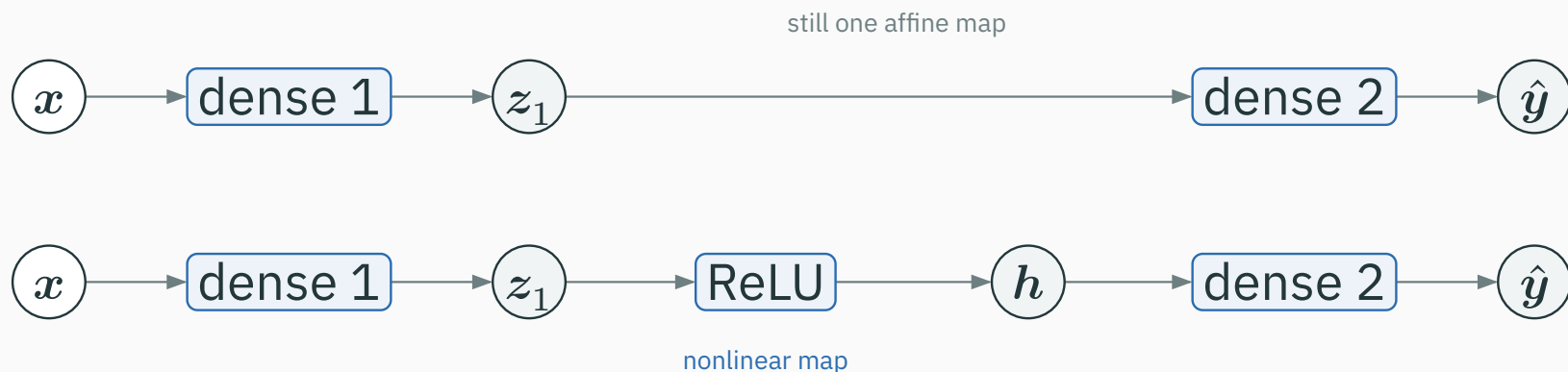
$$\begin{aligned} \mathbf{W}_2(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2 \\ = (\mathbf{W}_2\mathbf{W}_1)\mathbf{x} + (\mathbf{W}_2\mathbf{b}_1 + \mathbf{b}_2). \end{aligned}$$

ReLU is what prevents two dense layers from collapsing into one

Without a nonlinearity, two affine maps are still one affine map:

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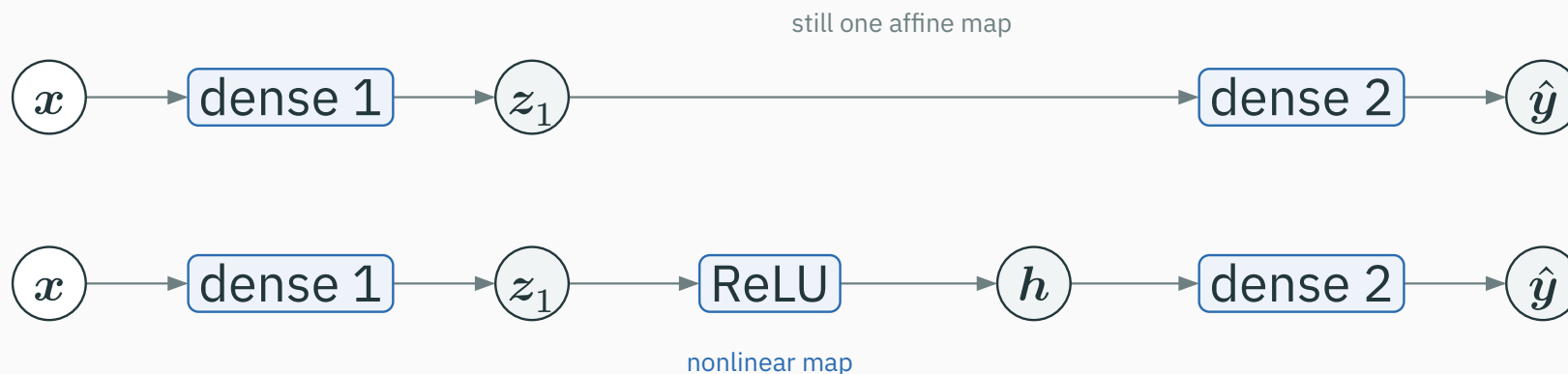


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ReLU makes the composition nonlinear; depth can now represent a richer function

A tiny MLP composes three vector blocks

The network now repeats the operations we already know: affine map, elementwise ReLU, affine map, scalar loss.

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$$z_1 = \mathbf{W}_1 x + b_1$$

$$h = \text{ReLU}(z_1)$$

$$\hat{y} = \mathbf{W}_2 h + b_2$$

$$\mathcal{L} = \sum_i (\hat{y}_i - y_i)^2$$

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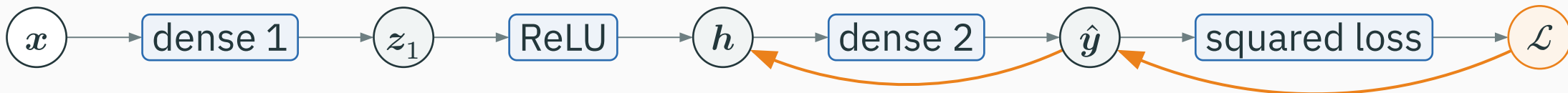
$$\hat{y} = W_2 h + b_2$$

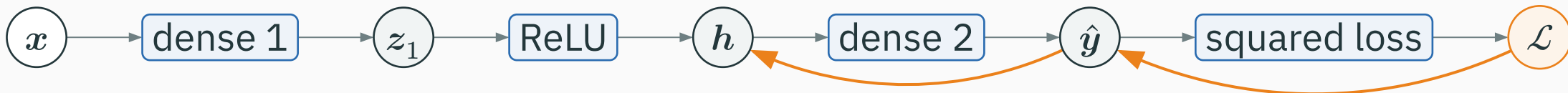
$$\mathcal{L} = \sum_i (\hat{y}_i - y_i)^2$$

dense → ReLU → dense → squared loss

Backward, part 1: loss $\rightarrow$ dense 2 $\rightarrow$ hidden activations

D DERIVATION

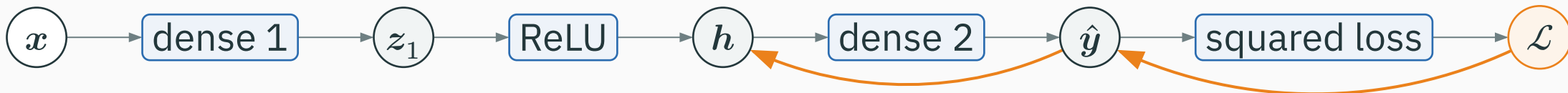




1. Squared loss. Start with the seed $\partial \mathcal{L} / \partial \mathcal{L} = 1$. The loss operation returns

$$g_{\hat{y}} = 2(\hat{y} - y).$$

This says how increasing each prediction coordinate would change the loss.



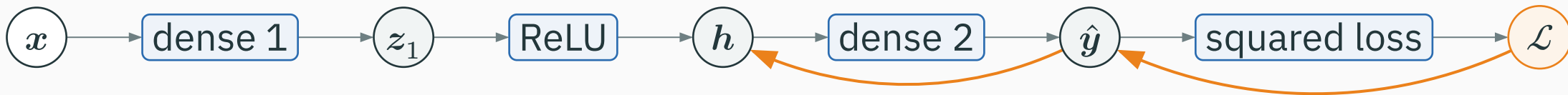
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$$g_{\hat{y}} = 2(\hat{y} - y).$$

This says how increasing each prediction coordinate would change the loss. **2.**

Second dense layer. It receives $g_{\hat{y}}$ and returns a gradient to its input h :

$$g_h = W_2^\top g_{\hat{y}}.$$



1. Squared loss. Start with the seed $\partial \mathcal{L} / \partial \mathcal{L} = 1$. The loss operation returns

$$g_{\hat{y}} = 2(\hat{y} - y).$$

This says how increasing each prediction coordinate would change the loss. **2.**

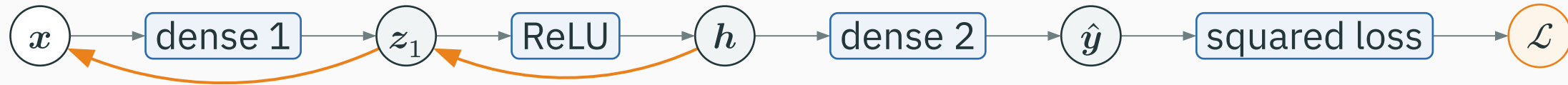
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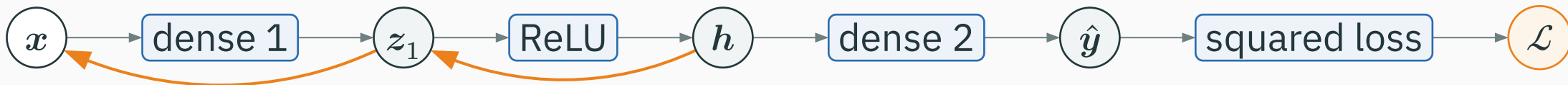
$$g_h = W_2^\top g_{\hat{y}}.$$

the returned g_h is now the arriving gradient at ReLU

Backward, part 2: ReLU $\rightarrow$ dense 1 $\rightarrow$ input

D DERIVATION

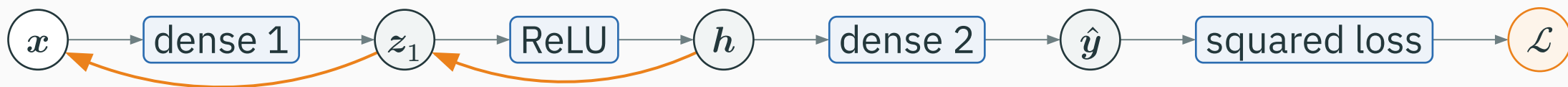




3. ReLU. Apply its local gate coordinate by coordinate:

$$g_{z_1} = g_h \odot \mathbb{1}[z_1 > 0].$$

An active unit passes its arriving gradient; an inactive unit returns zero.

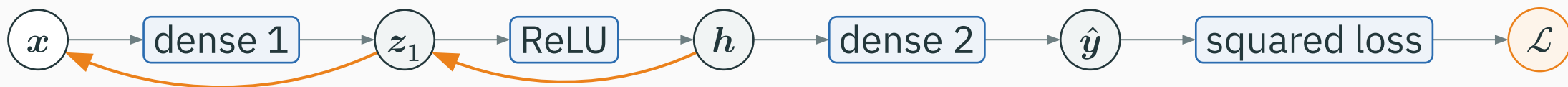


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$$g_x = W_1^\top g_{z_1}, \quad \partial \mathcal{L} / \partial W_1 = g_{z_1} x^\top, \quad \partial \mathcal{L} / \partial b_1 = g_{z_1}.$$



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each returned gradient becomes the arriving gradient for the block immediately to its left

The same tiny MLP in PyTorch

```
import torch
from torch import nn

model = nn.Sequential(
    nn.Linear(2, 3), nn.ReLU(), nn.Linear(3, 2)
)
x = torch.tensor([2., -1.])
y = torch.tensor([1., 0.])

y_hat = model(x)
loss = ((y_hat - y)**2).sum()
loss.backward()

for name, p in model.named_parameters():
    print(name, tuple(p.shape), tuple(p.grad.shape))
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PyTorch records the three blocks and applies their local rules in reverse

INTERACTIVE

↗ nipunbatra.github.io/interactive-articles/autograd

Step through the forward values, then follow one arriving gradient through a dense operation, a ReLU, and the preceding dense operation.

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For practice, predict each gradient's shape before revealing its value in the interactive.

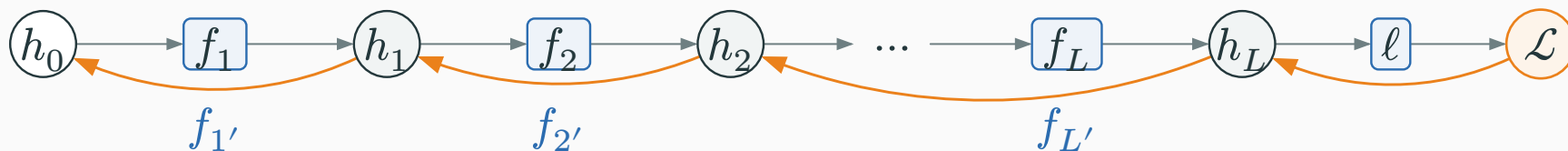
**When gradients cross many
layers**

Deep networks repeat the same multiplication

For a scalar chain $h_0 \rightarrow h_1 \rightarrow \dots \rightarrow h_L \rightarrow \mathcal{L}$:

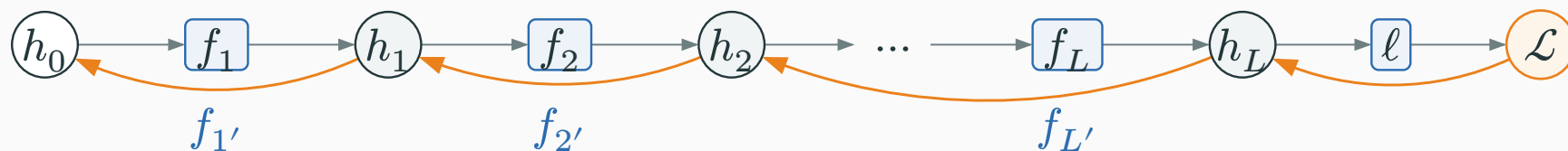
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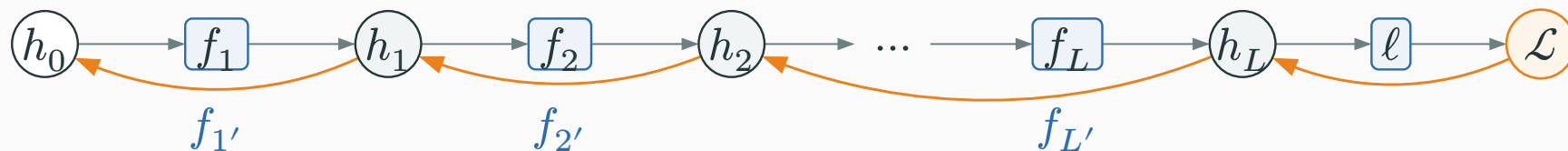
For a scalar chain $h_0 \rightarrow h_1 \rightarrow \dots \rightarrow h_L \rightarrow \mathcal{L}$:



$$\frac{\partial \mathcal{L}}{\partial h_0} = \frac{\partial \mathcal{L}}{\partial h_L} \cdot f_{L'}(h_{L-1}) \dots f_{1'}(h_0).$$

D DERIVATION

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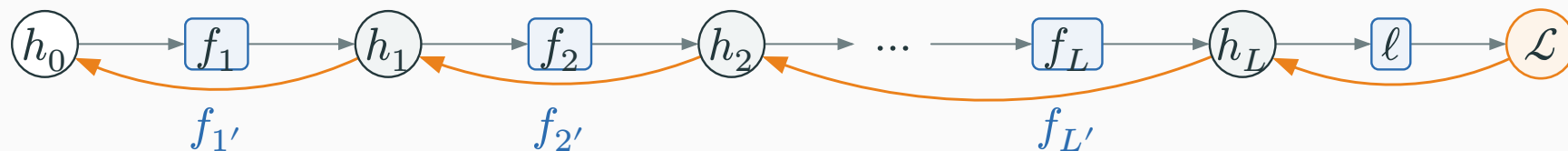


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depth creates a product of many local slopes

Vector layers do the same operation with matrix–vector products. The intuition is unchanged: repeatedly small factors shrink a gradient; repeatedly large factors grow it.

Ten ordinary-looking slopes can create three regimes

Start with an arriving loss derivative of 1 and multiply the same local slope ten times:

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Local slope	After 10 layers	Effect
0.5	$0.5^{10} \approx 0.001$	gradient nearly disappears
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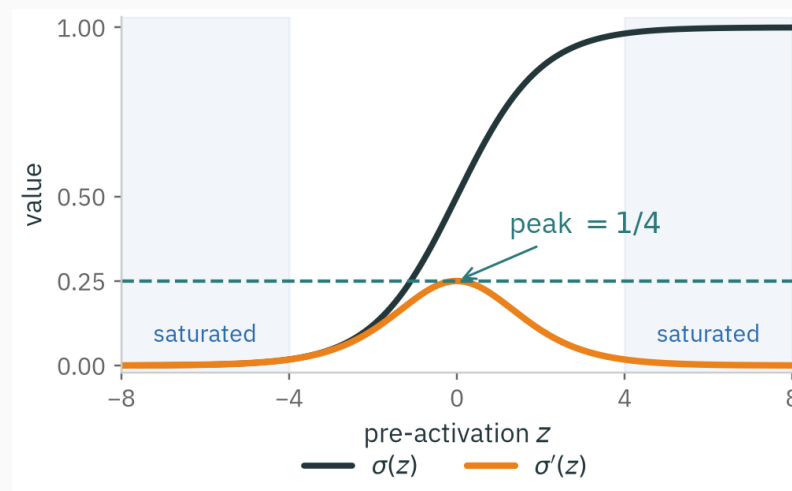
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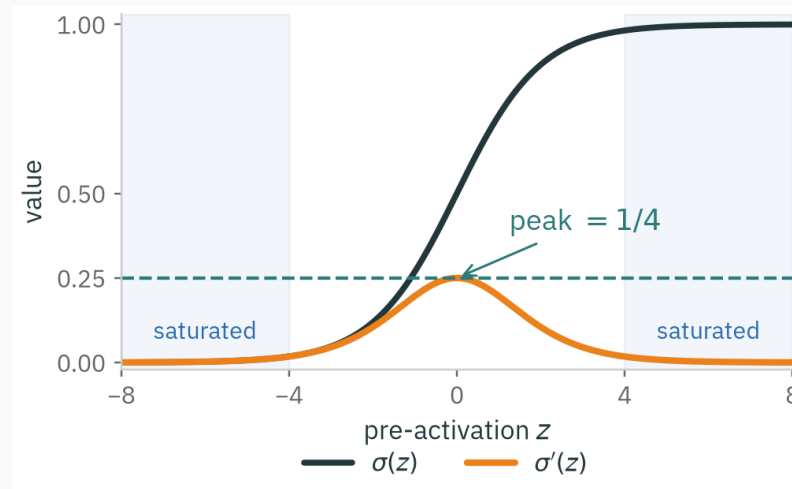
the chain rule explains both vanishing and exploding gradients

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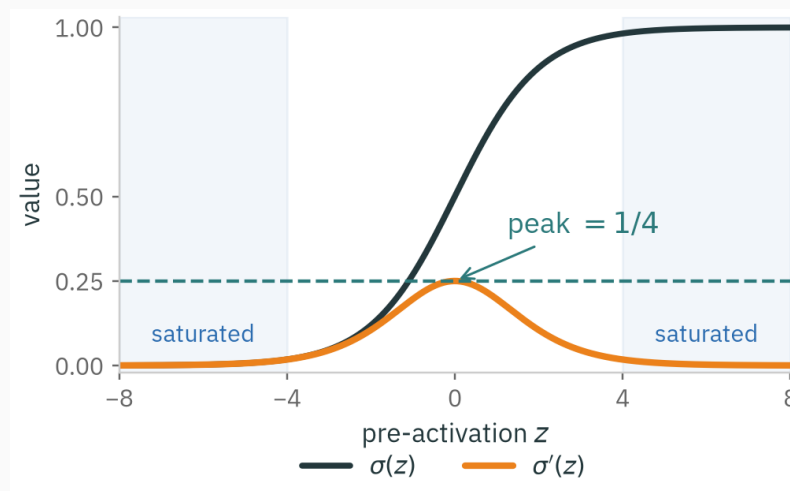


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each sigmoid layer multiplies the gradient by at most $1/4$

Repeated sigmoid derivatives can shrink the signal quickly. ReLU has slope 1 on active units and 0 on inactive units; weights and normalization also shape the full Jacobian.

INTERACTIVE

↗ nipunbatra.github.io/interactive-articles/vanishing-gradients

Sweep depth and activation function; watch the gradient magnitude at layer 0 collapse for sigmoid and survive for ReLU.

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Sweep depth and activation function; watch the gradient magnitude at layer 0 collapse for sigmoid and survive for ReLU.

Sweep depth to see repeated small local slopes rapidly erase an early-layer gradient.

Summary

Backprop in one sentence

Seed $\partial \mathcal{L} / \partial \mathcal{L} = 1$, then walk the graph **backward**, at each operation computing

downstream gradient = **upstream gradient** $\times$ **local derivative**,

and **adding** gradients wherever a variable branched.

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and **adding** gradients wherever a variable branched.

For vector operations, the **local derivative** can be a vector or matrix; the same color-coded chain rule applies.

Setting	Backward rule
scalar operation	$\frac{\partial \mathcal{L}}{\partial u} = \frac{\partial \mathcal{L}}{\partial v} \cdot \partial v / \partial u$
dense layer	$\frac{\partial \mathcal{L}}{\partial \mathbf{W}} = \frac{\partial \mathcal{L}}{\partial \mathbf{z}} \mathbf{x}^\top \frac{\partial \mathcal{L}}{\partial \mathbf{x}} = \mathbf{W}^\top \frac{\partial \mathcal{L}}{\partial \mathbf{z}}$
activation	$\frac{\partial \mathcal{L}}{\partial \mathbf{z}} = \frac{\partial \mathcal{L}}{\partial \mathbf{a}} \odot \varphi'(\mathbf{z})$
branch point	gradients add

We can compute $\partial \mathcal{L} / \partial \theta_j$ for every parameter.

Next: turn those gradients into reliable parameter updates.

Lecture 5 · Optimization for Deep Learning