CSE 493G1: Deep Learning
Revision 2: Backpropagation

Slides made by Shubhang Desai for CSE493G1 Spring 2023 offering.

Plan

- Background: the problem of gradient computation
- Intro to backpropagation algorithm
- Gradients of common computations
- Worked-thru examples
- What does it all mean?

Background

Refresher: Chain Rule

"Derivative of outside of inside equals derivative of outside times derivative of inside"

$$\frac{d}{dx}f(g(x)) = \frac{d}{dg(x)}f(g(x)) \times \frac{d}{dx}g(x)$$

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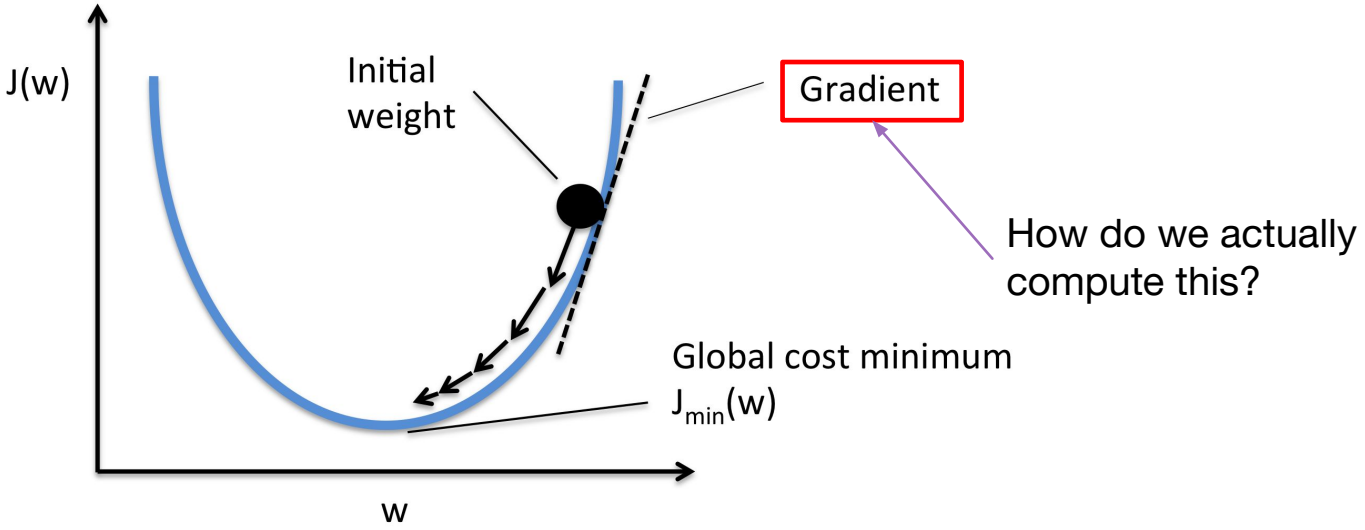
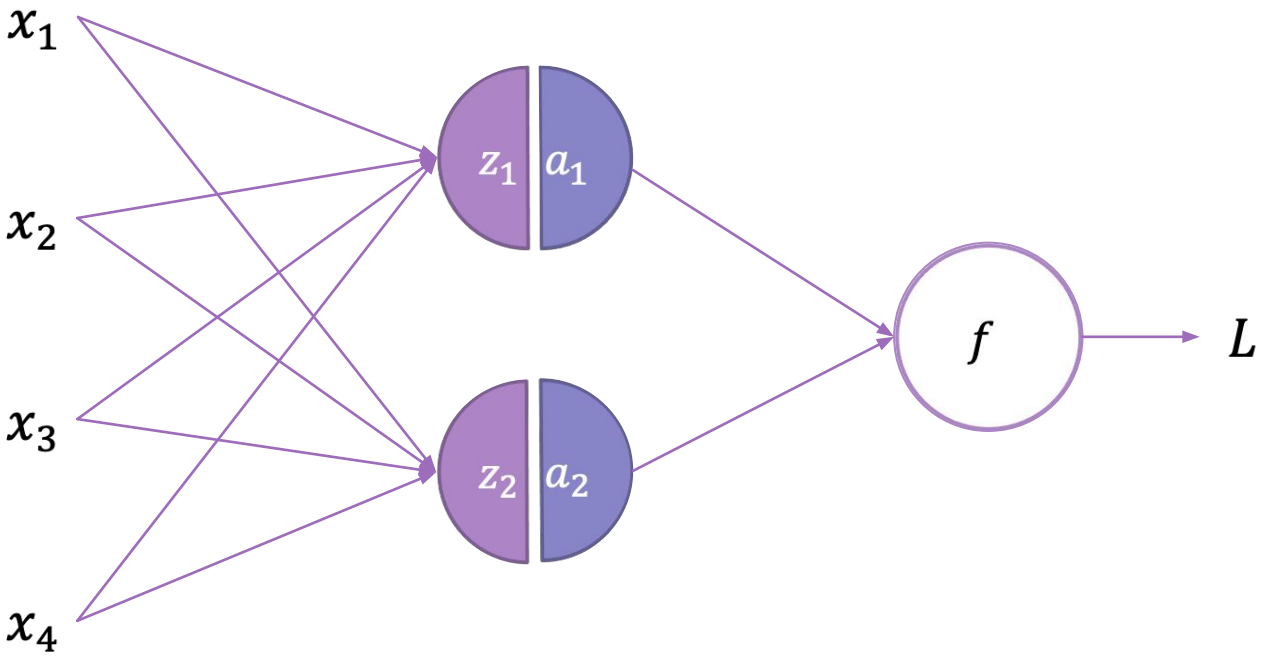
Refresher: Gradient Descent

Iteratively moving neural network weights in the direction of the gradient to minimize loss:

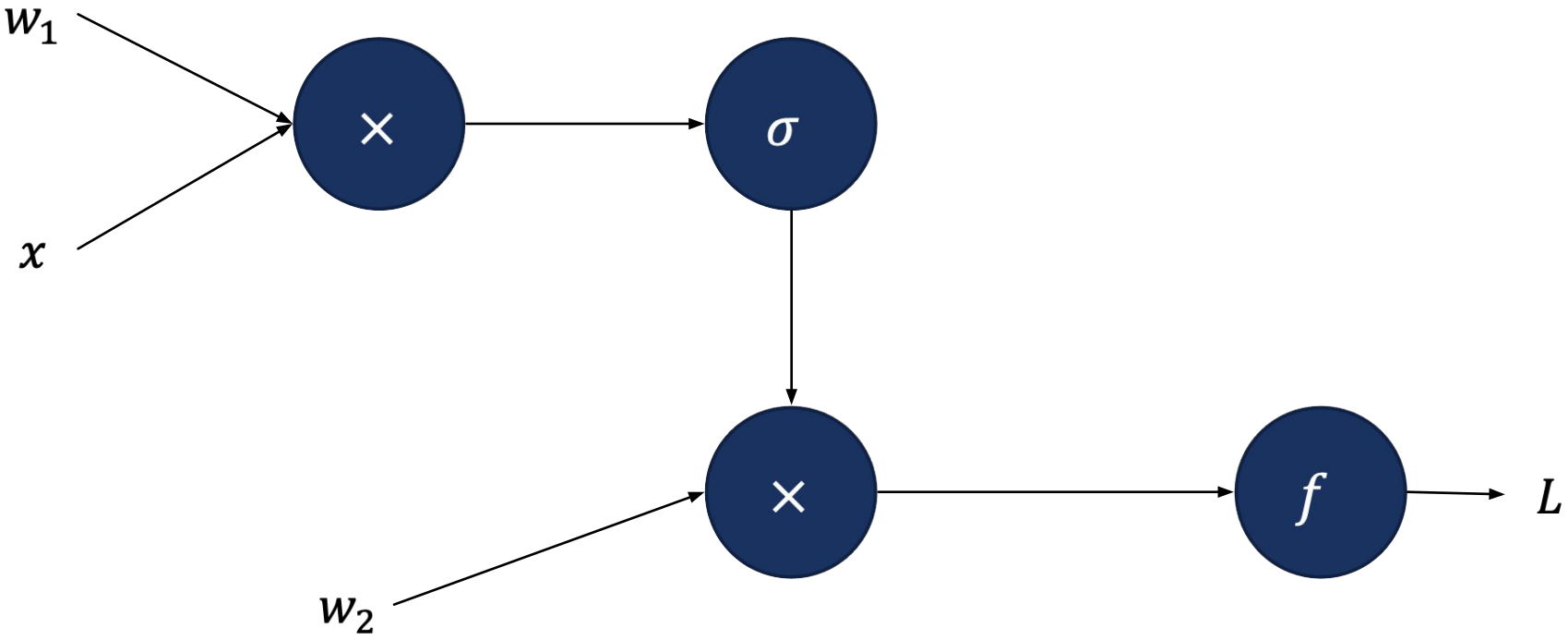


Intro to Backprop: A 2-Layer MLP

2-Layer MLP



$\hat{y} = w_2\sigma(w_1 x)$ and $L = f(\hat{y})$



2-Layer MLP Equations and Gradients

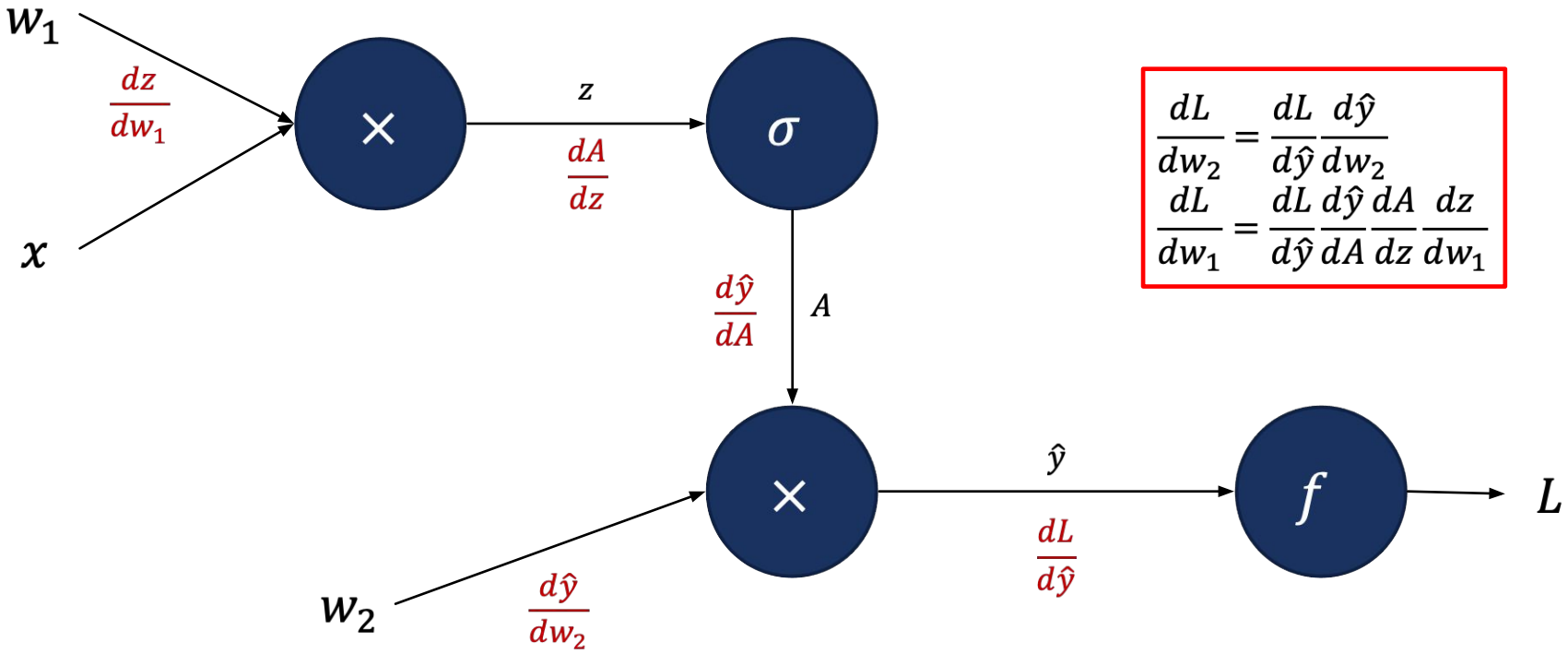
$L = f(\hat{y})$, where $\hat{y} = w_2 A$, $A = \sigma(z)$, and $z = w_1 x$

$$\frac{dL}{dw_1} = \frac{dL}{d\hat{y}}\frac{d\hat{y}}{dw_1} = \frac{dL}{d\hat{y}}\frac{d\hat{y}}{dA}\frac{dA}{dw_1} = \frac{dL}{d\hat{y}}\frac{d\hat{y}}{dA}\frac{dA}{dz}\frac{dz}{dw_1}$$

$$\frac{dL}{dw_2} = \frac{dL}{d\hat{y}}\frac{d\hat{y}}{dw_2}$$

Notice that this value is used in both gradient computations!

$\hat{y} = w_2\sigma(w_1 x)$ and $L = f(\hat{y})$



$$\frac{dL}{dw_2} = \frac{dL}{d\hat{y}}\frac{d\hat{y}}{dw_2}$$

$$\frac{dL}{dw_1} = \frac{dL}{d\hat{y}}\frac{d\hat{y}}{dA}\frac{dA}{dz}\frac{dz}{dw_1}$$

The Backpropagation Algorithm

- Treat entire network as a computational graph, each computation as a node
- We can independently compute local gradient at each node given node inputs
- Accumulate gradients from back (loss) to front (weights) using chain rule (simple multiplication!)

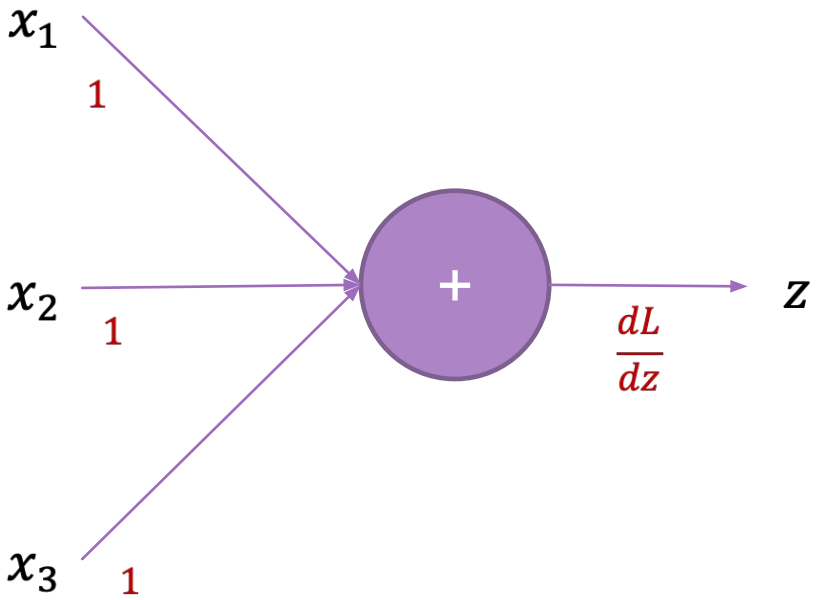
Computations and their Gradients

Summation

$$z = \sum_i x_i, L = f(Z)$$

$$\frac{\partial z}{\partial x_i} = 1$$

$$\frac{\partial L}{\partial x_i} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x_i} = \frac{\partial L}{\partial z}$$

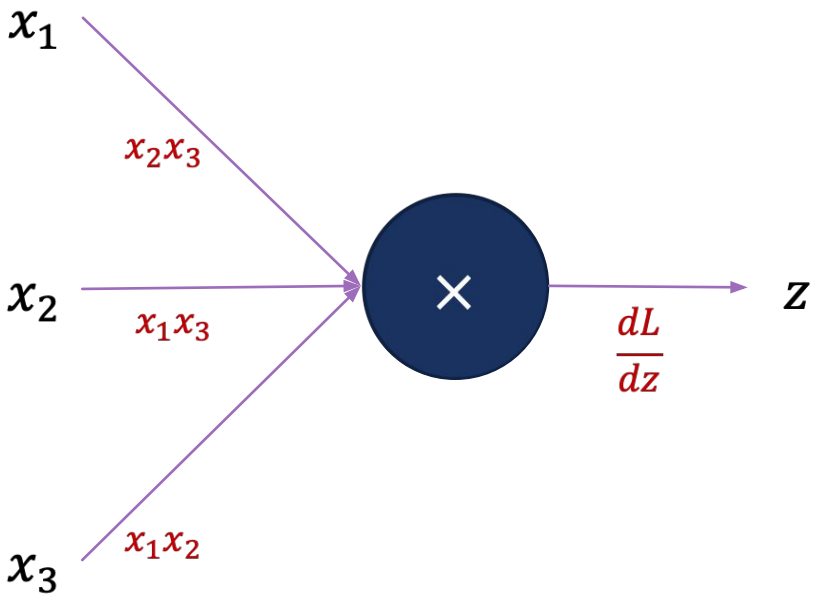


Multiplication

$$z = \prod_i x_i \, , L = f(Z)$$

$$\frac{\partial z}{\partial x_i} = \frac{z}{x_i}$$

$$\frac{\partial L}{\partial x_i} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x_i} = \frac{\partial L}{\partial z}\frac{z}{x_i}$$

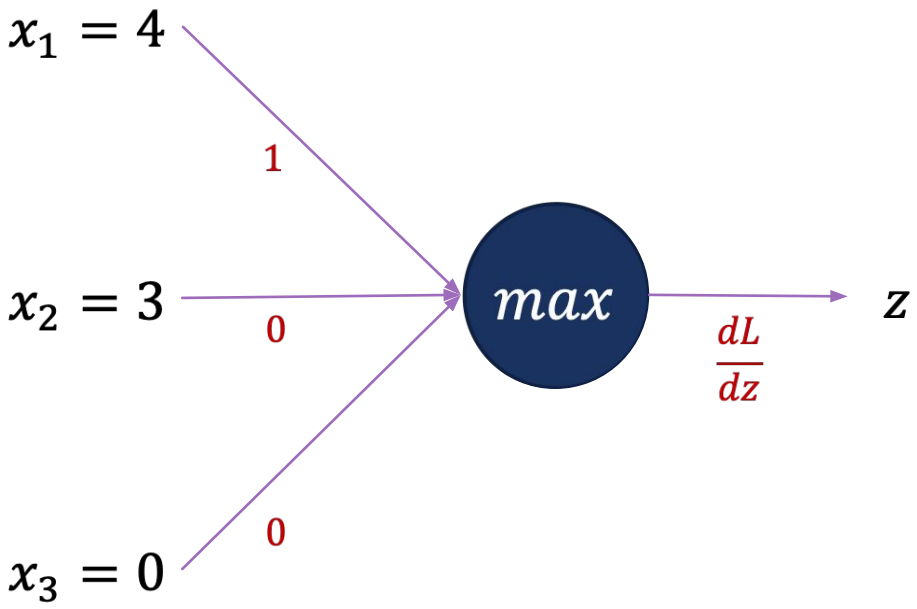


Min/Max

$$z = \max_i x_i, L = f(Z)$$

$$\frac{\partial z}{\partial x_i} = \mathbf{1}[x_i = z]$$

- $$\frac{\partial L}{\partial x_i} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x_i} = \frac{\partial L}{\partial z}\mathbf{1}[x_i = z]$$

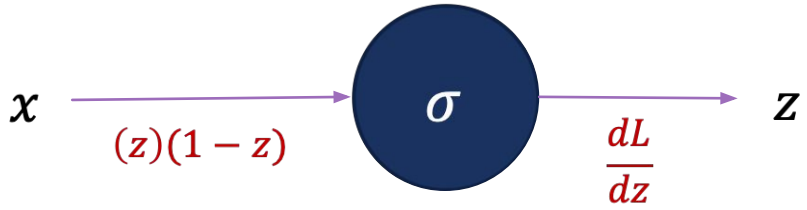


Sigmoid

$$z = \sigma(x), L = f(Z)$$

$$\frac{\partial z}{\partial x_i} = z(1-z)$$

- $$\frac{\partial L}{\partial x_i} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x_i} = \frac{\partial L}{\partial z} z(1-z)$$



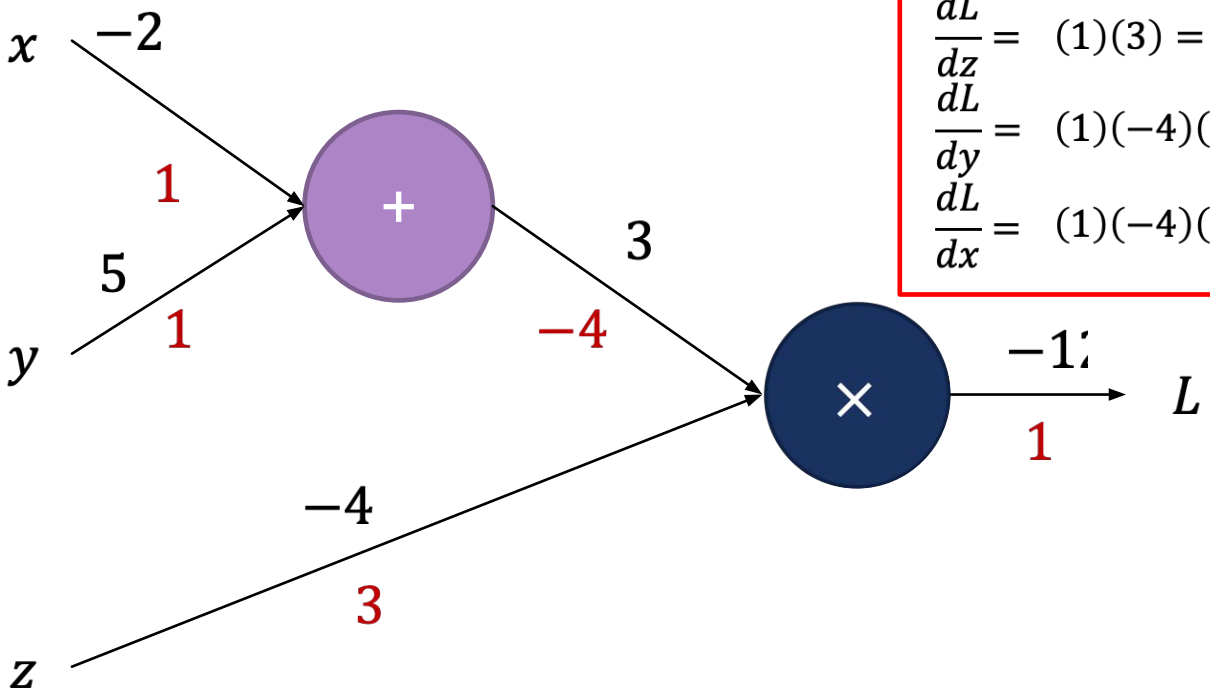
Computational Graph Example 1

$$L = (x + y)z$$

$$\frac{dL}{dz} = (1)(3) = 3$$

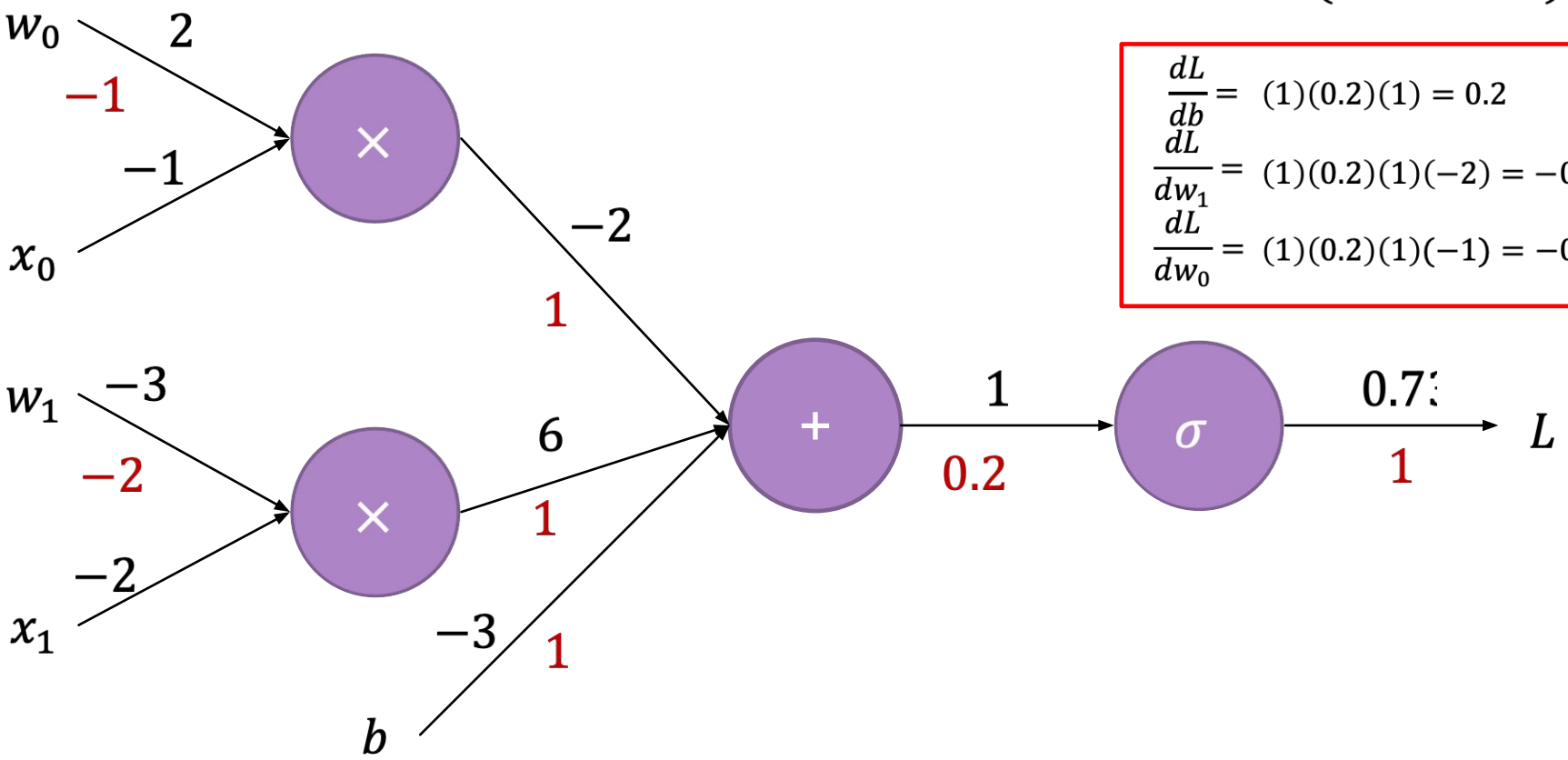
$$\frac{dL}{dy} = (1)(-4)(1) = -4$$

$$\frac{dL}{dx} = (1)(-4)(1) = -4$$



Computational Graph Example 2

$$L = \sigma(w^T x + b)$$



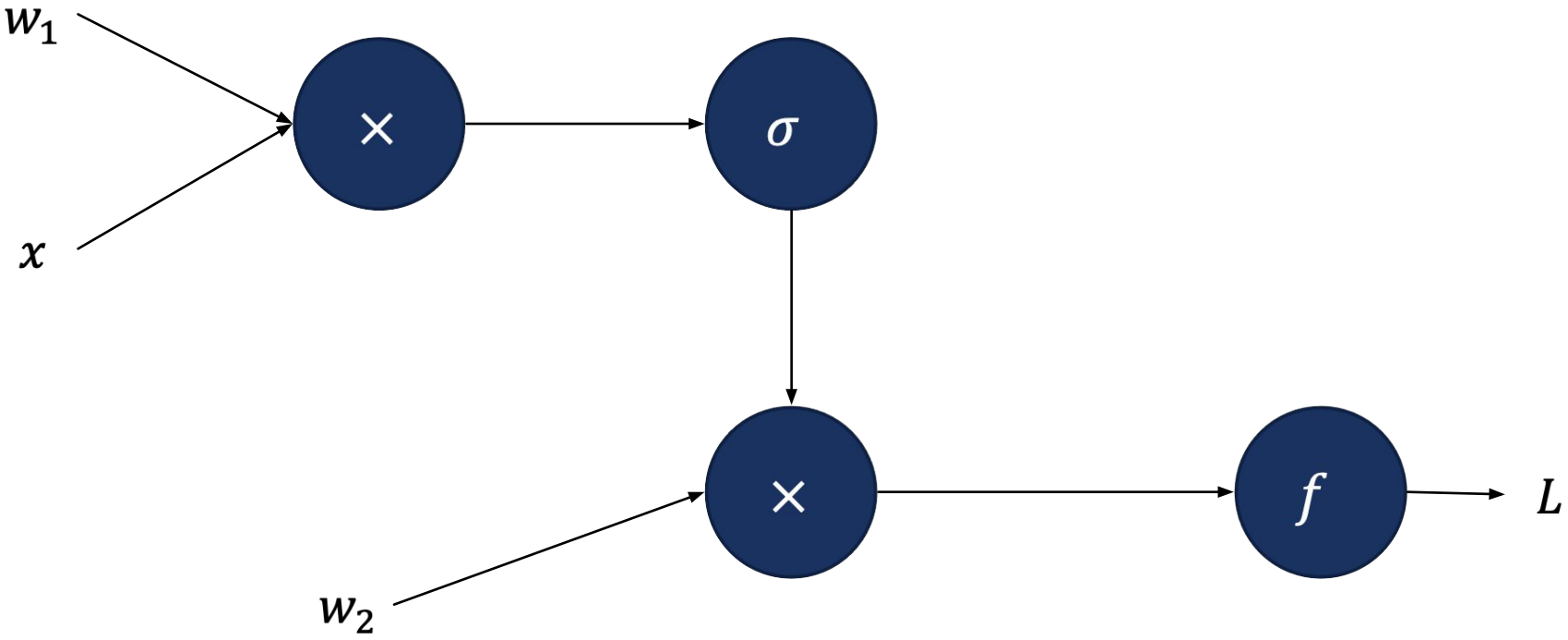
$$\frac{dL}{db} = (1)(0.2)(1) = 0.2$$

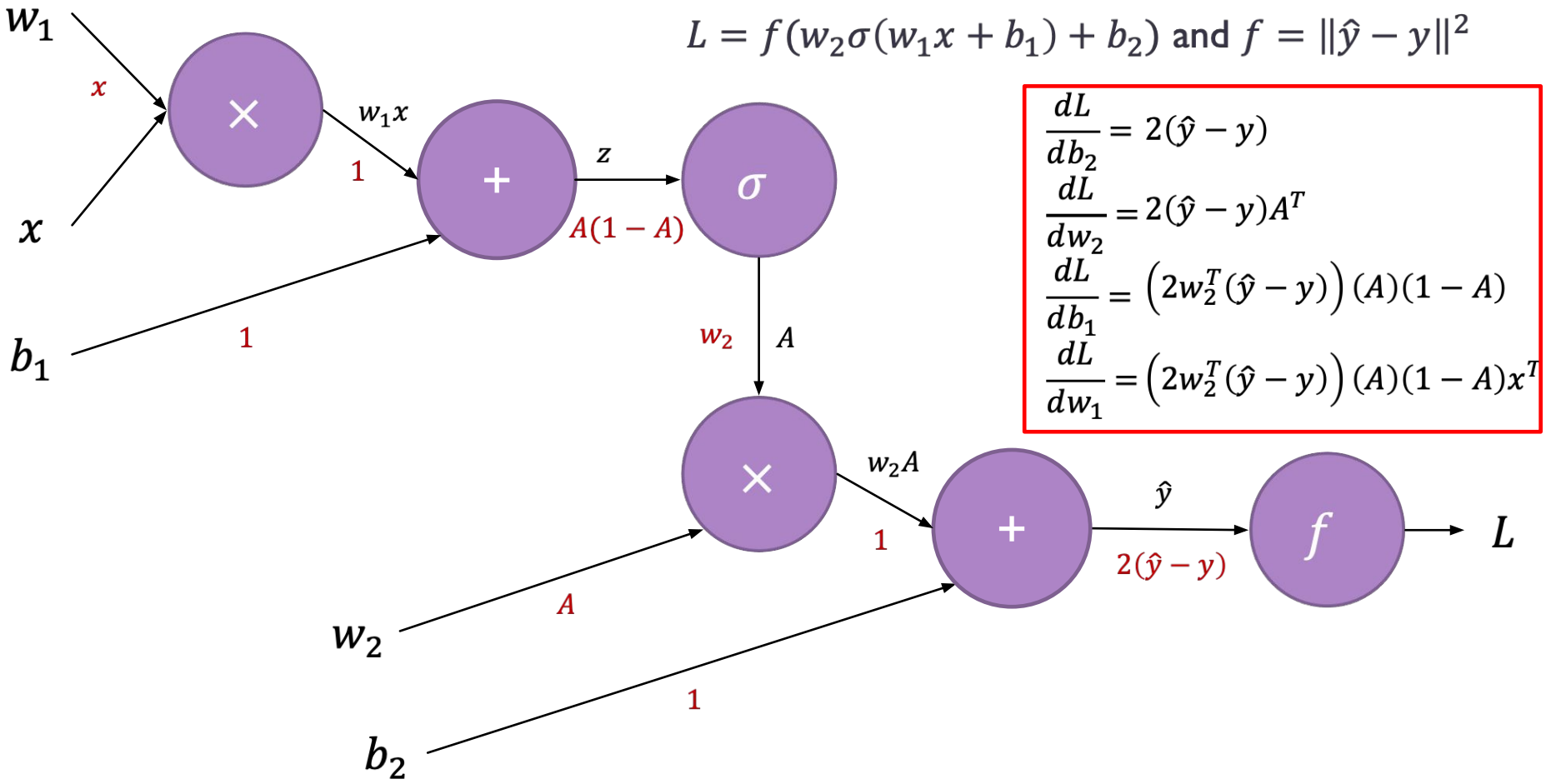
$$\frac{dL}{dw_1} = (1)(0.2)(1)(-2) = -0.4$$

$$\frac{dL}{dw_0} = (1)(0.2)(1)(-1) = -0.2$$

2-Layer MLP Example, Completed

$\hat{y} = w_2\sigma(w_1 x)$ and $L = f(\hat{y})$




$L = f(w_2\sigma(w_1x + b_1) + b_2)$ and $f = \|\hat{y} - y\|^2$
w_1
x
x
b_1
$\times$
w_1x
1
1
$+$
z
$A(1-A)$
σ
w_2
A
$\times$
w_2A
1
$+$
$\hat{y}$
$2(\hat{y}-y)$
f
L
w_2
A
b_2
1
$\frac{dL}{db_2} = 2(\hat{y} - y)$
$\frac{dL}{dw_2} = 2(\hat{y} - y)A^T$
$\frac{dL}{db_1} = \left(2w_2^T(\hat{y} - y)\right)(A)(1-A)$
$\frac{dL}{dw_1} = \left(2w_2^T(\hat{y} - y)\right)(A)(1-A)x^T$

More Mathematically…

Forward Prop	Backprop

What Does This All Mean For Us?

Not Much!

- Most NN ops can be broken down into simple computations with closed-form derivatives
- Frameworks like PyTorch and TensorFlow build the computational graph during the forward pass, and each node in the graph has its backward pass already written for us!
- As such, the framework can compute gradients automatically–a.k.a. auto-differentiation
  - Auto-diff allows us to focus on forward pass: if it's all differentiable, gradient comp. is taken care of
  - We may want to write the backward pass ourselves e.g. in C++ to speed it up, but this is rare
- It's still good to understand backprop at a theoretical level
  - Helps you debug when your model isn't converging!

Pseudocode

```
for X, y in train_dataset:
    y_hat = compute_prediction(model, X)
    l = compute_loss(y, y_hat)
    grads = compute_gradients(model, l)
    for name, grad in grads:
        model.take_update_step(name, grad)
```

Auto-diff enables us to compute gradients without writing any backwards pass code!

Real PyTorch Code

```
for X, y in train_dataset:
    y_hat = model(X)
    l = loss_fn(y, y_hat)
    l.backward()
    optim.step()
```

These APIs do gradient computation and weight update for you!

Summary

- Gradient descent requires gradient computation
- The popular method to do so in deep learning is backpropagation algorithm: greedily use chain rule to accumulate local gradients from “back to front”
- Frameworks such as PyTorch and TensorFlow do backprop for you (auto-differentiation)

In General…

For: $z^{[l]} = w^{[l]}A^{[l-1]} + b^{[l]}, \quad A^{[l]} = g^{[l]}(z^{[l]})$

Let: $\delta^{[l]} = \frac{\partial L}{\partial z^{[l]}} = \begin{cases} \frac{\partial L}{\partial \hat{y}} g'^{[l]}(z^{[l]}) & l \text{ is last layer} \\ ((w^{[l+1]})^T \delta^{[l+1]}) g'^{[l]}(z^{[l]}) & otherwise \end{cases}$

Then: $\frac{dL}{dw^{[l]}} = \delta^{[l]}(A^{[l-1]})^T, \quad \frac{dL}{db^{[l]}} = \delta^{[l]}u^T$