



# Lecture 07a

## Gradients

DL4DS – Spring 2025

How do we efficiently compute  
the gradient over deep  
networks?

# Loss function

- Training dataset of  $I$  pairs of input/output examples:

$$\{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^I$$

- Loss function or cost function measures how bad model is:

$$L[\phi, f[\mathbf{x}_i, \phi], \{\mathbf{x}_i, \mathbf{y}_i\}_{i=1}^I]$$

or for short:

$$L[\phi]$$

Returns a scalar that is smaller when model maps inputs to outputs better

# Gradient descent algorithm

**Step 1.** Compute the derivatives of the loss with respect to the parameters:

$$\frac{\partial L}{\partial \phi} = \begin{bmatrix} \frac{\partial L}{\partial \phi_0} \\ \frac{\partial L}{\partial \phi_1} \\ \vdots \\ \frac{\partial L}{\partial \phi_N} \end{bmatrix}. \quad \text{Also notated as } \nabla_w L$$

**Step 2.** Update the parameters according to the rule:

$$\phi \leftarrow \phi - \alpha \frac{\partial L}{\partial \phi},$$

where the positive scalar  $\alpha$  determines the magnitude of the change.

But so far, we looked at simple models that were easy to calculate gradients

For example, linear, 1-layer models.

$$\begin{aligned} L[\phi] &= \sum_{i=1}^I \ell_i = \sum_{i=1}^I (\mathbf{f}[x_i, \phi] - y_i)^2 \\ &= \sum_{i=1}^I (\phi_0 + \phi_1 x_i - y_i)^2 \end{aligned}$$

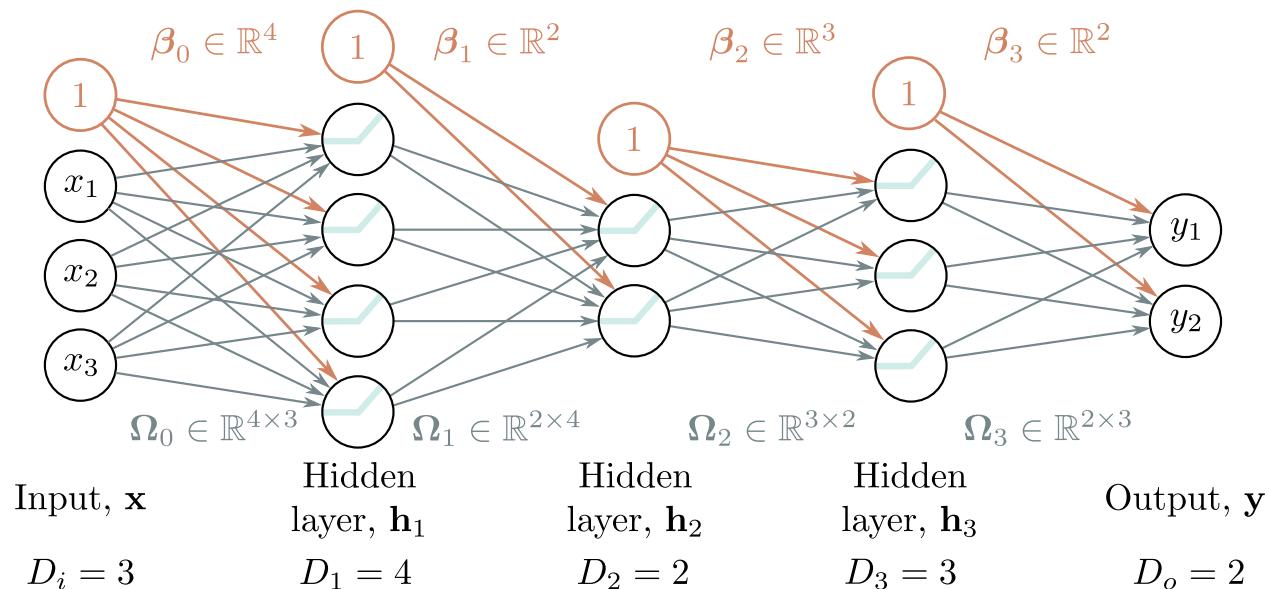
Least squares loss for linear regression

$$\frac{\partial L}{\partial \phi} = \frac{\partial}{\partial \phi} \sum_{i=1}^I \ell_i = \sum_{i=1}^I \frac{\partial \ell_i}{\partial \phi}$$

$$\frac{\partial \ell_i}{\partial \phi} = \begin{bmatrix} \frac{\partial \ell_i}{\partial \phi_0} \\ \frac{\partial \ell_i}{\partial \phi_1} \end{bmatrix} = \begin{bmatrix} 2(\phi_0 + \phi_1 x_i - y_i) \\ 2x_i(\phi_0 + \phi_1 x_i - y_i) \end{bmatrix}$$

Partial derivative w.r.t. each parameter

# What about deep learning models?



$$\begin{aligned}
 \mathbf{h}_1 &= \mathbf{a}[\beta_0 + \Omega_0 \mathbf{x}] \\
 \mathbf{h}_2 &= \mathbf{a}[\beta_1 + \Omega_1 \mathbf{h}_1] \\
 \mathbf{h}_3 &= \mathbf{a}[\beta_2 + \Omega_2 \mathbf{h}_2] \\
 \mathbf{f}[\mathbf{x}, \phi] &= \beta_3 + \Omega_3 \mathbf{h}_3
 \end{aligned}$$

We need to compute partial derivatives w.r.t.  
every parameter!

Loss: sum of individual terms:

$$L[\phi] = \sum_{i=1}^I \ell_i = \sum_{i=1}^I l[f[\mathbf{x}_i, \phi], y_i]$$

SGD Algorithm:

$$\phi_{t+1} \leftarrow \phi_t - \alpha \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\phi_t]}{\partial \phi}$$

*Millions* and even *billions* of  
parameters:

$$\phi = \{\beta_0, \Omega_0, \beta_1, \Omega_1, \beta_2, \Omega_2, \dots\}$$

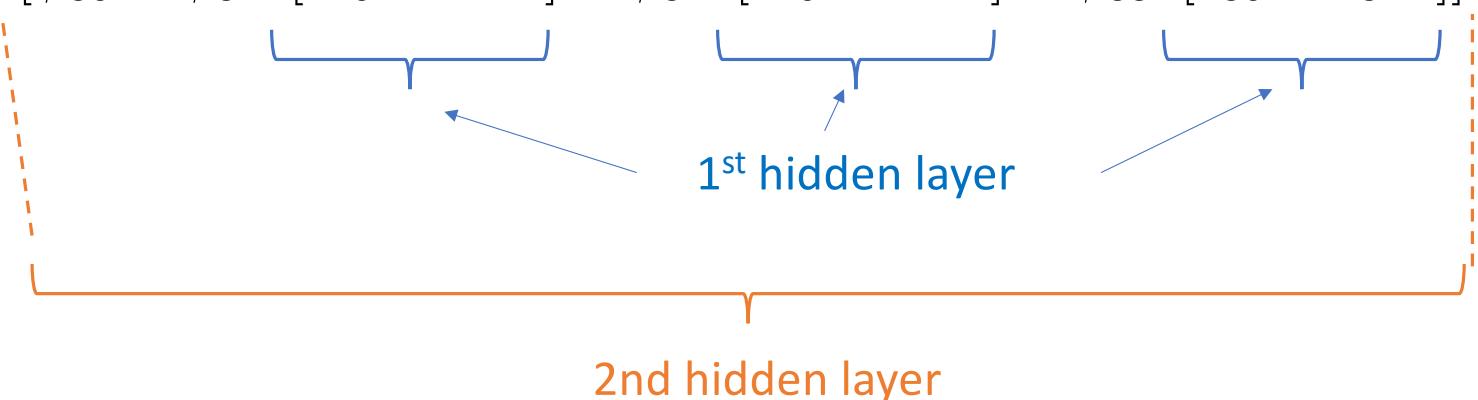
We need the partial derivative with  
respect to every weight and bias we  
want to update for every sample in  
the batch.

$$\frac{\partial \ell_i}{\partial \beta_k} \quad \text{and} \quad \frac{\partial \ell_i}{\partial \Omega_k}$$

# Network equation gets unwieldy even for small models

- Model equation for 2 hidden layers of 3 units each:

$$\begin{aligned}y' = & \phi'_0 + \phi'_1 a [\psi_{10} + \psi_{11} a[\theta_{10} + \theta_{11}x] + \psi_{12} a[\theta_{20} + \theta_{21}x] + \psi_{13} a[\theta_{30} + \theta_{31}x]] \\& + \phi'_2 a [\psi_{20} + \psi_{21} a[\theta_{10} + \theta_{11}x] + \psi_{22} a[\theta_{20} + \theta_{21}x] + \psi_{23} a[\theta_{30} + \theta_{31}x]] \\& + \phi'_3 a [\psi_{30} + \psi_{31} a[\theta_{10} + \theta_{11}x] + \psi_{32} a[\theta_{20} + \theta_{21}x] + \psi_{33} a[\theta_{30} + \theta_{31}x]]\end{aligned}$$



# Gradients

- Backpropagation intuition
- Toy model
- Matrix calculus
- Backpropagation matrix forward pass
- Backpropagation matrix backward pass

# Problem 1: Computing gradients

Loss: sum of individual terms:

$$L[\phi] = \sum_{i=1}^I \ell_i = \sum_{i=1}^I l[f[\mathbf{x}_i, \phi], y_i]$$

SGD Algorithm:

$$\phi_{t+1} \leftarrow \phi_t - \alpha \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\phi_t]}{\partial \phi}$$

Parameters:

$$\phi = \{\beta_0, \Omega_0, \beta_1, \Omega_1, \beta_2, \Omega_2, \beta_3, \Omega_3\}$$

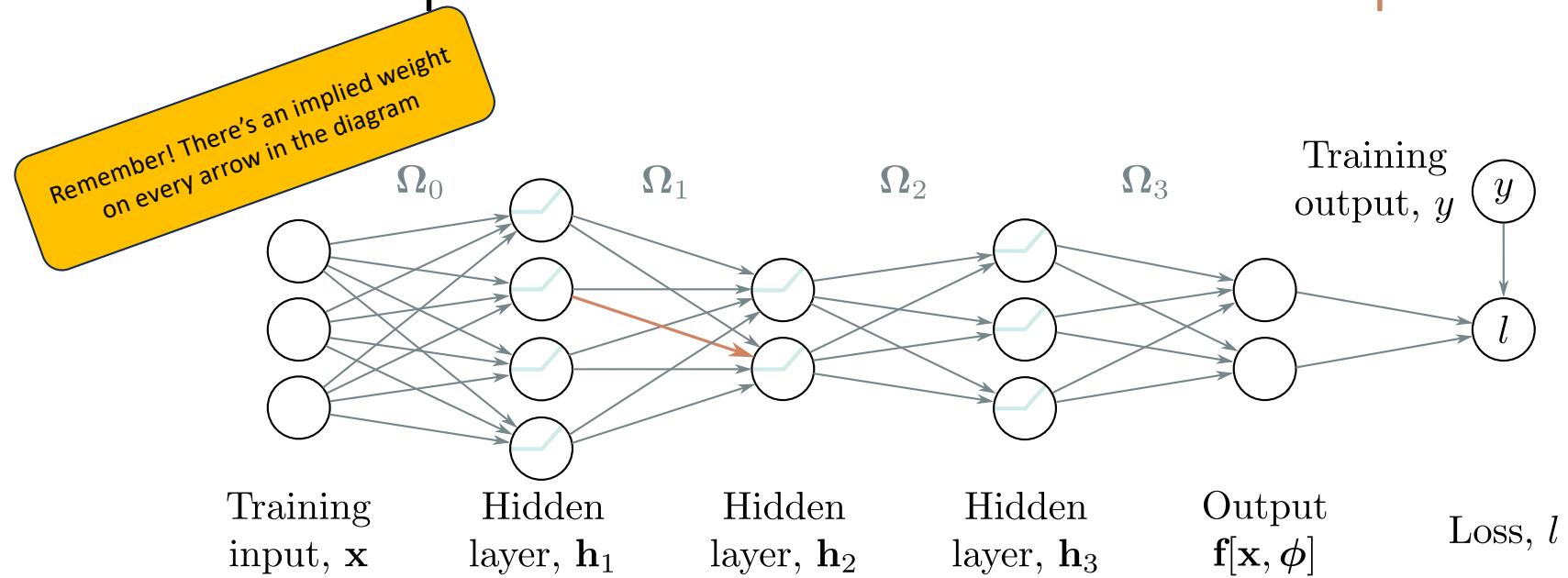
Need to compute gradients

$$\frac{\partial \ell_i}{\partial \beta_k} \quad \text{and} \quad \frac{\partial \ell_i}{\partial \Omega_k}$$

# Algorithm to compute gradient efficiently

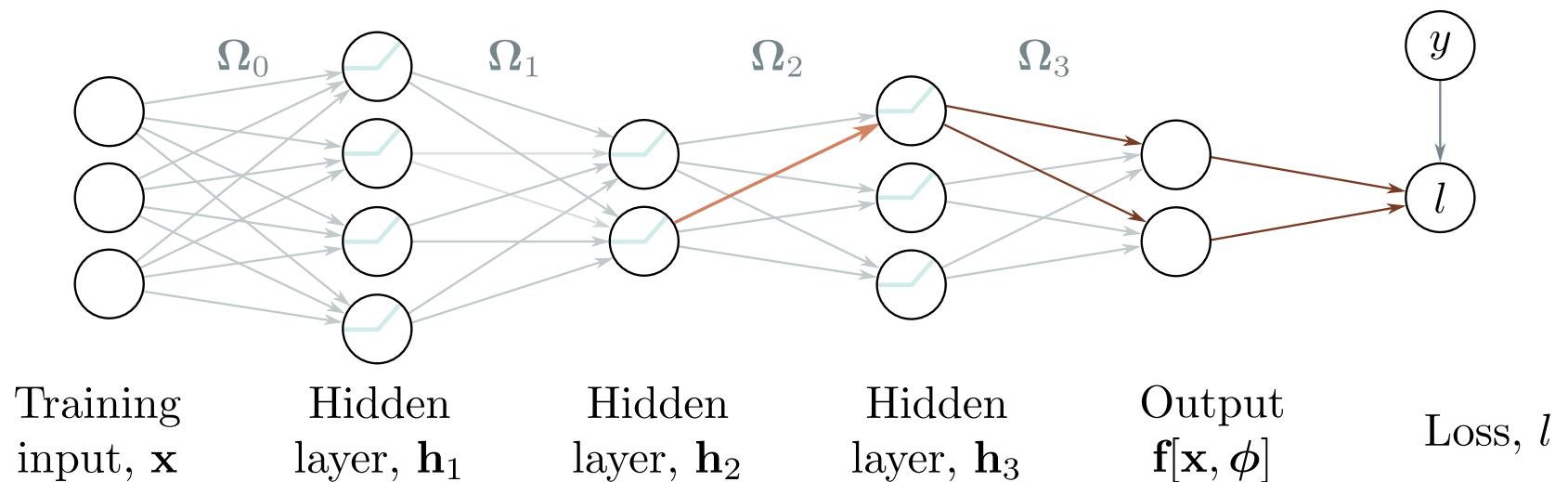
- “**Backpropagation algorithm**”
- Rumelhart, Hinton, and Williams (1986)

# BackProp intuition #1: the forward pass



- The weight on the orange arrow multiplies activation (ReLU output) of previous layer
- We want to know how change (*partial derivative*) in orange weight affects loss
- If we double activation in previous layer, weight will have twice the effect
- Conclusion: we need to know the activations at each layer.
- Put another way: we need to evaluate each partial derivatives for each input

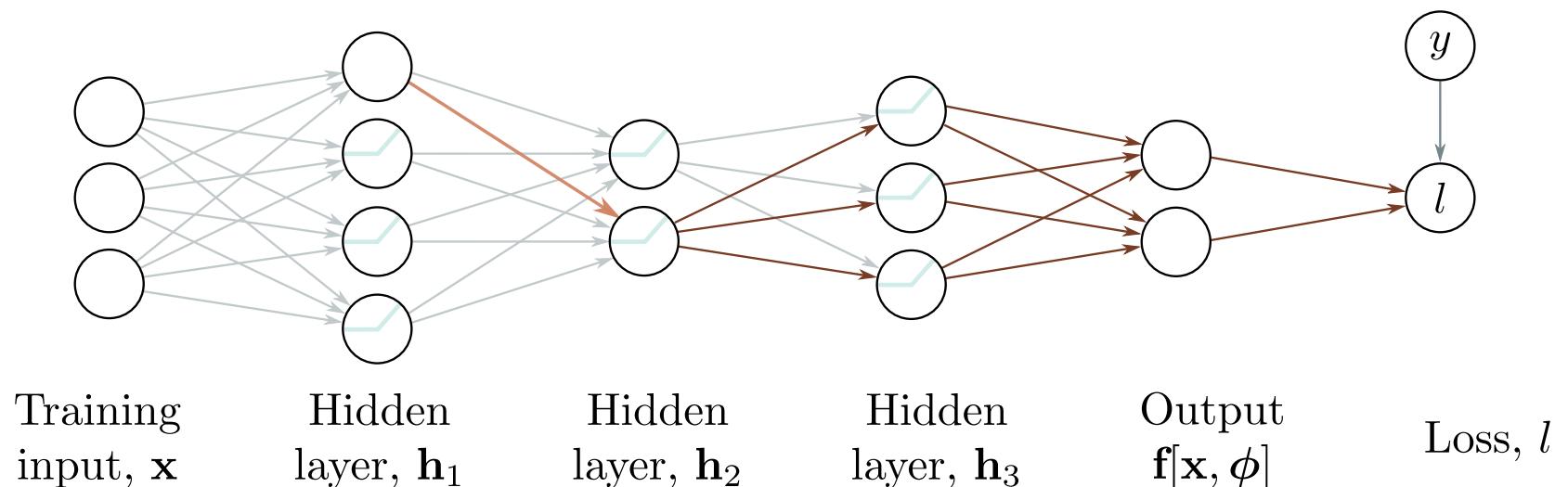
## BackProp intuition #2: the backward pass



To calculate how a small change in a weight or bias feeding into hidden layer  $\mathbf{h}_3$  modifies the loss, we need to know:

- how a change in layer  $\mathbf{h}_3$  changes the model output  $\mathbf{f}$
- how a change in the model output changes the loss  $l$

## BackProp intuition #2: the backward pass

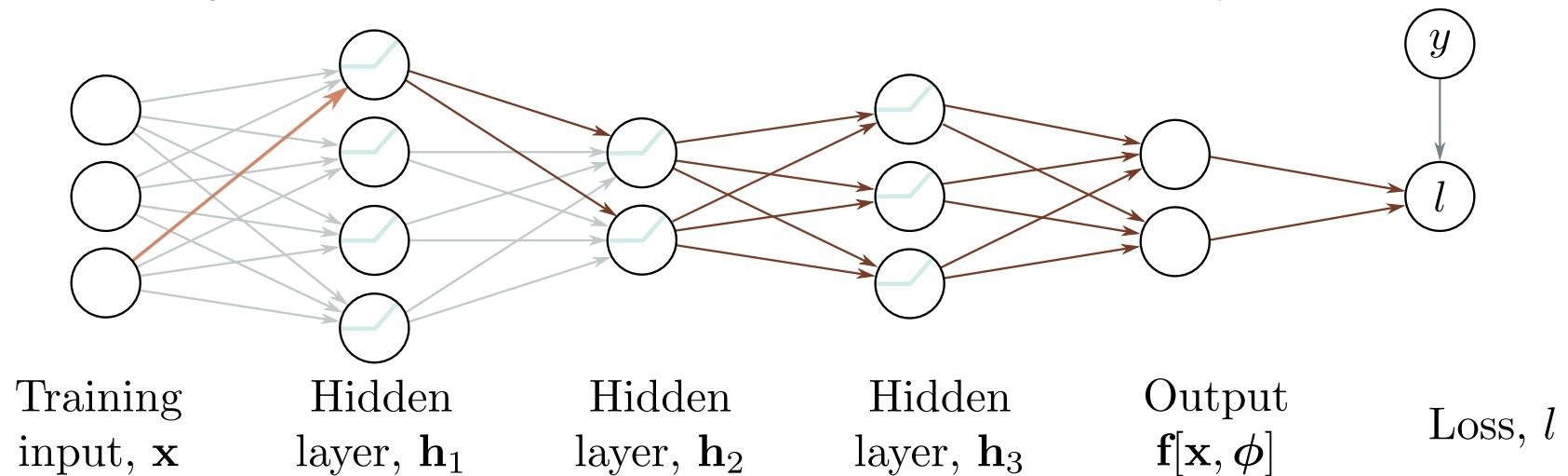


To calculate how a small change in a weight or bias feeding into hidden layer  $\mathbf{h}_2$  modifies the loss, we need to know:

- how a change in layer  $\mathbf{h}_2$  affects  $\mathbf{h}_3$
- how  $\mathbf{h}_3$  changes the model output  $\mathbf{f}$
- how a change in the model output  $\mathbf{f}$  changes the loss  $l$

We know this from the previous step

## BackProp intuition #2: the backward pass



To calculate how a small change in a weight or bias feeding into hidden layer  $\mathbf{h}_1$  modifies the loss, we need to know:

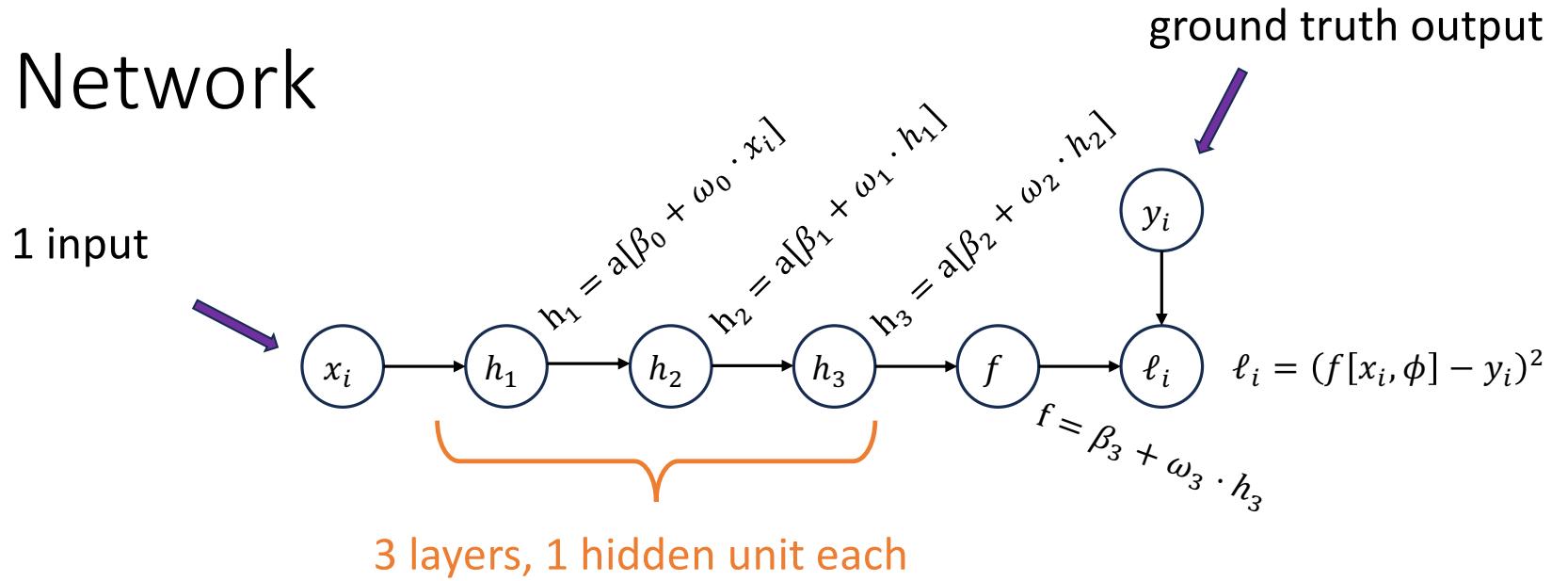
- how a change in layer  $\mathbf{h}_1$  affects  $\mathbf{h}_2$
- how a change in layer  $\mathbf{h}_2$  affects  $\mathbf{h}_3$
- how  $\mathbf{h}_3$  changes the model output  $\mathbf{f}$
- how a change in the model output  $\mathbf{f}$  changes the loss  $l$

We know these from the previous steps

# Gradients

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- Backpropagation matrix forward pass
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# Toy Network



$$f[x_i, \phi] = \beta_3 + \omega_3 \cdot a \left[ \beta_2 + \omega_2 \cdot a \left[ \beta_1 + \omega_1 \cdot a \left[ \beta_0 + \omega_0 \cdot x_i \right] \right] \right]$$

$$\ell_i = (f[x_i, \phi] - y_i)^2$$

# Gradients of toy function

$$f[x_i, \phi] = \beta_3 + \omega_3 \cdot a [\beta_2 + \omega_2 \cdot a [\beta_1 + \omega_1 \cdot a [\beta_0 + \omega_0 \cdot x_i]]]$$

$$\ell_i = (f[x_i, \phi] - y_i)^2$$

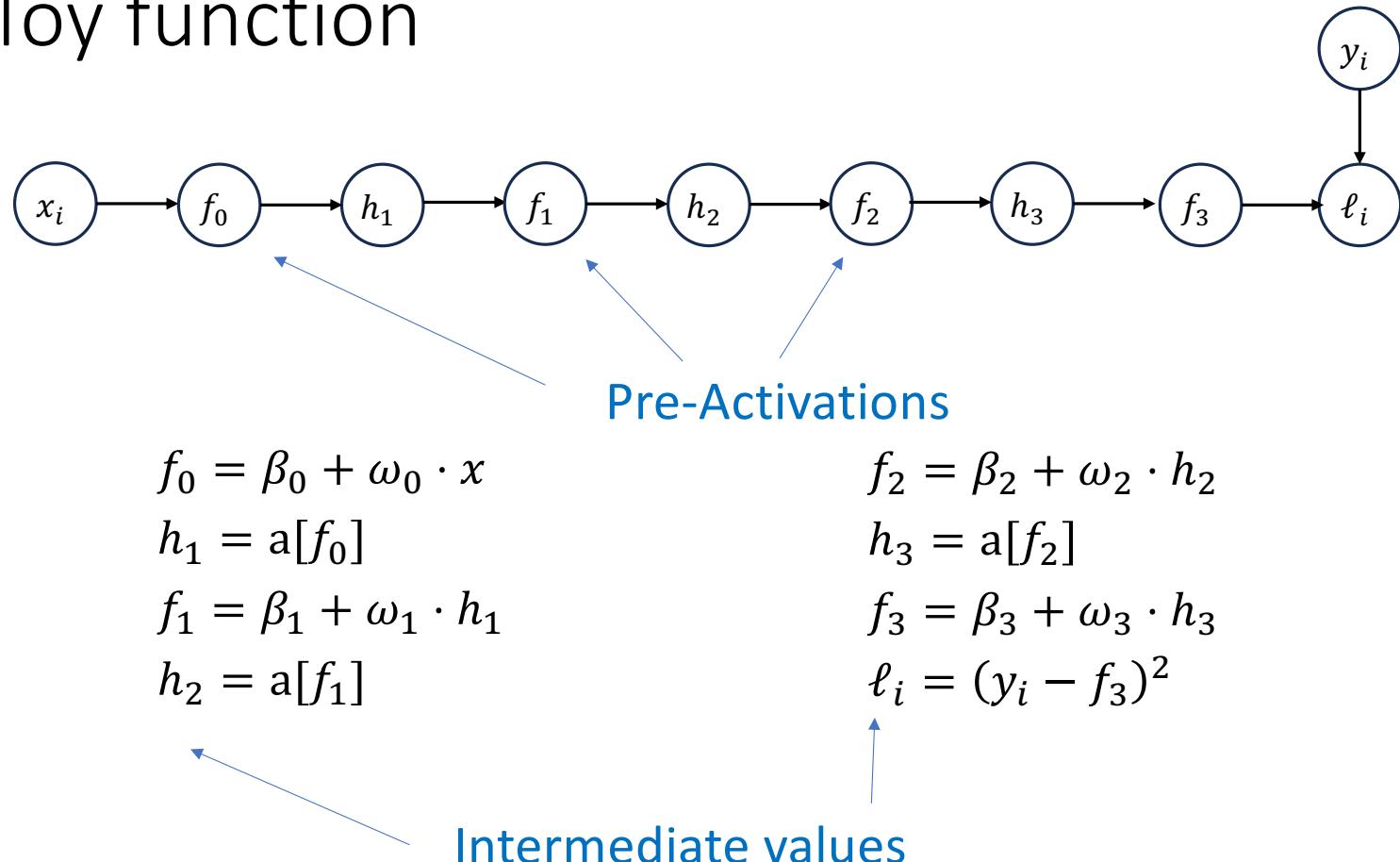
We want to calculate each partial:



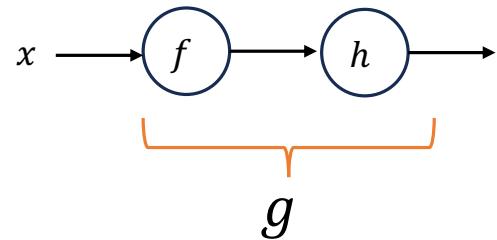
Tells us how a small change in  $\beta_i$  or  $\omega_i$  changes the loss  $\ell_i$  for the  $i^{\text{th}}$  example

$$\frac{\partial \ell_i}{\partial \beta_0}, \quad \frac{\partial \ell_i}{\partial \omega_0}, \quad \frac{\partial \ell_i}{\partial \beta_1}, \quad \frac{\partial \ell_i}{\partial \omega_1}, \quad \frac{\partial \ell_i}{\partial \beta_2}, \quad \frac{\partial \ell_i}{\partial \omega_2}, \quad \frac{\partial \ell_i}{\partial \beta_3}, \quad \text{and} \quad \frac{\partial \ell_i}{\partial \omega_3}$$

# Toy function



# Refresher: The Chain Rule



For  $g(x) = h(f(x))$

then  $g'(x) = h'(f(x)) f'(x)$ , where  $g'(x)$  is the derivative of  $g(x)$ .

Or can be written equivalently as

$$\frac{\partial g}{\partial x} = \frac{\partial h}{\partial f} \frac{\partial f}{\partial x}$$

Leibniz's Notation

Lagrange's Notation

# Forward pass

$$f[x_i, \phi] = \beta_3 + \omega_3 \cdot a [\beta_2 + \omega_2 \cdot a [\beta_1 + \omega_1 \cdot a [\beta_0 + \omega_0 \cdot x_i]]]$$

$$\ell_i = (f[x_i, \phi] - y_i)^2$$

1. Write this as a series of intermediate calculations

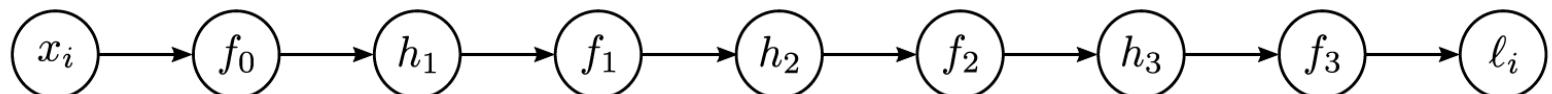
$$f_0 = \beta_0 + \omega_0 \cdot x_i \qquad \qquad f_2 = \beta_2 + \omega_2 \cdot h_2$$

2. Compute these intermediate quantities

$$h_1 = a[f_0] \qquad \qquad h_3 = a[f_2]$$

$$f_1 = \beta_1 + \omega_1 \cdot h_1 \qquad \qquad f_3 = \beta_3 + \omega_3 \cdot h_3$$

$$h_2 = a[f_1] \qquad \qquad \ell_i = (y_i - f_3)^2$$



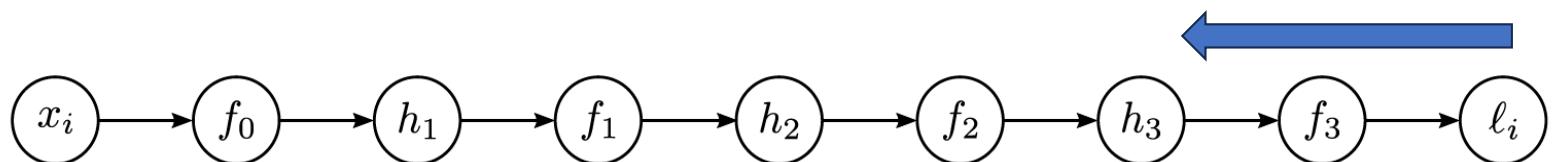
# Backward pass

$$f[x_i, \phi] = \beta_3 + \omega_3 \cdot a [\beta_2 + \omega_2 \cdot a [\beta_1 + \omega_1 \cdot a [\beta_0 + \omega_0 \cdot x_i]]]$$

$$\ell_i = (f[x_i, \phi] - y_i)^2$$

1. Compute the derivatives of the *loss* with respect to these intermediate quantities, but in reverse order.

$$\frac{\partial \ell_i}{\partial f_3}, \quad \frac{\partial \ell_i}{\partial h_3}, \quad \frac{\partial \ell_i}{\partial f_2}, \quad \frac{\partial \ell_i}{\partial h_2}, \quad \frac{\partial \ell_i}{\partial f_1}, \quad \frac{\partial \ell_i}{\partial h_1}, \quad \text{and} \quad \frac{\partial \ell_i}{\partial f_0}$$

# Backward pass

$$f[x_i, \phi] = \beta_3 + \omega_3 \cdot a [\beta_2 + \omega_2 \cdot a [\beta_1 + \omega_1 \cdot a [\beta_0 + \omega_0 \cdot x_i]]]$$

$$\ell_i = (f[x_i, \phi] - y_i)^2$$

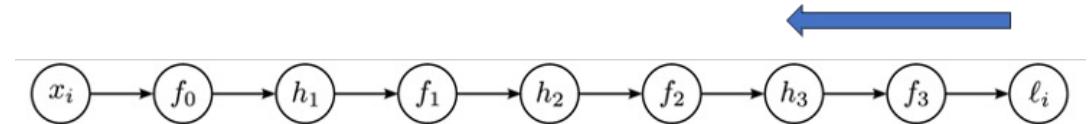
1. Compute the derivatives of the loss with respect to these intermediate quantities, but in reverse order.

$$\frac{\partial \ell_i}{\partial f_3}, \quad \frac{\partial \ell_i}{\partial h_3}, \quad \frac{\partial \ell_i}{\partial f_2}, \quad \frac{\partial \ell_i}{\partial h_2}, \quad \frac{\partial \ell_i}{\partial f_1}, \quad \frac{\partial \ell_i}{\partial h_1}, \quad \text{and} \quad \frac{\partial \ell_i}{\partial f_0}$$



# Backward pass

1. Compute the derivatives of the loss with respect to these intermediate quantities, but in reverse order.



$$\begin{array}{ll} f_0 = \beta_0 + \omega_0 \cdot x & f_2 = \beta_2 + \omega_2 \cdot h_2 \\ h_1 = a[f_0] & h_3 = a[f_2] \\ f_1 = \beta_1 + \omega_1 \cdot h_1 & f_3 = \beta_3 + \omega_3 \cdot h_3 \\ h_2 = a[f_1] & \ell_i = (f_3 - y_i)^2 \end{array}$$

- The first of these derivatives is trivial

$$\frac{\partial \ell_i}{\partial f_3} = 2(f_3 - y_i)$$

# Backward pass

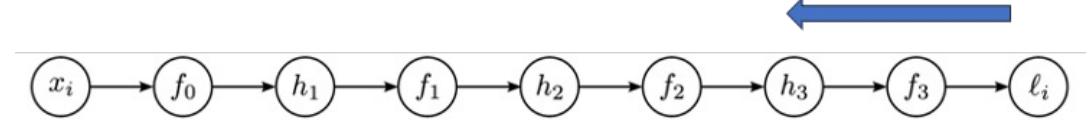
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- The second of these derivatives is computed via the chain rule

$$\frac{\partial \ell_i}{\partial h_3} = \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3}$$

How does a small change in  $h_3$  change  $\ell_i$ ?



# Backward pass

- 1. Compute the derivatives of the loss with respect to these intermediate quantities, but in reverse order.

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 f_0 = \beta_0 + \omega_0 \cdot x & f_2 = \beta_2 + \omega_2 \cdot h_2 \\
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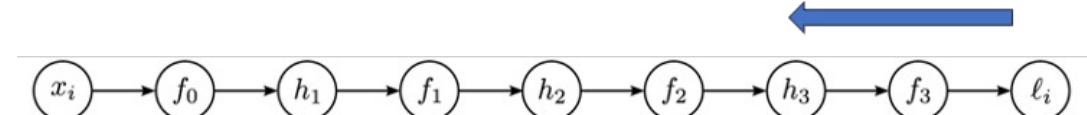
- The second derivative is computed via the chain rule

$$\frac{\partial \ell_i}{\partial h_3} = \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3}$$

How does a small change in  $h_3$  change  $\ell_i$ ?

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How does a small change in  $f_3$  change  $\ell_i$ ?



# Backward pass

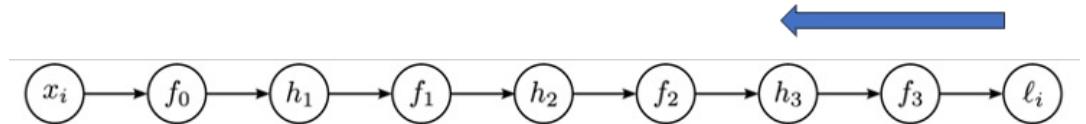
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- The second of these derivatives is computed via the chain rule

$$\frac{\partial \ell_i}{\partial h_3} = \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3}$$

Already computed!



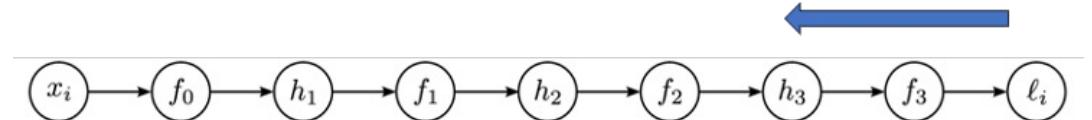
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1. Compute the derivatives of the loss with respect to these intermediate quantities, but in reverse order.

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- The remaining derivatives also calculated by further use of chain rule

$$\frac{\partial \ell_i}{\partial f_2} = \frac{\partial h_3}{\partial f_2} \left( \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right)$$



# Backward pass

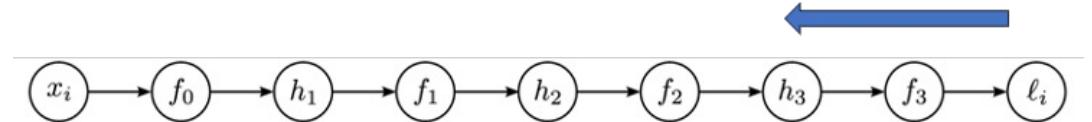
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 \end{array}$$

$$\frac{\partial \ell_i}{\partial f_2} = \frac{\partial h_3}{\partial f_2} \left( \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right)$$

Already computed!



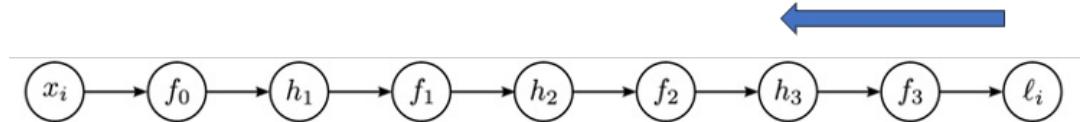
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$$\begin{aligned}\frac{\partial \ell_i}{\partial f_2} &= \frac{\partial h_3}{\partial f_2} \left( \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right) \\ \frac{\partial \ell_i}{\partial h_2} &= \frac{\partial f_2}{\partial h_2} \left( \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right)\end{aligned}$$

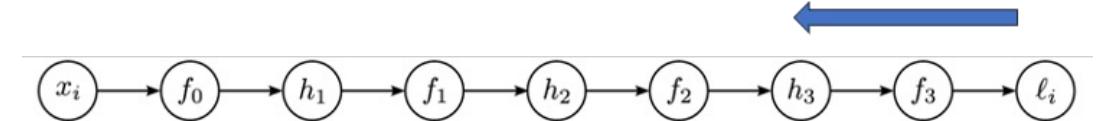


# Backward pass

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- The remaining derivatives also calculated by further use of chain rule

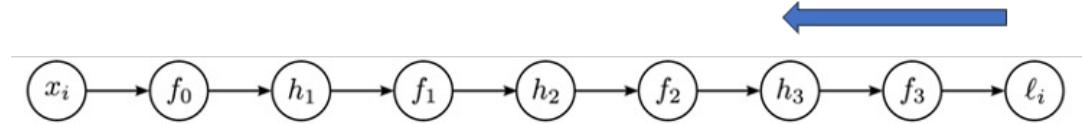


$$\begin{aligned}
 \frac{\partial \ell_i}{\partial f_2} &= \frac{\partial h_3}{\partial f_2} \left( \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right) \\
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 \frac{\partial \ell_i}{\partial f_0} &= \frac{\partial h_1}{\partial f_0} \left( \frac{\partial f_1}{\partial h_1} \frac{\partial h_2}{\partial f_1} \frac{\partial f_2}{\partial h_2} \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right)
 \end{aligned}$$

# Backward pass

1. Compute the derivatives of the loss with respect to these intermediate quantities, but in reverse order.

- The remaining derivatives also calculated by further use of chain rule



$$\frac{\partial \ell_i}{\partial f_3} = 2(f_3 - y_i)$$

$$\frac{\partial \ell_i}{\partial h_3} = \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3}$$

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$$\frac{\partial \ell_i}{\partial f_1} = \frac{\partial h_2}{\partial f_1} \left( \frac{\partial f_2}{\partial h_2} \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right)$$

$$\frac{\partial \ell_i}{\partial h_1} = \frac{\partial f_1}{\partial h_1} \left( \frac{\partial h_2}{\partial f_1} \frac{\partial f_2}{\partial h_2} \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right)$$

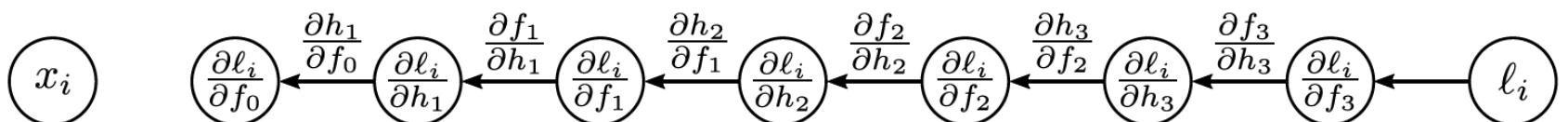
$$\frac{\partial \ell_i}{\partial f_0} = \frac{\partial h_1}{\partial f_0} \left( \frac{\partial f_1}{\partial h_1} \frac{\partial h_2}{\partial f_1} \frac{\partial f_2}{\partial h_2} \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right)$$

# Backward pass

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- The remaining derivatives also calculated by further use of chain rule

$$\begin{aligned}
 \frac{\partial \ell_i}{\partial f_3} &= 2(f_3 - y_i) \\
 \frac{\partial \ell_i}{\partial h_3} &= \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \\
 \frac{\partial \ell_i}{\partial f_2} &= \frac{\partial h_3}{\partial f_2} \left( \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right) \\
 \frac{\partial \ell_i}{\partial h_2} &= \frac{\partial f_2}{\partial h_2} \left( \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right) \\
 \frac{\partial \ell_i}{\partial f_1} &= \frac{\partial h_2}{\partial f_1} \left( \frac{\partial f_2}{\partial h_2} \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right) \\
 \frac{\partial \ell_i}{\partial h_1} &= \frac{\partial f_1}{\partial h_1} \left( \frac{\partial h_2}{\partial f_1} \frac{\partial f_2}{\partial h_2} \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right) \\
 \frac{\partial \ell_i}{\partial f_0} &= \frac{\partial h_1}{\partial f_0} \left( \frac{\partial f_1}{\partial h_1} \frac{\partial h_2}{\partial f_1} \frac{\partial f_2}{\partial h_2} \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right)
 \end{aligned}$$



We extend this to get to the parameters  $\omega$ 's and  $\beta$ 's

# Backward pass

- 2. Find how the loss changes as a function of the parameters  $\beta$  and  $\omega$ .

$$\begin{array}{ll} f_0 = \beta_0 + \omega_0 \cdot x & f_2 = \beta_2 + \omega_2 \cdot h_2 \\ h_1 = a[f_0] & h_3 = a[f_2] \\ f_1 = \beta_1 + \omega_1 \cdot h_1 & f_3 = \beta_3 + \omega_3 \cdot h_3 \\ h_2 = a[f_1] & \ell_i = (y_i - f_3)^2 \end{array}$$

- Another application of the chain rule

$$\frac{\partial \ell_i}{\partial \omega_k} = \frac{\partial f_k}{\partial \omega_k} \frac{\partial \ell_i}{\partial f_k}$$

How does a small change in  $\omega_k$  change  $\ell_i$ ?

How does a small change in  $\omega_k$  change  $f_k$ ?

How does a small change in  $f_k$  change  $\ell_i$ ?

# Backward pass

2. Find how the loss changes as a function of the parameters  $\beta$  and  $\omega$ .

$$f_0 = \beta_0 + \omega_0 \cdot x$$

$$h_1 = a[f_0]$$

$$f_1 = \beta_1 + \omega_1 \cdot h_1$$

$$h_2 = a[f_1]$$

$$f_2 = \beta_2 + \omega_2 \cdot h_2$$

$$h_3 = a[f_2]$$

$$f_3 = \beta_3 + \omega_3 \cdot h_3$$

$$\ell_i = (y_i - f_3)^2$$

- Another application of the chain rule

$$\frac{\partial \ell_i}{\partial \omega_k} = \frac{\partial f_k}{\partial \omega_k} \frac{\partial \ell_i}{\partial f_k}$$

How does a small change in  $\omega_k$  change  $\ell_i$ ?

$$\frac{\partial f_k}{\partial \omega_k} = h_k$$

Already calculated in part 1.

# Backward pass

2. Find how the loss changes as a function of the parameters  $\beta$  and  $\omega$ .

$$\begin{array}{ll} f_0 = \beta_0 + \omega_0 \cdot x & f_2 = \beta_2 + \omega_2 \cdot h_2 \\ h_1 = a[f_0] & h_3 = a[f_2] \\ f_1 = \beta_1 + \omega_1 \cdot h_1 & f_3 = \beta_3 + \omega_3 \cdot h_3 \\ h_2 = a[f_1] & \ell_i = (y_i - f_3)^2 \end{array}$$

- Another application of the chain rule
- Similarly for  $\beta$  parameters

$$\frac{\partial \ell_i}{\partial \omega_k} = \frac{\partial f_k}{\partial \omega_k} \frac{\partial \ell_i}{\partial f_k}$$

$$\frac{\partial \ell_i}{\partial \beta_k} = \cancel{\frac{\partial f_k}{\partial \beta_k}} \frac{\partial \ell_i}{\partial f_k}$$

1

# Backward pass

2. Find how the loss changes as a function of the parameters  $\beta$  and  $\omega$ .

$$f_0 = \beta_0 + \omega_0 \cdot x$$

$$h_1 = a[f_0]$$

$$f_1 = \beta_1 + \omega_1 \cdot h_1$$

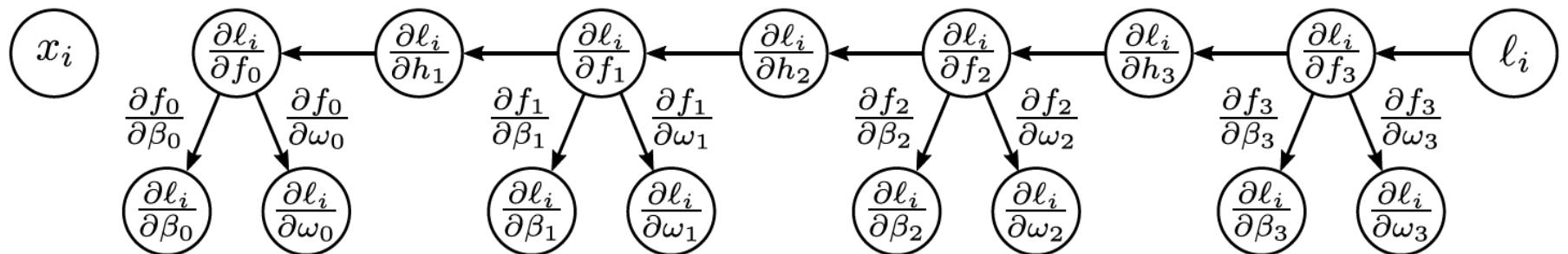
$$h_2 = a[f_1]$$

$$f_2 = \beta_2 + \omega_2 \cdot h_2$$

$$h_3 = a[f_2]$$

$$f_3 = \beta_3 + \omega_3 \cdot h_3$$

$$\ell_i = (y_i - f_3)^2$$



The Slido logo consists of the word "slido" in a lowercase, sans-serif font, with a small green square icon containing a white "S" character positioned above the letter "l".

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**Backpropagation is the process of computing gradients using the chain rule of differentiation.**

- ① Start presenting to display the poll results on this slide.

# Gradients

- Backpropagation intuition
- Toy model
- Matrix calculus
- Backpropagation matrix forward pass
- Backpropagation matrix backward pass

# Matrix calculus

Scalar function  $f[\cdot]$  of a *vector*  $\mathbf{a}$

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix}$$

$$\frac{\partial f}{\partial \mathbf{a}} = \begin{bmatrix} \frac{\partial f}{\partial a_1} \\ \frac{\partial f}{\partial a_2} \\ \frac{\partial f}{\partial a_3} \\ \frac{\partial f}{\partial a_4} \end{bmatrix}$$

The derivative is a vector of shape  $\mathbf{a}$

# Matrix calculus

Scalar function  $f[\cdot]$  of a *matrix*  $\mathbf{a}$

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \end{bmatrix}$$

$$\frac{\partial f}{\partial \mathbf{A}} = \begin{bmatrix} \frac{\partial f}{\partial a_{11}} & \frac{\partial f}{\partial a_{12}} & \frac{\partial f}{\partial a_{13}} \\ \frac{\partial f}{\partial a_{21}} & \frac{\partial f}{\partial a_{22}} & \frac{\partial f}{\partial a_{23}} \\ \frac{\partial f}{\partial a_{31}} & \frac{\partial f}{\partial a_{32}} & \frac{\partial f}{\partial a_{33}} \\ \frac{\partial f}{\partial a_{41}} & \frac{\partial f}{\partial a_{42}} & \frac{\partial f}{\partial a_{43}} \end{bmatrix}$$

The derivative is a matrix of shape  $\mathbf{a}$

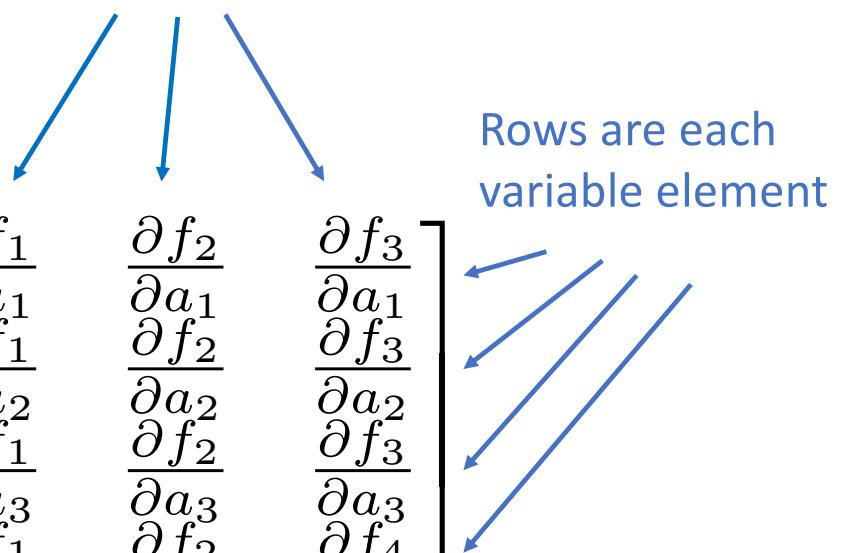
# Matrix calculus

Vector function  $\mathbf{f}[\cdot]$  of a vector  $\mathbf{a}$

$$\mathbf{f} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} \quad \mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix}$$

Vector of scalar  
valued functions

Columns are each  
element function

$$\frac{\partial \mathbf{f}}{\partial \mathbf{a}} = \begin{bmatrix} \frac{\partial f_1}{\partial a_1} & \frac{\partial f_2}{\partial a_1} & \frac{\partial f_3}{\partial a_1} \\ \frac{\partial f_1}{\partial a_2} & \frac{\partial f_2}{\partial a_2} & \frac{\partial f_3}{\partial a_2} \\ \frac{\partial f_1}{\partial a_3} & \frac{\partial f_2}{\partial a_3} & \frac{\partial f_3}{\partial a_3} \\ \frac{\partial f_1}{\partial a_4} & \frac{\partial f_2}{\partial a_4} & \frac{\partial f_4}{\partial a_4} \end{bmatrix}$$


# Comparing vector and matrix

Scalar derivatives:

$$f_3 = \beta_3 + \omega_3 h_3 \quad \frac{\partial f_3}{\partial h_3} = \frac{\partial}{\partial h_3} (\beta_3 + \omega_3 h_3) = \omega_3$$

# Comparing vector and matrix

Scalar derivatives:

$$f_3 = \beta_3 + \omega_3 h_3$$

$$\frac{\partial f_3}{\partial h_3} = \frac{\partial}{\partial h_3} (\beta_3 + \omega_3 h_3) = \omega_3$$

Matrix derivatives:

$$\mathbf{f}_3 = \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3$$

$$\frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} = \frac{\partial}{\partial \mathbf{h}_3} (\boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3) = \boldsymbol{\Omega}_3^T$$

# Comparing vector and matrix

Scalar derivatives:

$$f_3 = \beta_3 + \omega_3 h_3 \quad \frac{\partial f_3}{\partial \beta_3} = \frac{\partial}{\partial \omega_3} \beta_3 + \omega_3 h_3 = 1$$

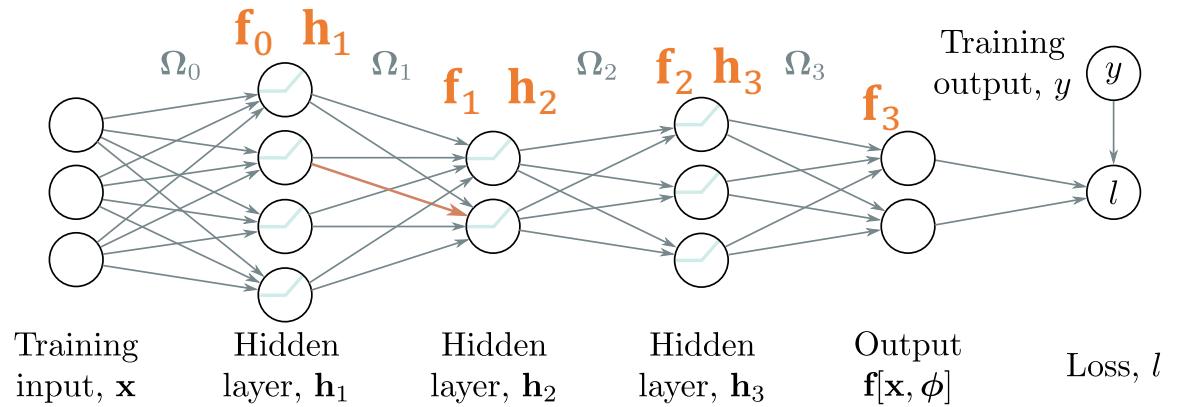
Matrix derivatives:

$$\mathbf{f}_3 = \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \quad \frac{\partial \mathbf{f}_3}{\partial \boldsymbol{\beta}_3} = \frac{\partial}{\partial \boldsymbol{\beta}_3} (\boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3) = \mathbf{I}$$

# Gradients

- Backpropagation intuition
- Toy model
- Matrix calculus
- Backpropagation matrix forward pass
- Backpropagation matrix backward pass

# The forward pass



1. Write this as a series of intermediate calculations

$$\mathbf{f}_0 = \beta_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i$$

$$\mathbf{h}_1 = \mathbf{a}[\mathbf{f}_0]$$

$$\mathbf{f}_1 = \beta_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1$$

$$\mathbf{h}_2 = \mathbf{a}[\mathbf{f}_1]$$

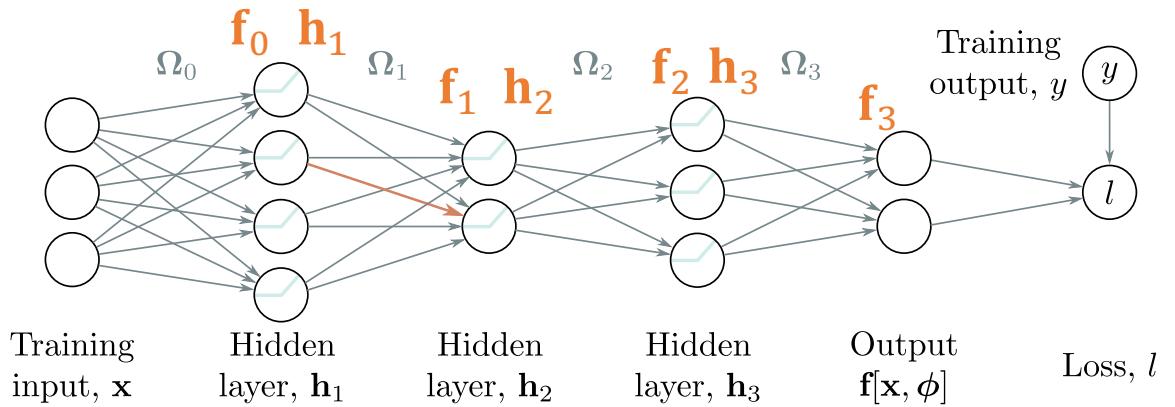
$$\mathbf{f}_2 = \beta_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2$$

$$\mathbf{h}_3 = \mathbf{a}[\mathbf{f}_2]$$

$$\mathbf{f}_3 = \beta_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3$$

$$l_i = l[\mathbf{f}_3, y_i]$$

# The forward pass



1. Write this as a series of intermediate calculations

$$\mathbf{f}_0 = \beta_0 + \Omega_0 \mathbf{x}_i$$

$$\mathbf{h}_1 = \mathbf{a}[\mathbf{f}_0]$$

$$\mathbf{f}_1 = \beta_1 + \Omega_1 \mathbf{h}_1$$

$$\mathbf{h}_2 = \mathbf{a}[\mathbf{f}_1]$$

$$\mathbf{f}_2 = \beta_2 + \Omega_2 \mathbf{h}_2$$

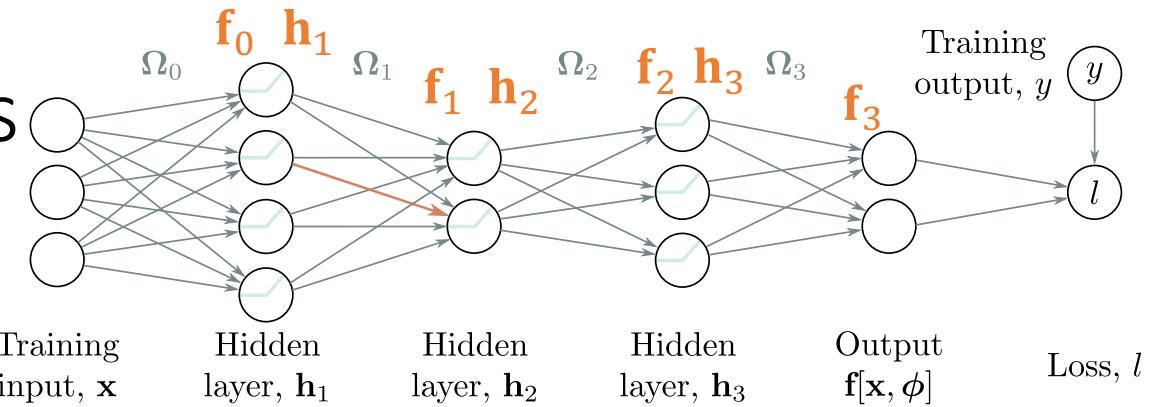
$$\mathbf{h}_3 = \mathbf{a}[\mathbf{f}_2]$$

$$\mathbf{f}_3 = \beta_3 + \Omega_3 \mathbf{h}_3$$

$$l_i = l[\mathbf{f}_3, y_i]$$

2. Compute these intermediate quantities

# The backward pass



1. Write this as a series of intermediate calculations

$$\mathbf{f}_0 = \beta_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i$$

2. Compute these intermediate quantities

$$\mathbf{h}_1 = \mathbf{a}[\mathbf{f}_0]$$

$$\mathbf{f}_1 = \beta_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1$$

$$\mathbf{h}_2 = \mathbf{a}[\mathbf{f}_1]$$

$$\mathbf{f}_2 = \beta_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2$$

$$\mathbf{h}_3 = \mathbf{a}[\mathbf{f}_2]$$

$$\mathbf{f}_3 = \beta_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3$$

$$\ell_i = l[\mathbf{f}_3, y_i]$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_2} = \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

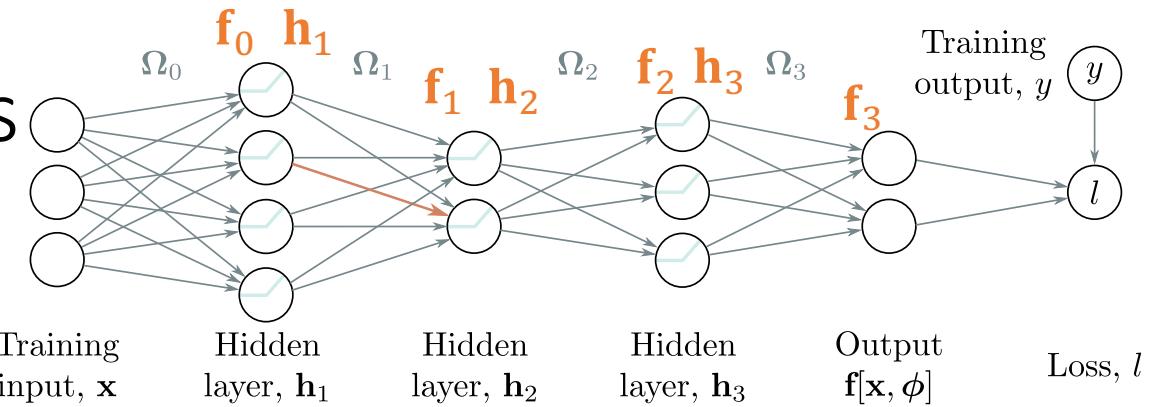
$$\frac{\partial \ell_i}{\partial \mathbf{f}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \left( \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_0} = \frac{\partial \mathbf{h}_1}{\partial \mathbf{f}_0} \frac{\partial \mathbf{f}_1}{\partial \mathbf{h}_1} \left( \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

# Gradients

- Backpropagation intuition
- Toy model
- Matrix calculus
- Backpropagation matrix forward pass
- Backpropagation matrix backward pass

# The backward pass



1. Write this as a series of intermediate calculations

$$\mathbf{f}_0 = \beta_0 + \Omega_0 \mathbf{x}_i$$

2. Compute these intermediate quantities

$$\mathbf{h}_1 = \mathbf{a}[\mathbf{f}_0]$$

$$\mathbf{f}_1 = \beta_1 + \Omega_1 \mathbf{h}_1$$

$$\mathbf{h}_2 = \mathbf{a}[\mathbf{f}_1]$$

$$\mathbf{f}_2 = \beta_2 + \Omega_2 \mathbf{h}_2$$

$$\mathbf{h}_3 = \mathbf{a}[\mathbf{f}_2]$$

$$\mathbf{f}_3 = \beta_3 + \Omega_3 \mathbf{h}_3$$

$$\ell_i = l[\mathbf{f}_3, y_i]$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_2} = \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \boxed{\frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3}} \frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \left( \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_0} = \frac{\partial \mathbf{h}_1}{\partial \mathbf{f}_0} \frac{\partial \mathbf{f}_1}{\partial \mathbf{h}_1} \left( \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

# Yikes!

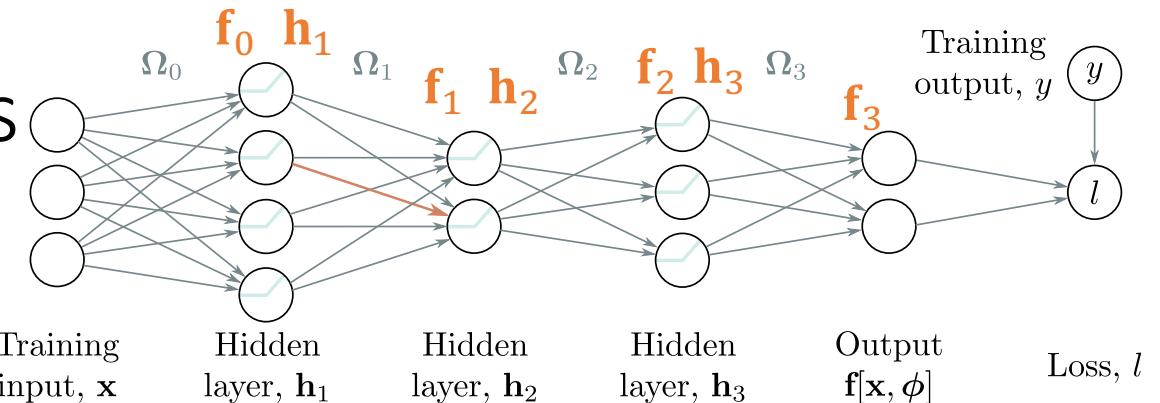
- But:

$$\frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} = \frac{\partial}{\partial \mathbf{h}_3} (\boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3) = \boldsymbol{\Omega}_3^T$$

- Quite similar to:

$$\frac{\partial f_3}{\partial h_3} = \frac{\partial}{\partial h_3} (\beta_3 + \omega_3 h_3) = \omega_3$$

# The backward pass



1. Write this as a series of intermediate calculations

$$\mathbf{f}_0 = \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i$$

2. Compute these intermediate quantities

$$\mathbf{h}_1 = \mathbf{a}[\mathbf{f}_0]$$

$$\mathbf{f}_1 = \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1$$

$$\mathbf{h}_2 = \mathbf{a}[\mathbf{f}_1]$$

$$\mathbf{f}_2 = \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2$$

$$\mathbf{h}_3 = \mathbf{a}[\mathbf{f}_2]$$

$$\mathbf{f}_3 = \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3$$

$$\ell_i = l[\mathbf{f}_3, y_i]$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

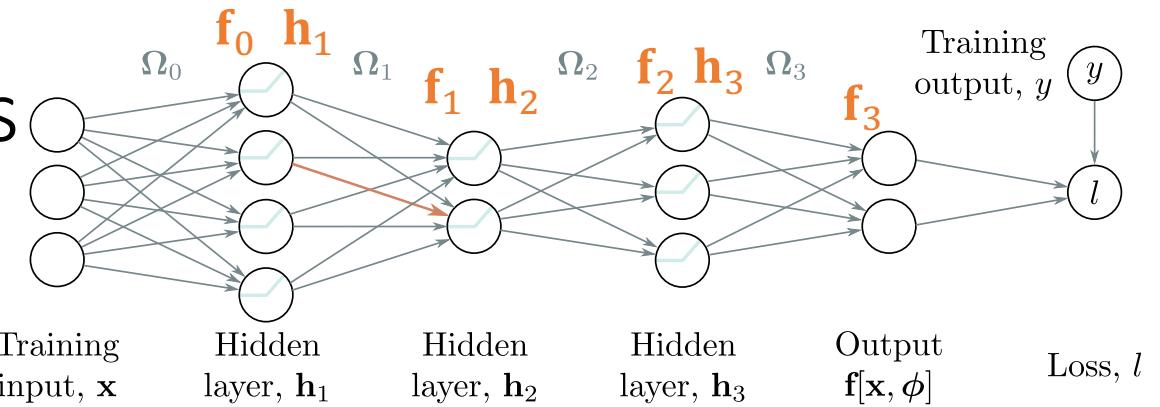
$$\boxed{\frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} = \frac{\partial}{\partial \mathbf{h}_3} (\boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3) = \boldsymbol{\Omega}_3^T}$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_2} = \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \boxed{\frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3}} \frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \left( \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_0} = \frac{\partial \mathbf{h}_1}{\partial \mathbf{f}_0} \frac{\partial \mathbf{f}_1}{\partial \mathbf{h}_1} \left( \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

# The backward pass



1. Write this as a series of intermediate calculations

$$\mathbf{f}_0 = \beta_0 + \Omega_0 \mathbf{x}_i$$

2. Compute these intermediate quantities

$$\mathbf{h}_1 = \mathbf{a}[\mathbf{f}_0]$$

$$\mathbf{f}_1 = \beta_1 + \Omega_1 \mathbf{h}_1$$

$$\mathbf{h}_2 = \mathbf{a}[\mathbf{f}_1]$$

$$\mathbf{f}_2 = \beta_2 + \Omega_2 \mathbf{h}_2$$

$$\mathbf{h}_3 = \mathbf{a}[\mathbf{f}_2]$$

$$\mathbf{f}_3 = \beta_3 + \Omega_3 \mathbf{h}_3$$

$$\ell_i = l[\mathbf{f}_3, y_i]$$

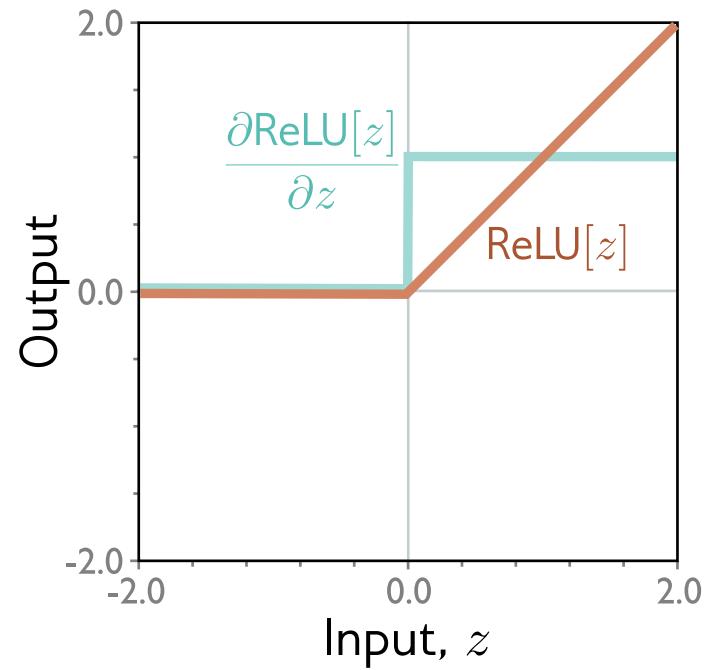
$$\frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_2} = \boxed{\frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2}} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

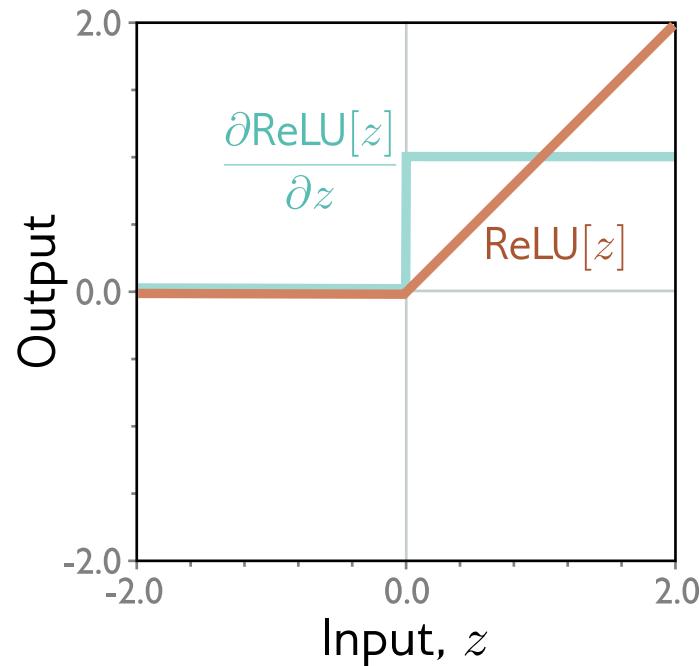
$$\frac{\partial \ell_i}{\partial \mathbf{f}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \left( \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_0} = \frac{\partial \mathbf{h}_1}{\partial \mathbf{f}_0} \frac{\partial \mathbf{f}_1}{\partial \mathbf{h}_1} \left( \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

# Derivative of ReLU



# Derivative of ReLU



$$\text{ReLU}[z] = \max(0, z)$$

$$\frac{\partial \text{ReLU}[z]}{\partial z} = \mathbb{I}[z > 0]$$

“Indicator function”

# Derivative of RELU

1. Consider:

$$\mathbf{a} = \text{ReLU}[\mathbf{b}]$$

where:

$$\mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

2. We could equivalently write:

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} \text{ReLU}[b_1] \\ \text{ReLU}[b_2] \\ \text{ReLU}[b_3] \end{bmatrix}$$

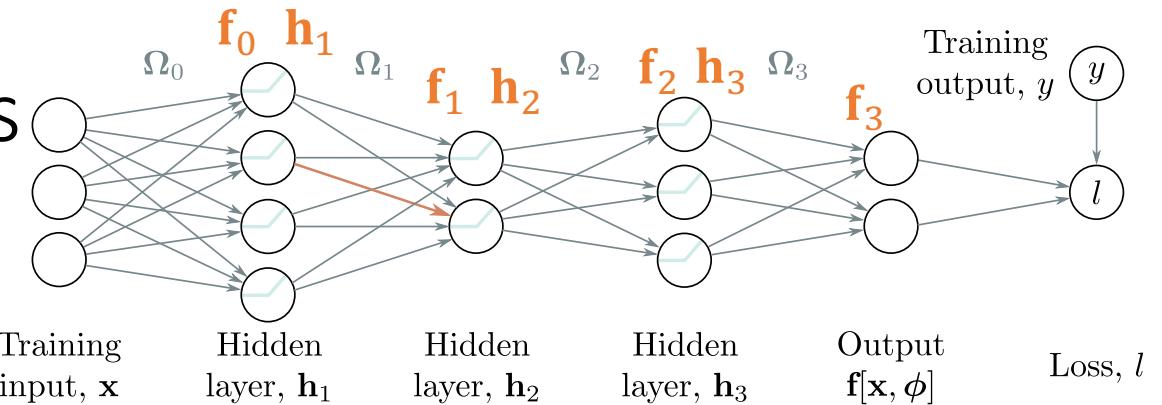
3. Taking the derivative

$$\frac{\partial \mathbf{a}}{\partial \mathbf{b}} = \begin{bmatrix} \frac{\partial a_1}{\partial b_1} & \frac{\partial a_2}{\partial b_1} & \frac{\partial a_3}{\partial b_1} \\ \frac{\partial a_1}{\partial b_2} & \frac{\partial a_2}{\partial b_2} & \frac{\partial a_3}{\partial b_2} \\ \frac{\partial a_1}{\partial b_3} & \frac{\partial a_2}{\partial b_3} & \frac{\partial a_3}{\partial b_3} \end{bmatrix} = \begin{bmatrix} \mathbb{I}[b_1 > 0] & 0 & 0 \\ 0 & \mathbb{I}[b_2 > 0] & 0 \\ 0 & 0 & \mathbb{I}[b_3 > 0] \end{bmatrix}$$

4. We can equivalently pointwise multiply by diagonal

$$\mathbb{I}[\mathbf{b} > 0] \odot$$

# The backward pass



1. Write this as a series of intermediate calculations

$$\mathbf{f}_0 = \beta_0 + \Omega_0 \mathbf{x}_i$$

$$\mathbf{h}_1 = \mathbf{a}[\mathbf{f}_0]$$

$$\mathbf{f}_1 = \beta_1 + \Omega_1 \mathbf{h}_1$$

$$\mathbf{h}_2 = \mathbf{a}[\mathbf{f}_1]$$

$$\mathbf{f}_2 = \beta_2 + \Omega_2 \mathbf{h}_2$$

$$\mathbf{h}_3 = \mathbf{a}[\mathbf{f}_2]$$

$$\mathbf{f}_3 = \beta_3 + \Omega_3 \mathbf{h}_3$$

$$\ell_i = l[\mathbf{f}_3, y_i]$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

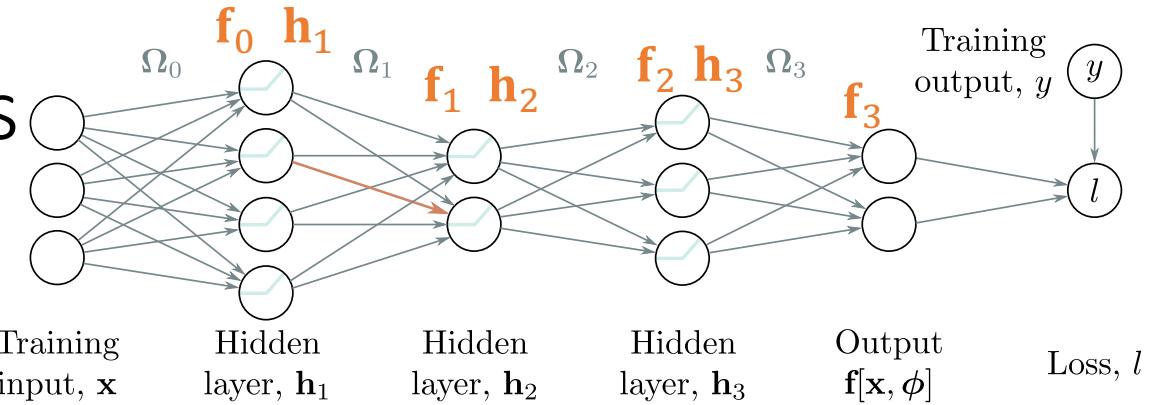
$$\frac{\partial \ell_i}{\partial \mathbf{f}_2} = \boxed{\frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2}} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \left( \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

$$\frac{\partial \ell_i}{\partial \mathbf{f}_0} = \frac{\partial \mathbf{h}_1}{\partial \mathbf{f}_0} \frac{\partial \mathbf{f}_1}{\partial \mathbf{h}_1} \left( \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3} \right)$$

$\mathbb{I}[\mathbf{f}_2 > 0]$

# The backward pass



1. Write this as a series of intermediate calculations
2. Compute these intermediate quantities
3. Take derivatives of output with respect to intermediate quantities
4. Take derivatives w.r.t. parameters

$$\mathbf{f}_0 = \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i$$

$$\mathbf{h}_1 = \mathbf{a}[\mathbf{f}_0]$$

$$\mathbf{f}_1 = \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1$$

$$\mathbf{h}_2 = \mathbf{a}[\mathbf{f}_1]$$

$$\mathbf{f}_2 = \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2$$

$$\mathbf{h}_3 = \mathbf{a}[\mathbf{f}_2]$$

$$\mathbf{f}_3 = \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3$$

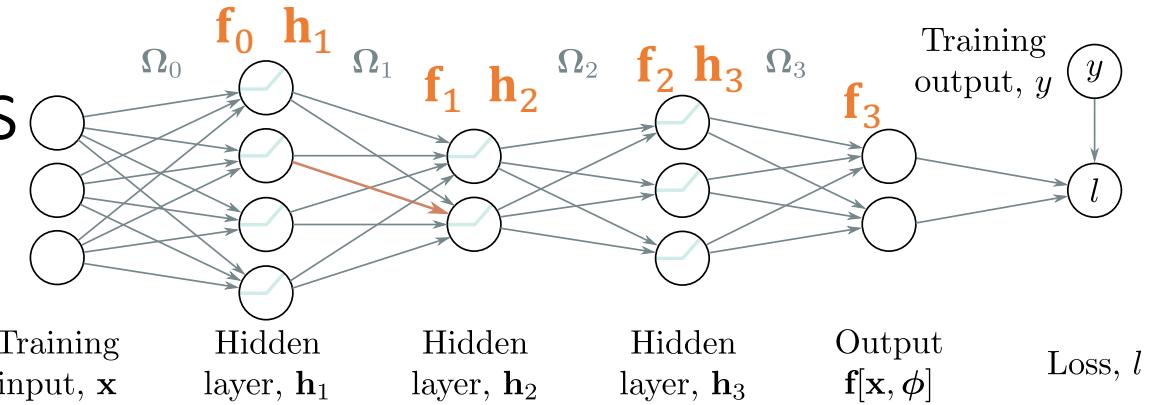
$$\ell_i = l[\mathbf{f}_3, y_i]$$

$$\frac{\partial \ell_i}{\partial \boldsymbol{\beta}_k} = \frac{\partial \mathbf{f}_k}{\partial \boldsymbol{\beta}_k} \frac{\partial \ell_i}{\partial \mathbf{f}_k}$$

$$= \frac{\partial}{\partial \boldsymbol{\beta}_k} (\boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathbf{h}_k) \frac{\partial \ell_i}{\partial \mathbf{f}_k}$$

$$= \frac{\partial \ell_i}{\partial \mathbf{f}_k},$$

# The backward pass



1. Write this as a series of intermediate calculations
2. Compute these intermediate quantities
3. Take derivatives of output with respect to intermediate quantities
4. Take derivatives w.r.t. parameters

$$\mathbf{f}_0 = \beta_0 + \Omega_0 \mathbf{x}_i$$

$$\mathbf{h}_1 = \mathbf{a}[\mathbf{f}_0]$$

$$\mathbf{f}_1 = \beta_1 + \Omega_1 \mathbf{h}_1$$

$$\mathbf{h}_2 = \mathbf{a}[\mathbf{f}_1]$$

$$\mathbf{f}_2 = \beta_2 + \Omega_2 \mathbf{h}_2$$

$$\mathbf{h}_3 = \mathbf{a}[\mathbf{f}_2]$$

$$\mathbf{f}_3 = \beta_3 + \Omega_3 \mathbf{h}_3$$

$$\ell_i = l[\mathbf{f}_3, y_i]$$

$$\frac{\partial \ell_i}{\partial \Omega_k} = \frac{\partial \mathbf{f}_k}{\partial \Omega_k} \frac{\partial \ell_i}{\partial \mathbf{f}_k}$$

$$= \frac{\partial}{\partial \Omega_k} (\beta_k + \Omega_k \mathbf{h}_k) \frac{\partial \ell_i}{\partial \mathbf{f}_k}$$

$$= \frac{\partial \ell_i}{\partial \mathbf{f}_k} \mathbf{h}_k^T$$

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**The backpropagation algorithm updates all weights in a neural network simultaneously using matrix operations.**

- ① Start presenting to display the poll results on this slide.

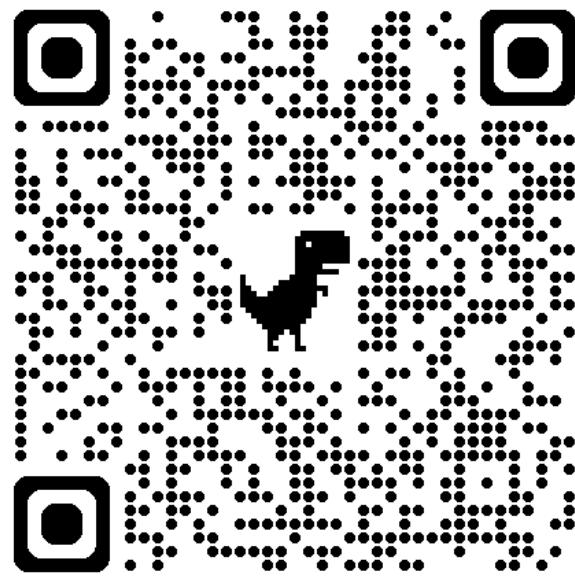
# Gradients

- Backpropagation intuition
- Toy model
- Matrix calculus
- Backpropagation matrix forward pass
- Backpropagation matrix backward pass
- **Matrix backprop summary**

# Pros and cons

- Extremely efficient
  - Only need matrix multiplication and thresholding for ReLU functions
- Memory hungry – must store all the intermediate quantities
- Sequential
  - can process multiple batches in parallel
  - but things get harder if the whole model doesn't fit on one machine.

Feedback?



[Link](#)