



Lecture 07a

Gradients

DL4DS – Spring 2024

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 α 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.

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

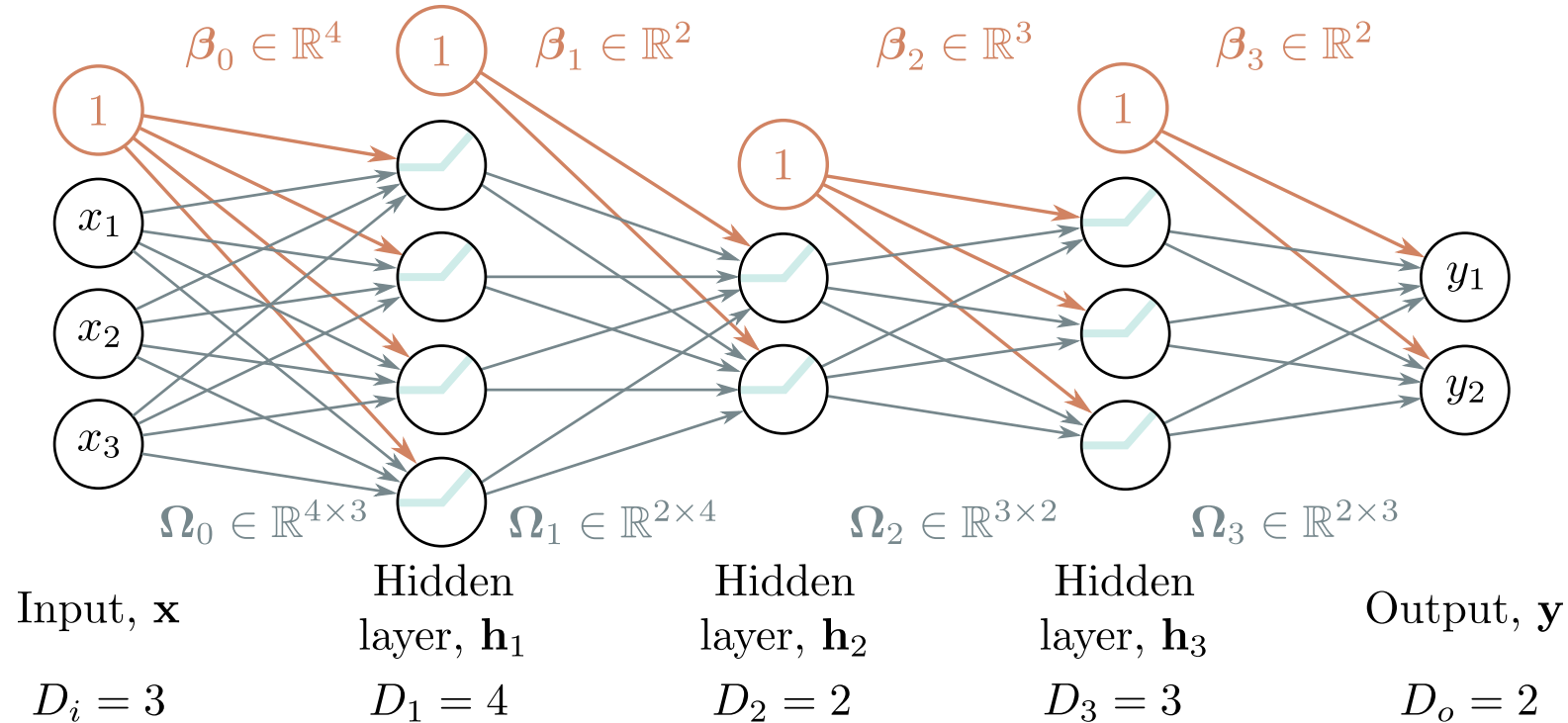
Least squares loss for linear regression

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

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

Partial derivative w.r.t. each parameter

What about deep learning models?



$$\mathbf{h}_1 = \mathbf{a}[\beta_0 + \Omega_0 \mathbf{x}]$$

$$\mathbf{h}_2 = \mathbf{a}[\beta_1 + \Omega_1 \mathbf{h}_1]$$

$$\mathbf{h}_3 = \mathbf{a}[\beta_2 + \Omega_2 \mathbf{h}_2]$$

$$\mathbf{f}[\mathbf{x}, \phi] = \beta_3 + \Omega_3 \mathbf{h}_3$$

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
- Jupyter notebook example of backprop and autograd
- 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

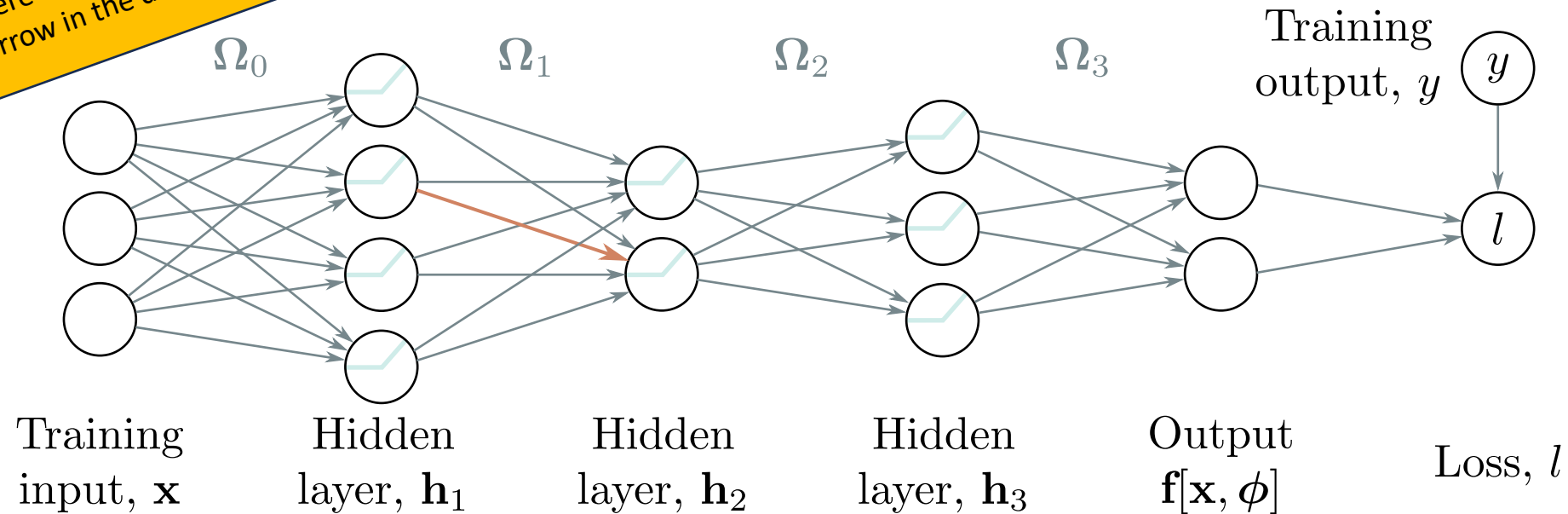
$$\frac{\partial \ell_i}{\partial \beta_k} \quad \text{and} \quad \frac{\partial \ell_i}{\partial \Omega_k}$$

Algorithm to compute gradient efficiently

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

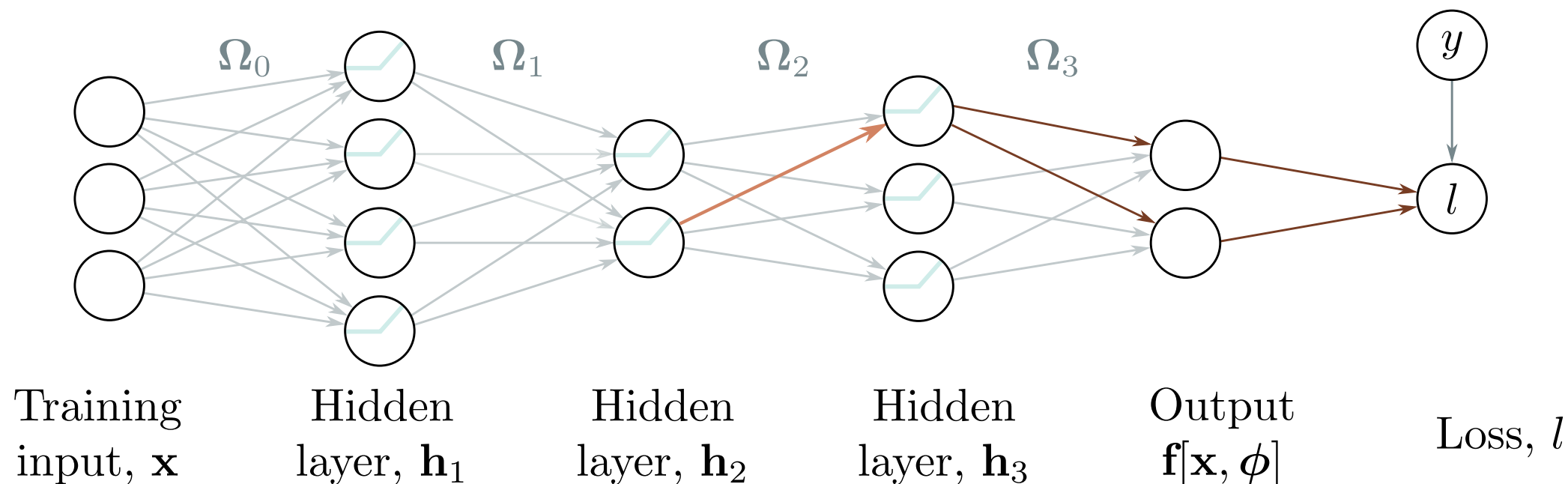
BackProp intuition #1: the forward pass

Remember! There's an implied weight on every arrow in the diagram



- The weight on the orange arrow multiplies activation (ReLU output) of previous layer
- We want to know how change 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.**

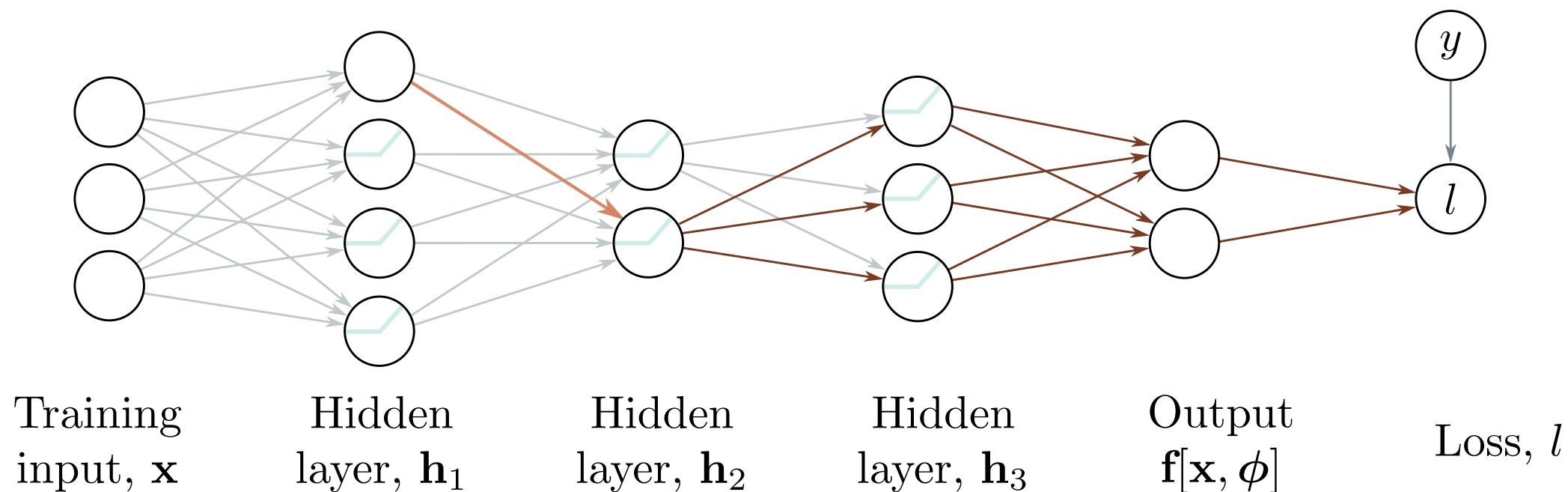
BackProp intuition #2: the backward pass



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



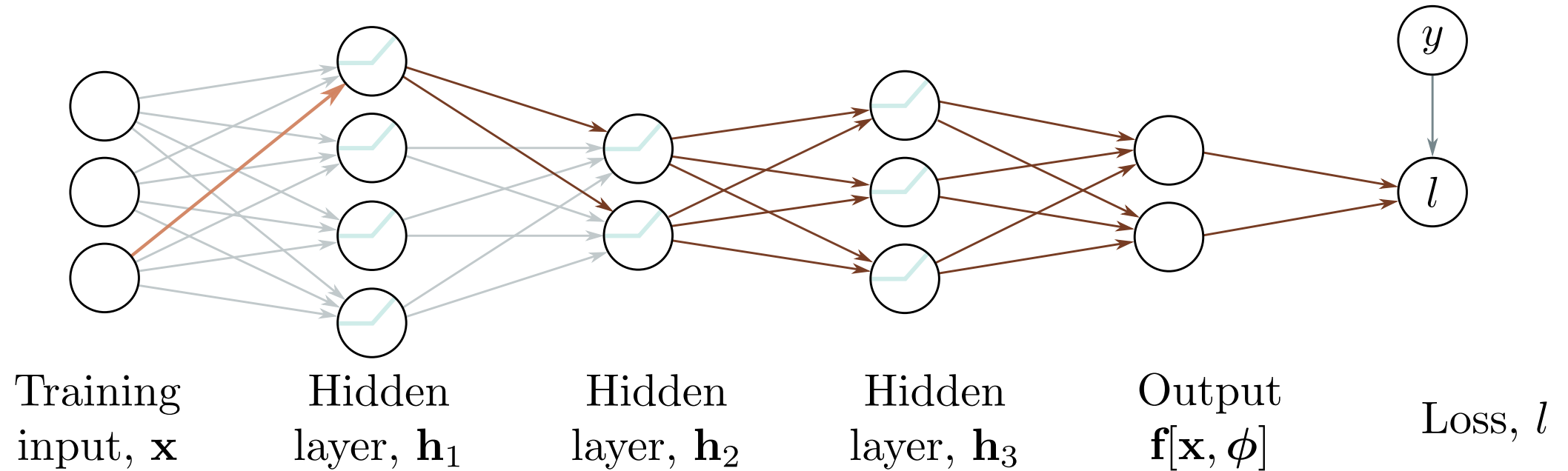
To calculate how a small change in a weight or bias feeding into hidden layer \mathbf{h}_2 modifies the loss, we need to know:

- 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:

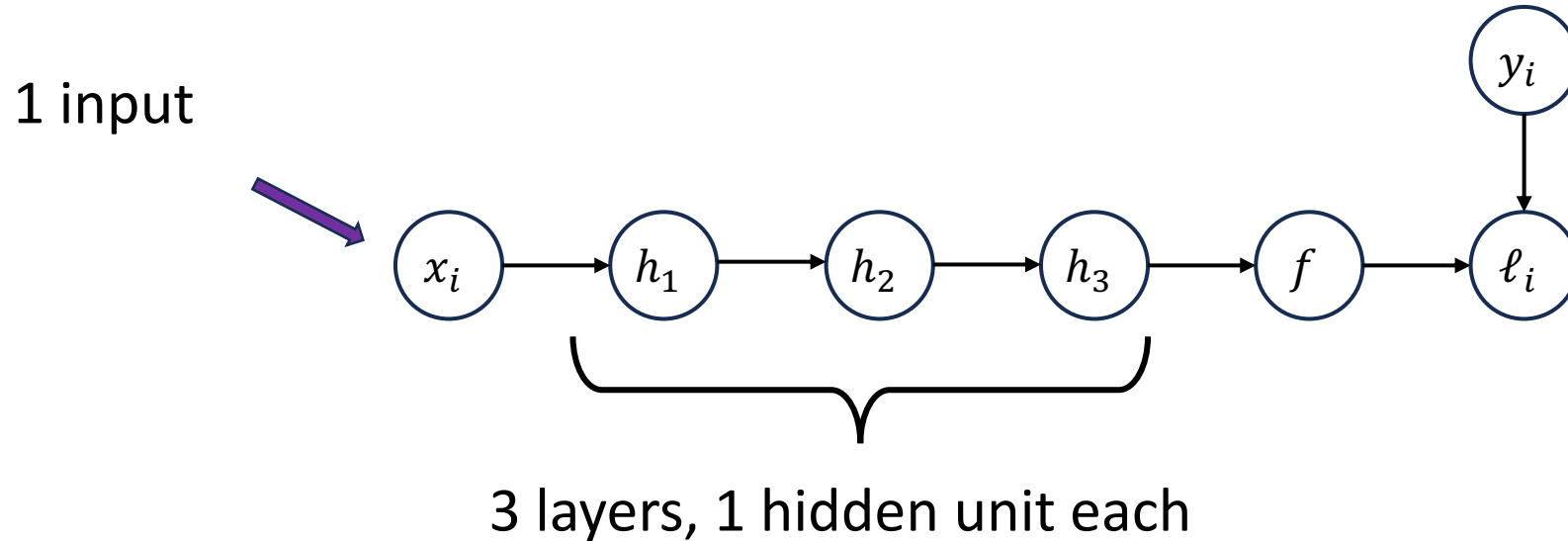
- how a change in layer \mathbf{h}_1 affects \mathbf{h}_2
- how a change in layer \mathbf{h}_2 affects \mathbf{h}_3
- how \mathbf{h}_3 changes the model output \mathbf{f}
- how a change in the model output \mathbf{f} changes the loss l

We know these from the previous steps

Gradients

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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

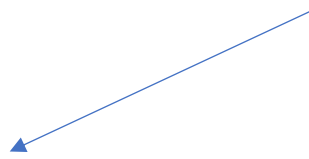
$$f[x_i, \phi] = \beta_3 + \omega_3 \cdot a \left[\beta_2 + \omega_2 \cdot a \left[\beta_1 + \omega_1 \cdot a \left[\beta_0 + \omega_0 \cdot x_i \right] \right] \right]$$

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

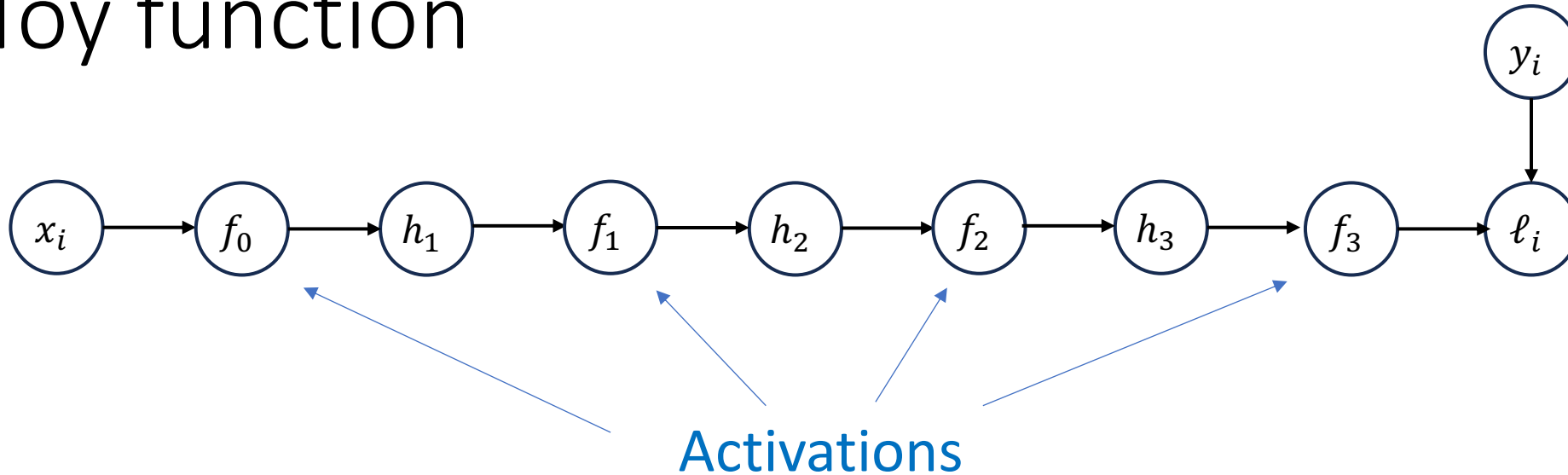
We want to calculate:

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

Tells us how a small change in β_i or ω_i change the loss ℓ_i for the i^{th} example



Toy function



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

$$h_1 = a[f_0]$$

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

$$h_2 = a[f_1]$$

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

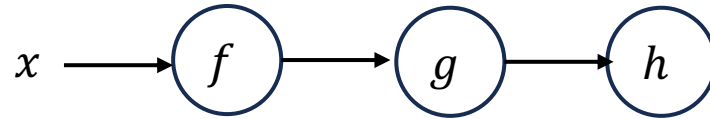
$$h_3 = a[f_2]$$

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

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

Intermediate values

Refresher: The Chain Rule



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

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

Or can be written as

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

Forward pass

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

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

1. Write this as a series of intermediate calculations

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

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

2. Compute these intermediate quantities

$$h_1 = a[f_0]$$

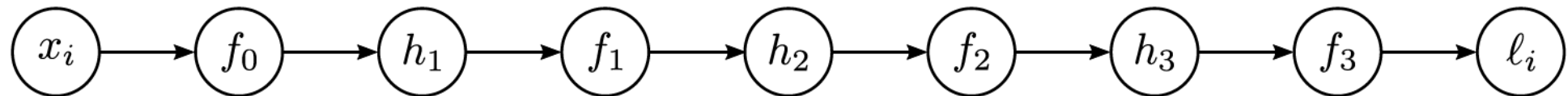
$$h_3 = a[f_2]$$

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

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

$$h_2 = a[f_1]$$

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



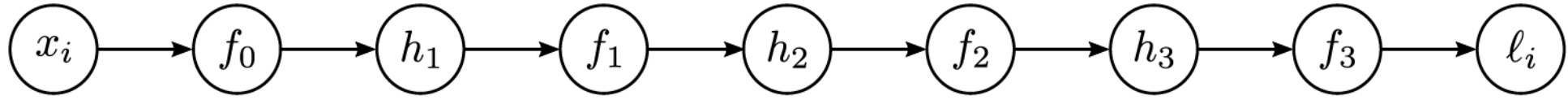
Backward pass

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

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

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

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



Backward pass

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

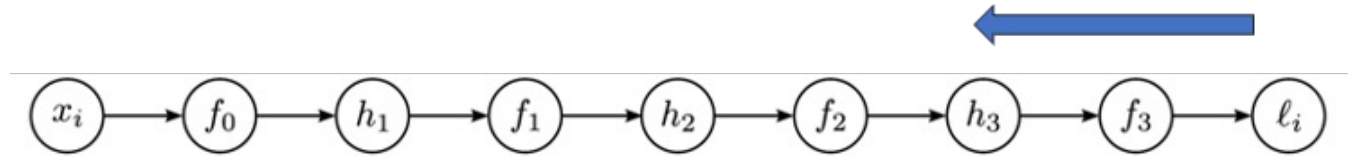
$$\ell_i = (f[x_i, \phi] - y_i)^2$$

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.

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

$$h_1 = a[f_0]$$

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

$$h_2 = a[f_1]$$

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

$$h_3 = a[f_2]$$

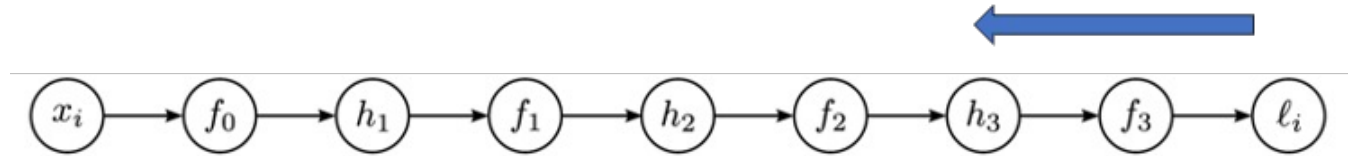
$$f_3 = \beta_3 + \omega_3 \cdot h_3$$

$$l_i = (f_3 - y_i)^2$$

- The first of these derivatives is trivial

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

Backward pass



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

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

$$h_1 = a[f_0]$$

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

$$h_2 = a[f_1]$$

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$$h_3 = a[f_2]$$

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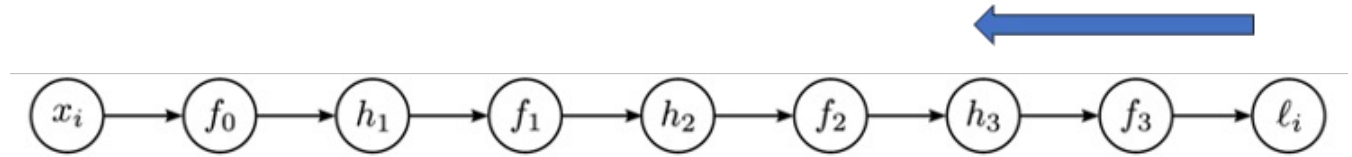
$$l_i = (y_i - f_3)^2$$

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

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

How does a small change in h_3 change l_i ?

Backward pass



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

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

$$h_1 = a[f_0]$$

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

$$h_2 = a[f_1]$$

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

$$h_3 = a[f_2]$$

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

$$l_i = (y_i - f_3)^2$$

- The second derivative is computed via the chain rule

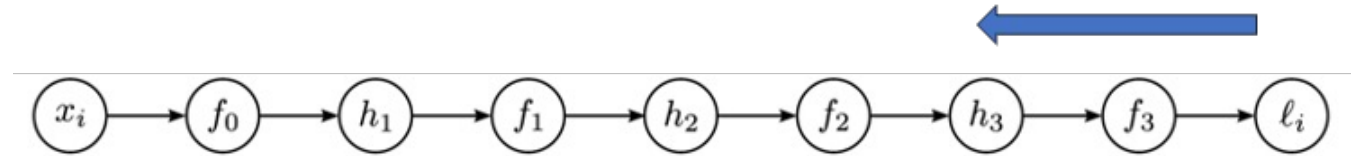
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How does a small change in h_3 change l_i ?

How does a small change in h_3 change f_3 ?

How does a small change in f_3 change l_i ?

Backward pass



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

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

$$h_1 = a[f_0]$$

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$$h_3 = a[f_2]$$

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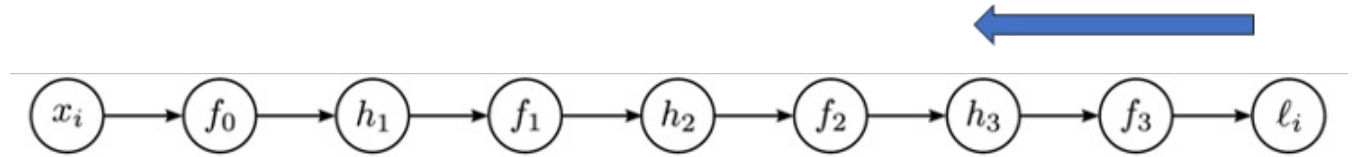
$$l_i = (y_i - f_3)^2$$

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

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

Already computed!

Backward pass



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

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

$$h_1 = a[f_0]$$

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

$$h_2 = a[f_1]$$

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

$$h_3 = a[f_2]$$

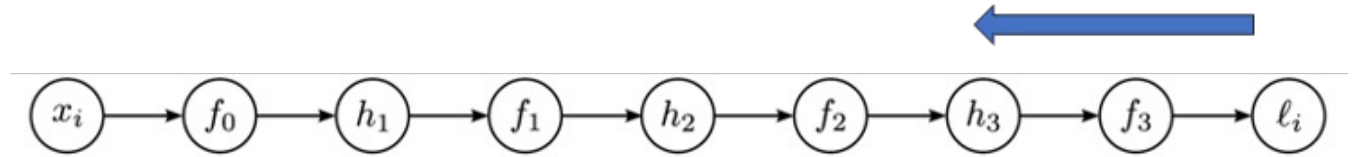
$$f_3 = \beta_3 + \omega_3 \cdot h_3$$

$$l_i = (y_i - f_3)^2$$

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

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

Backward pass



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

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

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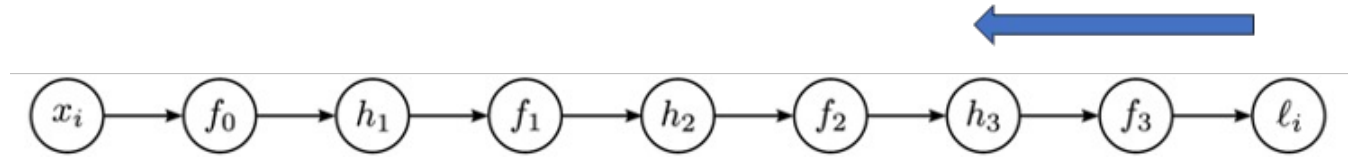
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Already computed!

Backward pass



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

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

$$h_1 = a[f_0]$$

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

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$$h_3 = a[f_2]$$

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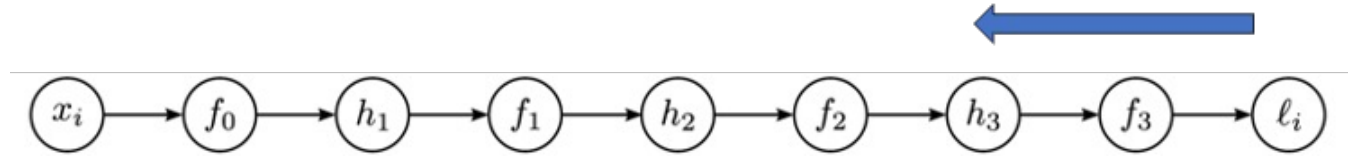
$$l_i = (y_i - f_3)^2$$

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

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Backward pass



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

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

$$h_1 = a[f_0]$$

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

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

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

$$l_i = (y_i - f_3)^2$$

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

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

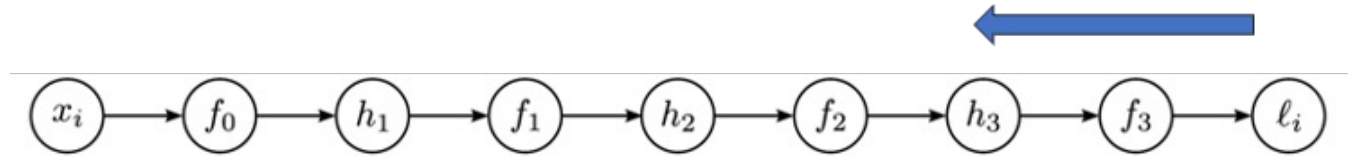
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$$\frac{\partial l_i}{\partial f_0} = \frac{\partial h_1}{\partial f_0} \left(\frac{\partial f_1}{\partial h_1} \frac{\partial h_2}{\partial f_1} \frac{\partial f_2}{\partial h_2} \frac{\partial h_3}{\partial f_2} \frac{\partial f_3}{\partial h_3}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

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

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

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

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Backward pass

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

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

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

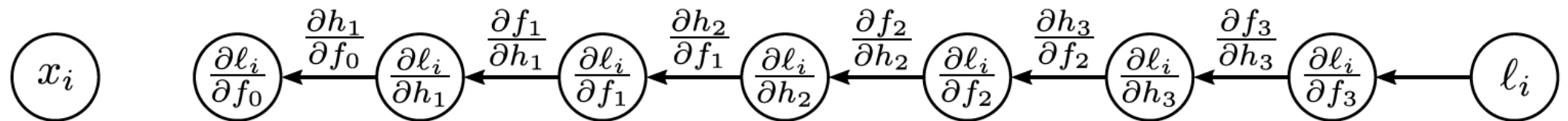
$$\frac{\partial l_i}{\partial f_2} = \frac{\partial h_3}{\partial f_2} \left(\frac{\partial f_3}{\partial h_3} \frac{\partial l_i}{\partial f_3} \right)$$

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

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

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

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



We extend this to get to the parameters ω 's and β 's

Backward pass

2. Find how the loss changes as a function of the parameters β and ω .

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

$$h_1 = a[f_0]$$

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

$$h_2 = a[f_1]$$

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

$$h_3 = a[f_2]$$

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

$$l_i = (y_i - f_3)^2$$

- Another application of the chain rule

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

How does a small change in ω_k change l_i ?

How does a small change in ω_k change f_k ?

How does a small change in f_k change l_i ?

Backward pass

2. Find how the loss changes as a function of the parameters β and ω .

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

$$h_1 = a[f_0]$$

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

$$h_2 = a[f_1]$$

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

$$h_3 = a[f_2]$$

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

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

- 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 ω_k change ℓ_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 β and ω .

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

$$h_1 = a[f_0]$$

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

$$h_2 = a[f_1]$$

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

$$h_3 = a[f_2]$$

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

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

- Another application of the chain rule
- Similarly for β parameters

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

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

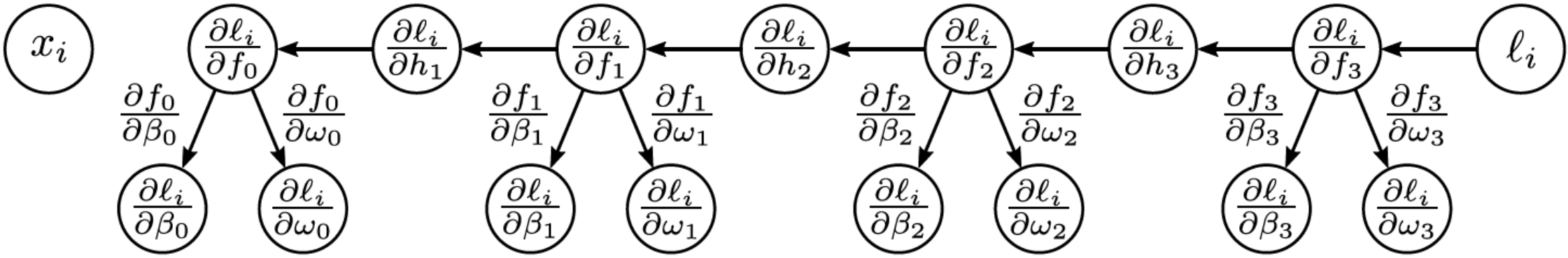
1

Backward pass

2. Find how the loss changes as a function of the parameters β and ω .

$$\begin{aligned} f_0 &= \beta_0 + \omega_0 \cdot x \\ h_1 &= a[f_0] \\ f_1 &= \beta_1 + \omega_1 \cdot h_1 \\ h_2 &= a[f_1] \end{aligned}$$

$$\begin{aligned} f_2 &= \beta_2 + \omega_2 \cdot h_2 \\ h_3 &= a[f_2] \\ f_3 &= \beta_3 + \omega_3 \cdot h_3 \\ \ell_i &= (y_i - f_3)^2 \end{aligned}$$

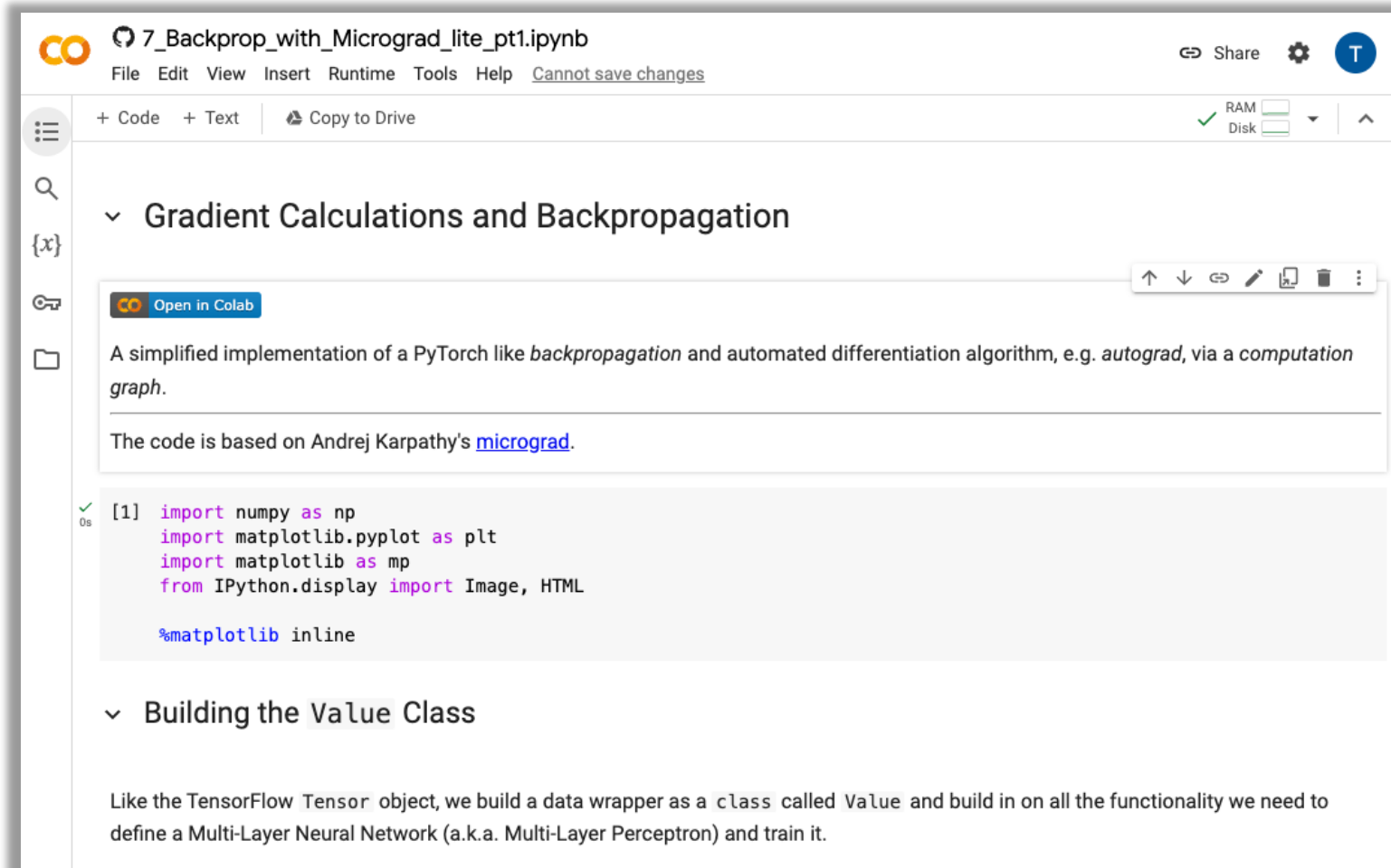


Gradients

- Backpropagation intuition
- Toy model
- [Jupyter notebook example of backprop and autograd](#)
- Matrix calculus
- Backpropagation matrix forward pass
- Backpropagation matrix backward pass

Jupyter Notebook Example

[7 Backprop with Micrograd lite pt1.ipynb](#)



7_Backprop_with_Micrograd_lite_pt1.ipynb

File Edit View Insert Runtime Tools Help [Cannot save changes](#)

+ Code + Text Copy to Drive

RAM Disk

Gradient Calculations and Backpropagation

[Open in Colab](#)

A simplified implementation of a PyTorch like *backpropagation* and automated differentiation algorithm, e.g. *autograd*, via a *computation graph*.

The code is based on Andrej Karpathy's [micrograd](#).

```
[1] import numpy as np
import matplotlib.pyplot as plt
import matplotlib as mp
from IPython.display import Image, HTML

%matplotlib inline
```

Building the Value Class

Like the TensorFlow `Tensor` object, we build a data wrapper as a `class` called `Value` and build in on all the functionality we need to define a Multi-Layer Neural Network (a.k.a. Multi-Layer Perceptron) and train it.

Gradients

- Backpropagation intuition
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- **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}

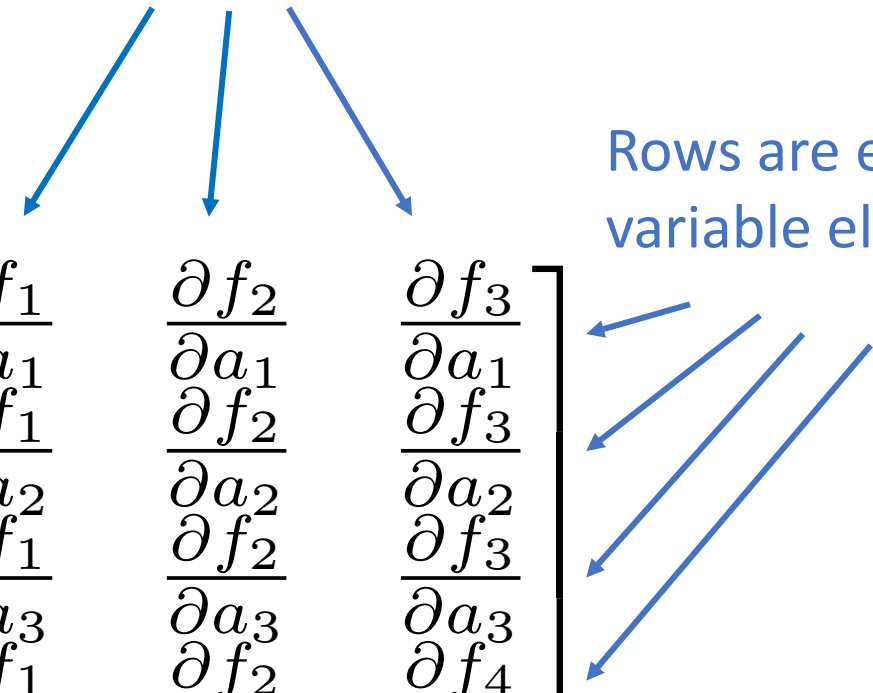
$$\mathbf{f} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} \quad \mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix}$$

Vector of scalar
valued functions

Columns are each
element function

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

Rows are each
variable element



Comparing vector and matrix

Scalar derivatives:

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

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

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:

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

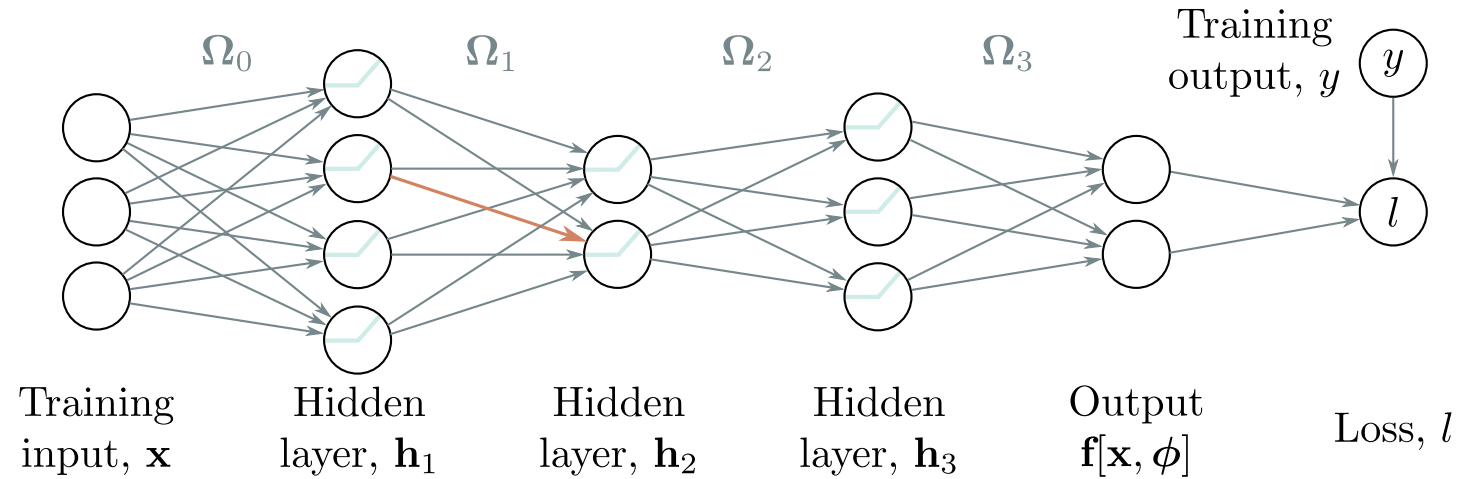
Matrix derivatives:

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

Gradients

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The forward pass



1. Write this as a series of intermediate calculations

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

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

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

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

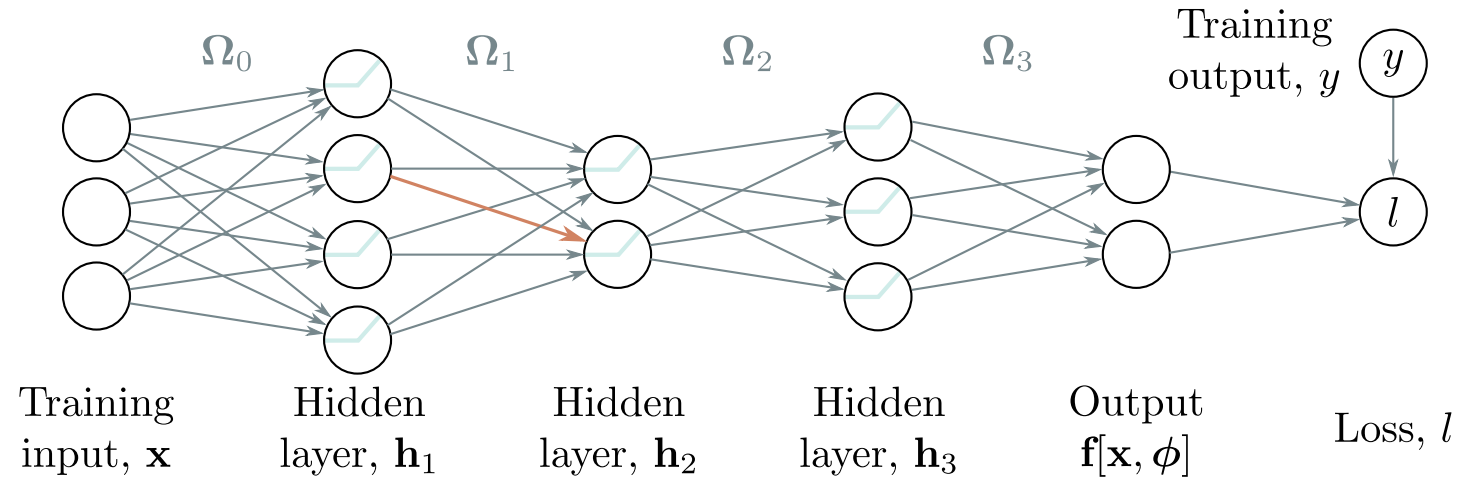
$$\mathbf{f}_2 = \beta_2 + \Omega_2 \mathbf{h}_2$$

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

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

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

The forward 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

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

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

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

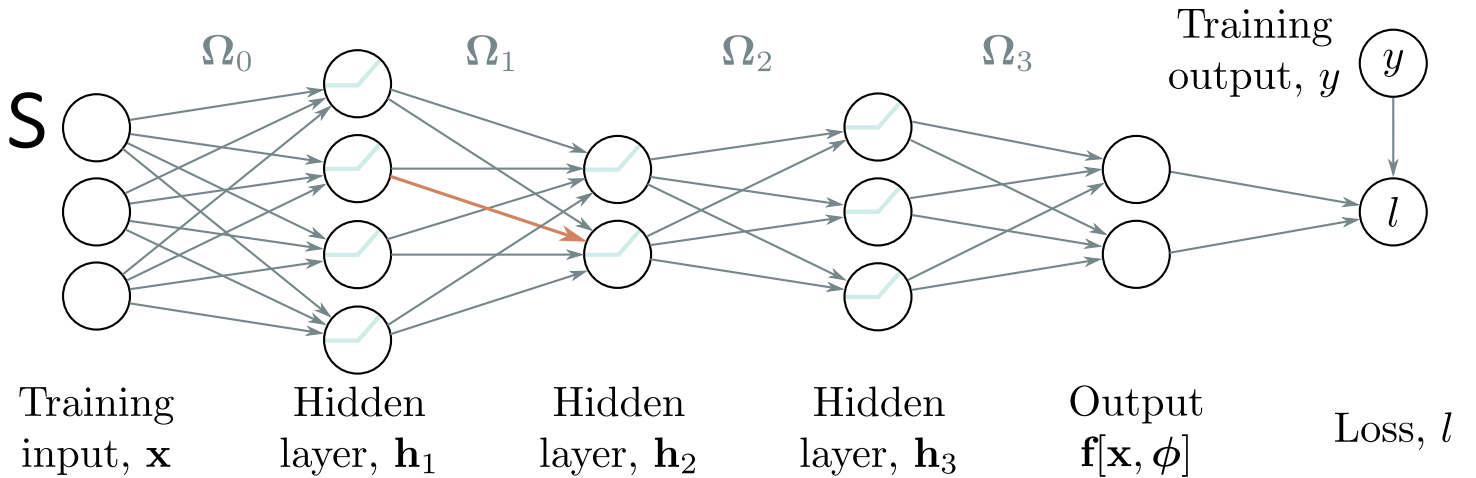
$$\mathbf{f}_2 = \beta_2 + \Omega_2 \mathbf{h}_2$$

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

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

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

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

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

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

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

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

3. Take derivatives of output with respect to intermediate quantities

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

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

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

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

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

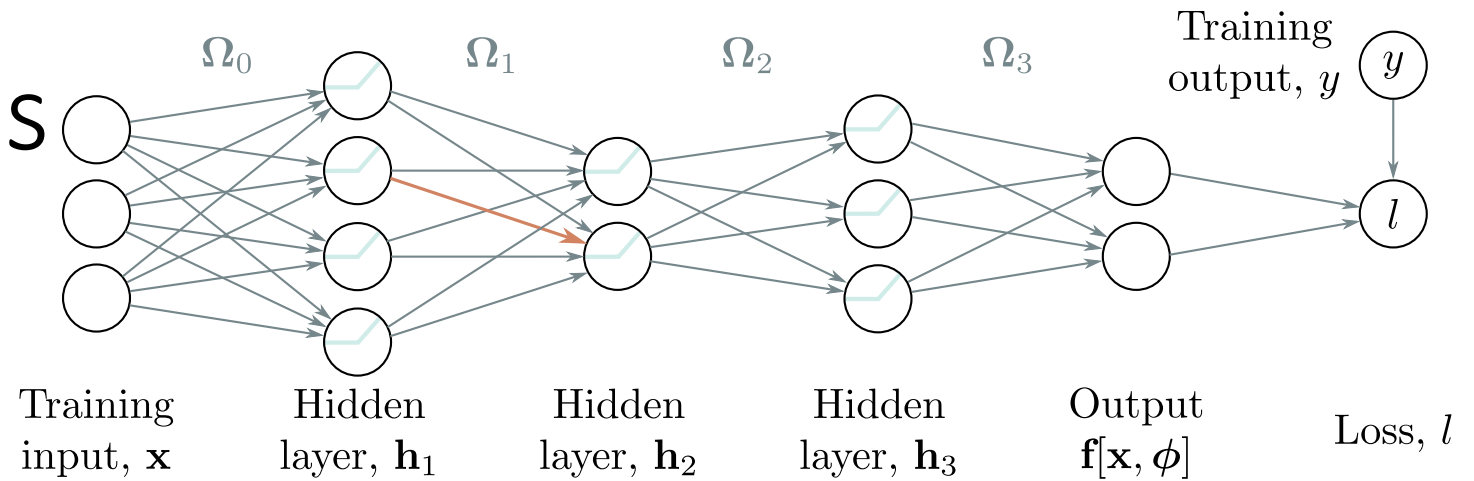
$$\frac{\partial l_i}{\partial \mathbf{f}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \left(\frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial l_i}{\partial \mathbf{f}_3}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

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

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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

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

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

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

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

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

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

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

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

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

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

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

Yikes!

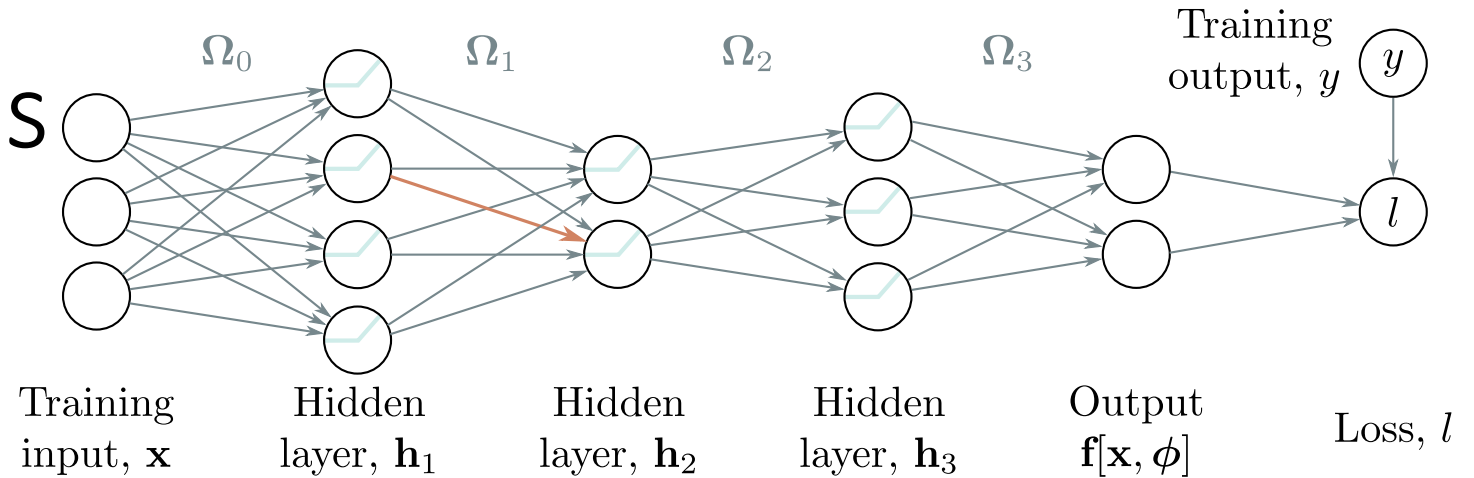
- But:

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

- 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

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

2. Compute these intermediate quantities

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

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

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

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

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

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

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

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

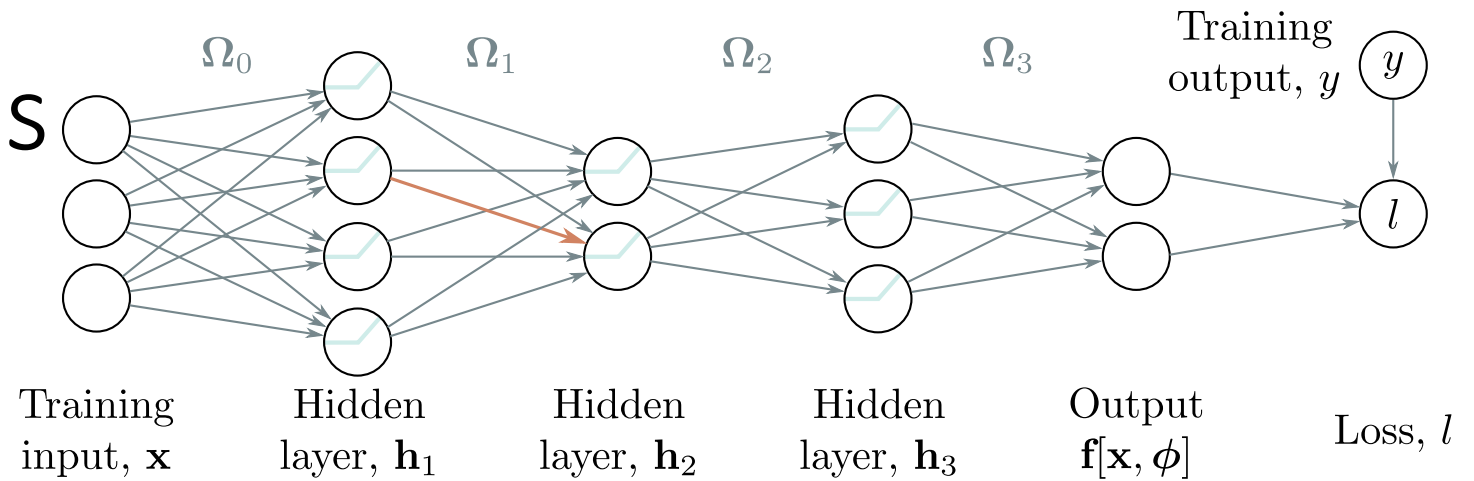
$$\frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} = \frac{\partial}{\partial \mathbf{h}_3} (\beta_3 + \mathbf{\Omega}_3 \mathbf{h}_3) = \mathbf{\Omega}_3^T$$

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

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

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

The backward pass



1. Write this as a series of intermediate calculations

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

2. Compute these intermediate quantities

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

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

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

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

3. Take derivatives of output with respect to intermediate quantities

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

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

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

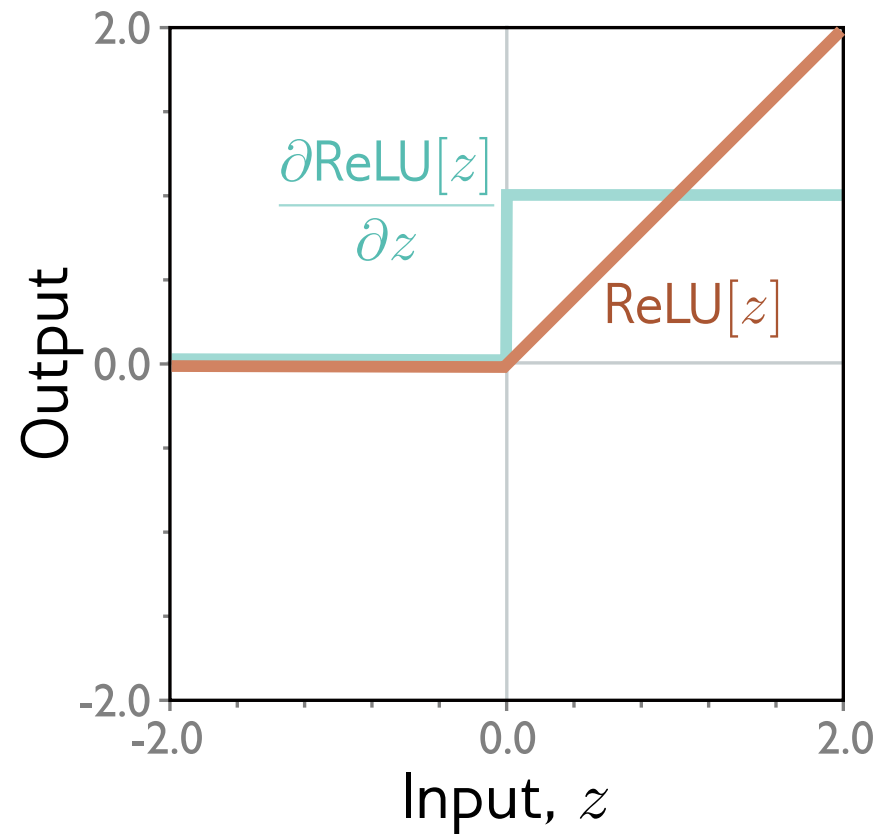
$$\frac{\partial l_i}{\partial \mathbf{f}_3}$$

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

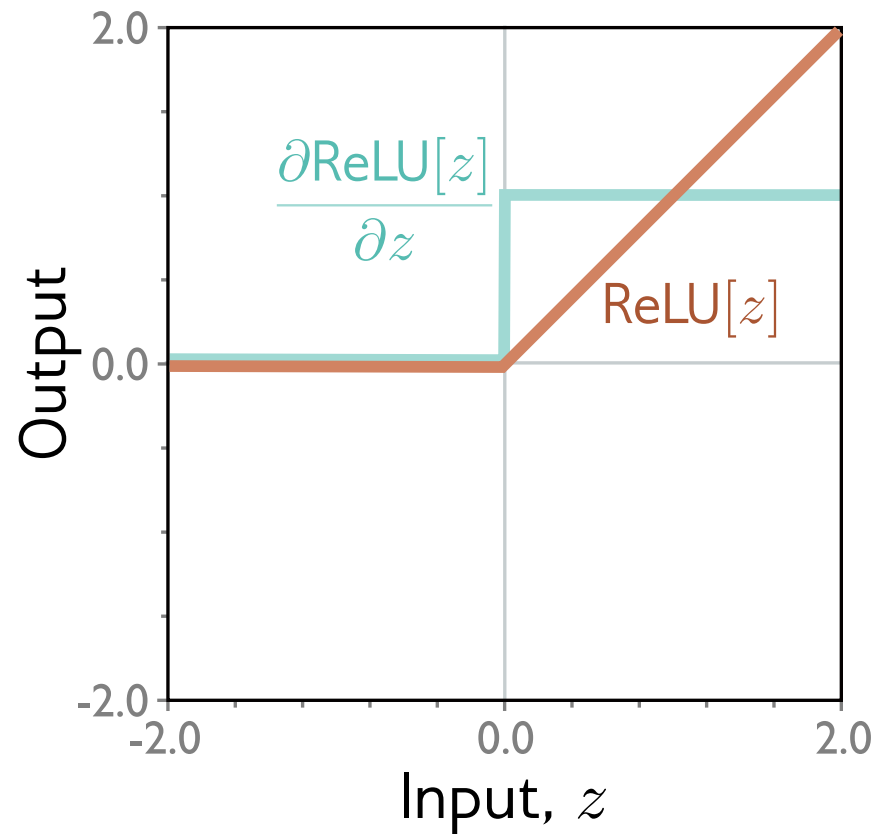
$$\frac{\partial l_i}{\partial \mathbf{f}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \left(\frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial l_i}{\partial \mathbf{f}_3}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

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

Derivative of ReLU



Derivative of ReLU



$$\mathbb{I}[z > 0]$$

“Indicator function”

Derivative of ReLU

1. Consider:

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

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:

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

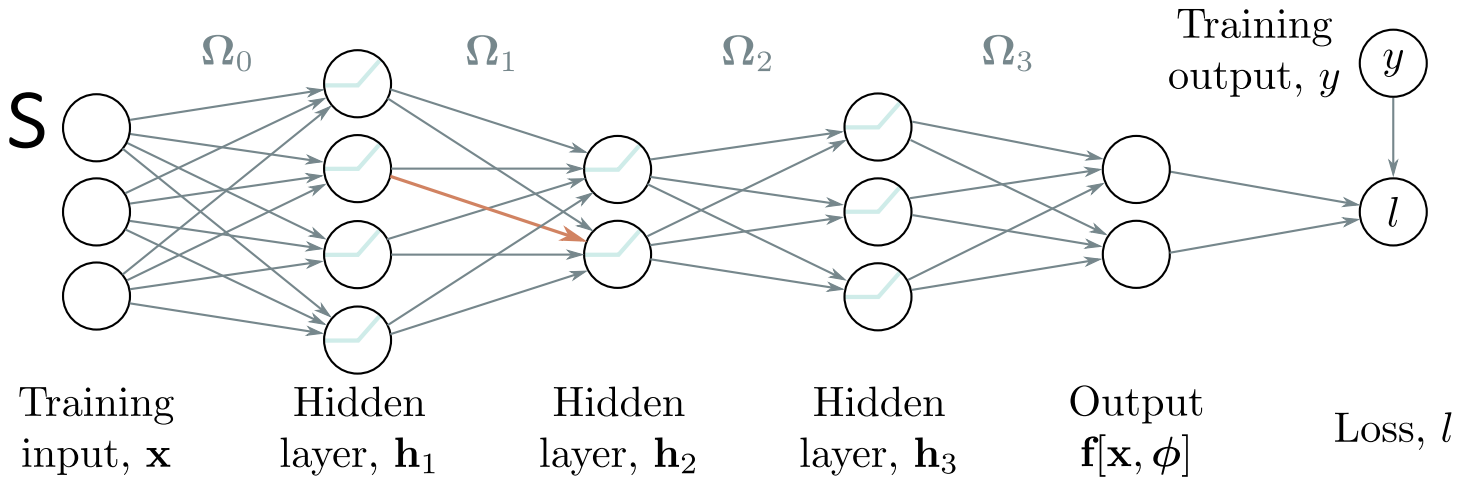
3. Taking the derivative

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

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

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

2. Compute these intermediate quantities

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

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

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

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

3. Take derivatives of output with respect to intermediate quantities

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

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

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

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

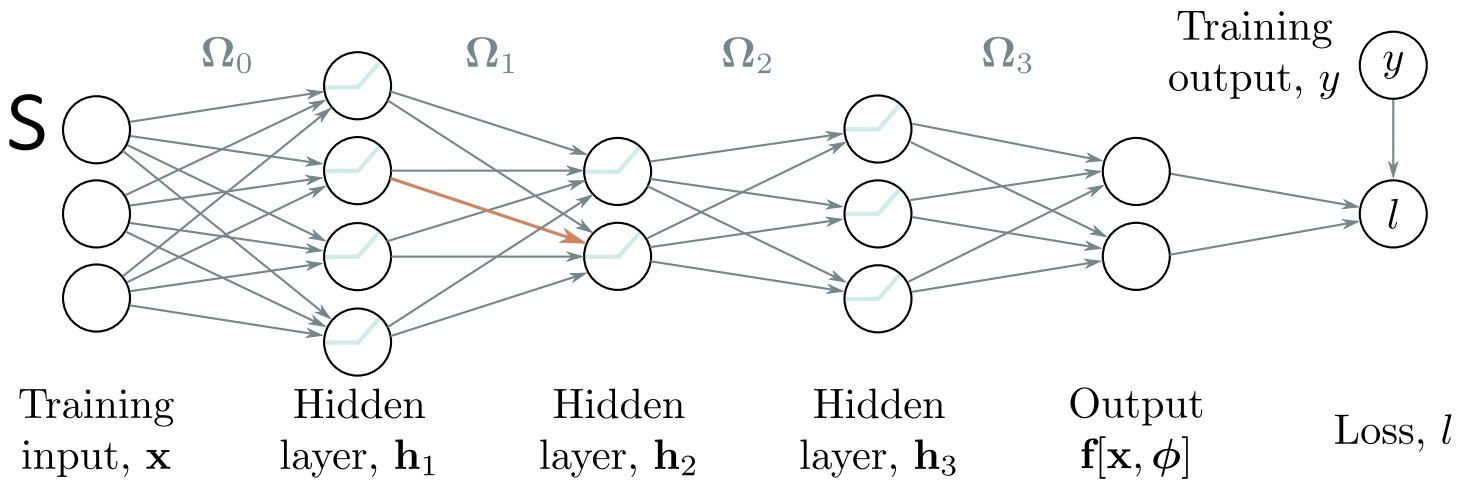
$$\frac{\partial l_i}{\partial \mathbf{f}_2} = \frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial l_i}{\partial \mathbf{f}_3}$$

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

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

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

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

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

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

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

3. Take derivatives of output with respect to intermediate quantities

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

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

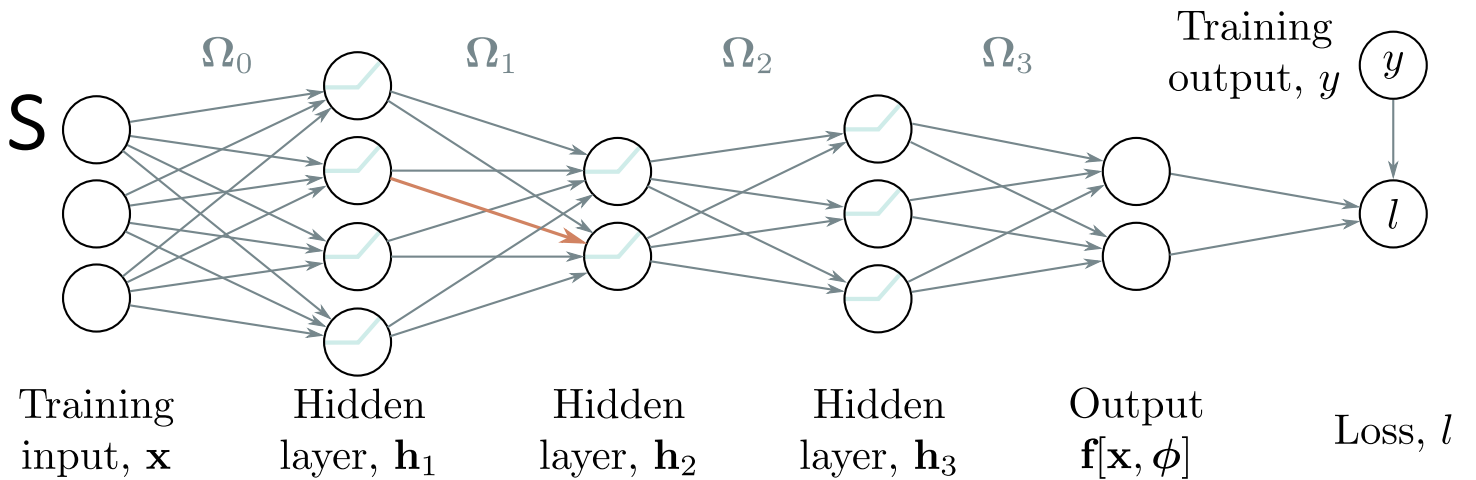
4. Take derivatives w.r.t. parameters

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

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

$$\begin{aligned} \frac{\partial l_i}{\partial \beta_k} &= \frac{\partial \mathbf{f}_k}{\partial \beta_k} \frac{\partial l_i}{\partial \mathbf{f}_k} \\ &= \frac{\partial}{\partial \beta_k} (\beta_k + \Omega_k \mathbf{h}_k) \frac{\partial l_i}{\partial \mathbf{f}_k} \\ &= \frac{\partial l_i}{\partial \mathbf{f}_k}, \end{aligned}$$

The backward pass



1. Write this as a series of intermediate calculations

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

2. Compute these intermediate quantities

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

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

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

3. Take derivatives of output with respect to intermediate quantities

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

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

4. Take derivatives w.r.t. parameters

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

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

$$\begin{aligned} \frac{\partial l_i}{\partial \mathbf{\Omega}_k} &= \frac{\partial \mathbf{f}_k}{\partial \mathbf{\Omega}_k} \frac{\partial l_i}{\partial \mathbf{f}_k} \\ &= \frac{\partial}{\partial \mathbf{\Omega}_k} (\beta_k + \mathbf{\Omega}_k \mathbf{h}_k) \frac{\partial l_i}{\partial \mathbf{f}_k} \\ &= \frac{\partial l_i}{\partial \mathbf{f}_k} \mathbf{h}_k^T \end{aligned}$$

Gradients

- Backpropagation intuition
- Toy model
- Jupyter notebook example of backprop and autograd
- 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?

