BOSTON UNIVERSITY

Deep Learning for Data Science
DS 542

https://dl4ds.github.io/sp2026/

Backpropagation

Plan for Today

- Motivation for backpropagation
- Intuition for backpropagation
- Toy model
- Matrix calculus
- Neural network forward pass
- Neural network backward pass

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:

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

or for short:

$$L\left[\phi\right]$$

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:

$$\frac{\partial L}{\partial \phi} = \begin{bmatrix} \frac{\partial L}{\partial \phi_0} \\ \frac{\partial L}{\partial \phi_1} \\ \vdots \\ \frac{\partial L}{\partial \phi_N} \end{bmatrix}.$$

Also notated as $\nabla_w L$

Step 2. Update the parameters according to the rule:

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

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.

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

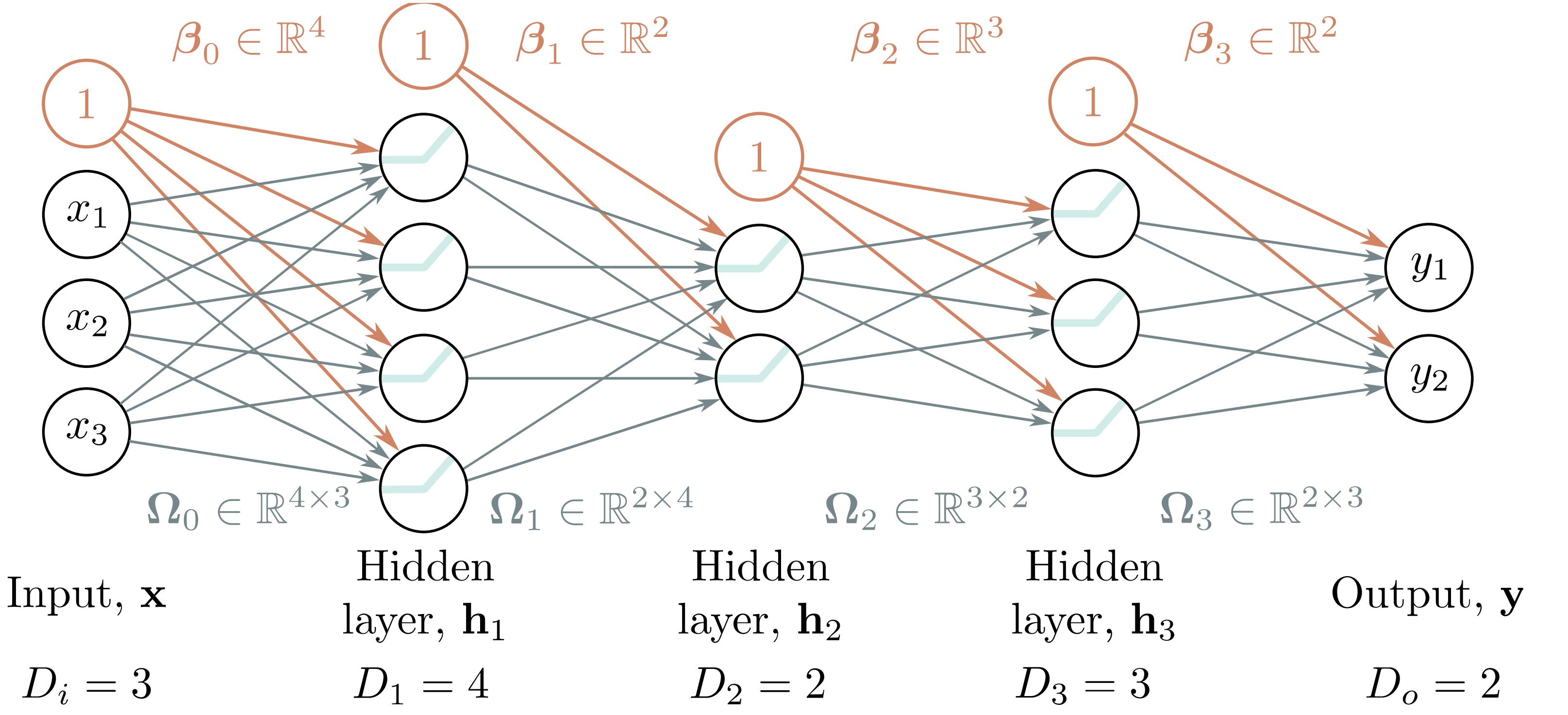
Least squares loss for linear regression

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

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

Partial derivative w.r.t. each parameter

What about deep learning models?



$$
\begin{aligned}
\mathbf{h}_1 &= \mathbf{a}[\boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}] \\
\mathbf{h}_2 &= \mathbf{a}[\boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1] \\
\mathbf{h}_3 &= \mathbf{a}[\boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2] \\
\mathbf{f}[\mathbf{x}, \boldsymbol{\phi}] &= \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3
\end{aligned}
$$

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

Loss: sum of individual terms:

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

SGD Algorithm:

$$\boldsymbol{\phi}_{t+1} \longleftarrow \boldsymbol{\phi}_t - \alpha \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}$$

Millions and even *billions* of parameters:

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

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

$$\frac{\partial \ell_i}{\partial \boldsymbol{\beta}_k} \qquad \text{and} \qquad \frac{\partial \ell_i}{\partial \boldsymbol{\Omega}_k}$$

Network equation gets unwieldy even for small models

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

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

1st hidden layer

2nd hidden layer

Don’t We Have Auto Grad?

- The backpropagation formulas for gradients are going to guide us to better initializations next lecture.

- Many problems with neural network training are due to poor gradient management.

Gradients

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

Problem 1: Computing gradients

Loss: sum of individual terms:

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

SGD Algorithm:

$$\boldsymbol{\phi}_{t+1} \longleftarrow \boldsymbol{\phi}_t - \alpha \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i[\boldsymbol{\phi}_t]}{\partial \boldsymbol{\phi}}$$

Parameters:

$$\boldsymbol{\phi} = \{\boldsymbol{\beta}_0, \boldsymbol{\Omega}_0, \boldsymbol{\beta}_1, \boldsymbol{\Omega}_1, \boldsymbol{\beta}_2, \boldsymbol{\Omega}_2, \boldsymbol{\beta}_3, \boldsymbol{\Omega}_3\}$$

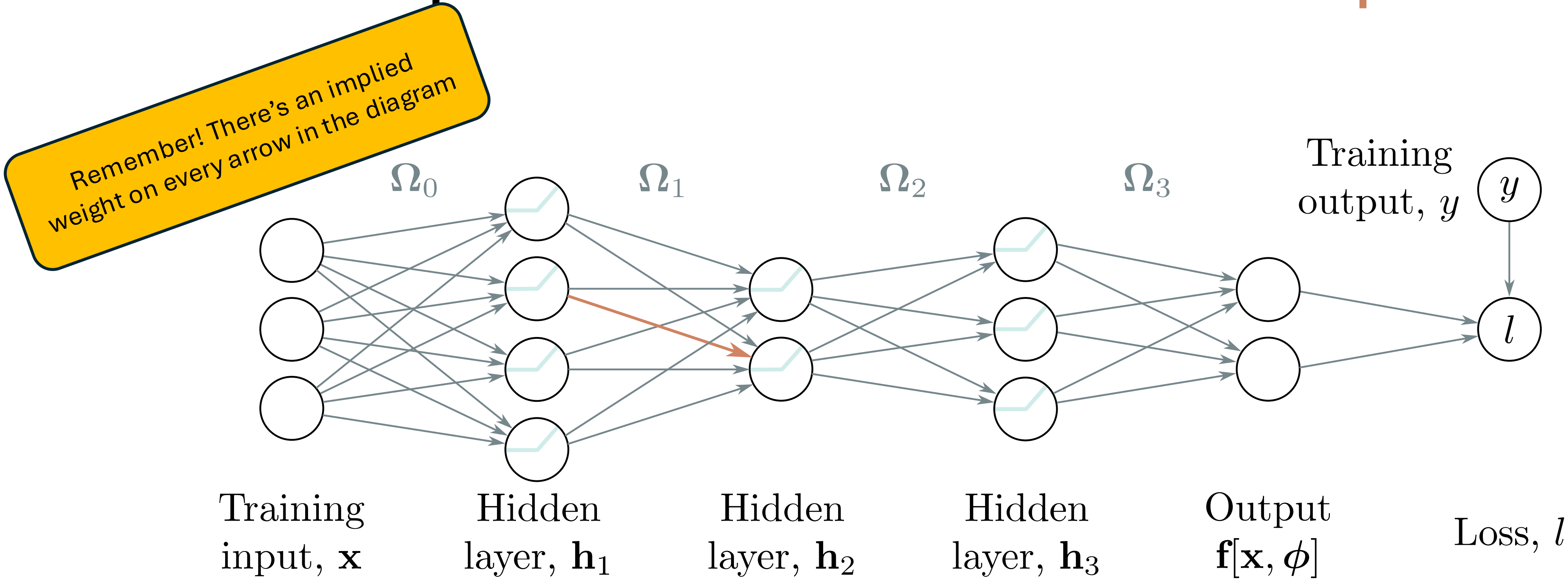
Need to compute gradients

$$\frac{\partial \ell_i}{\partial \boldsymbol{\beta}_k} \quad \text{and} \quad \frac{\partial \ell_i}{\partial \boldsymbol{\Omega}_k}$$

Algorithm to compute gradient efficiently

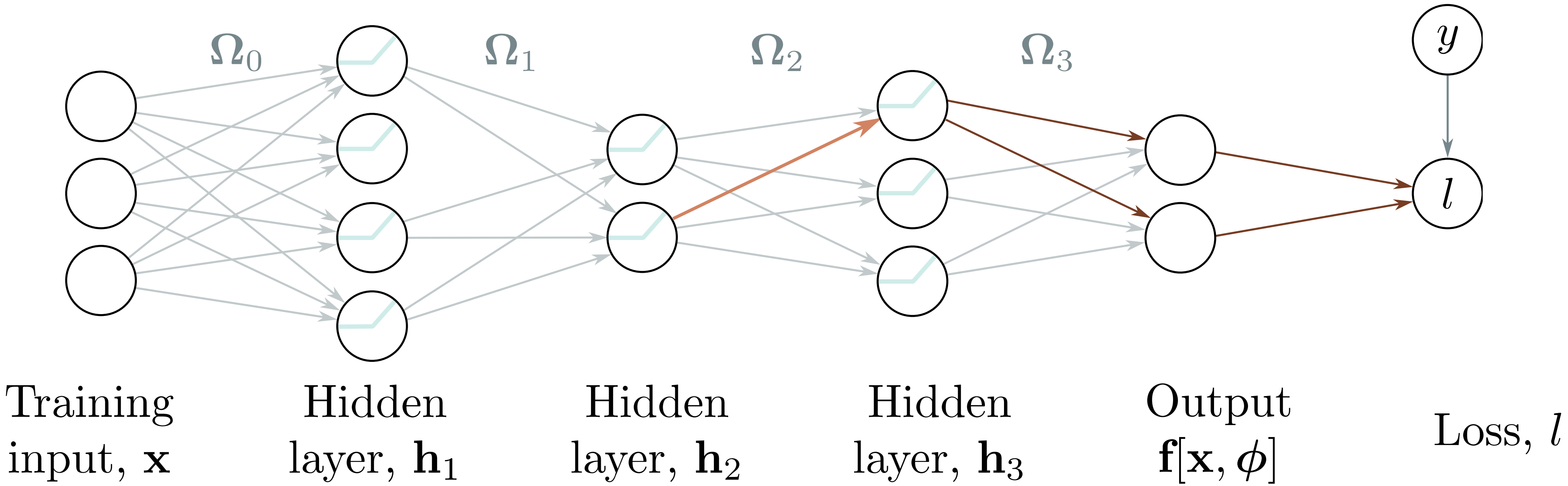
- “Backpropagation algorithm”
- Rumelhart, Hinton, and Williams (1986)

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

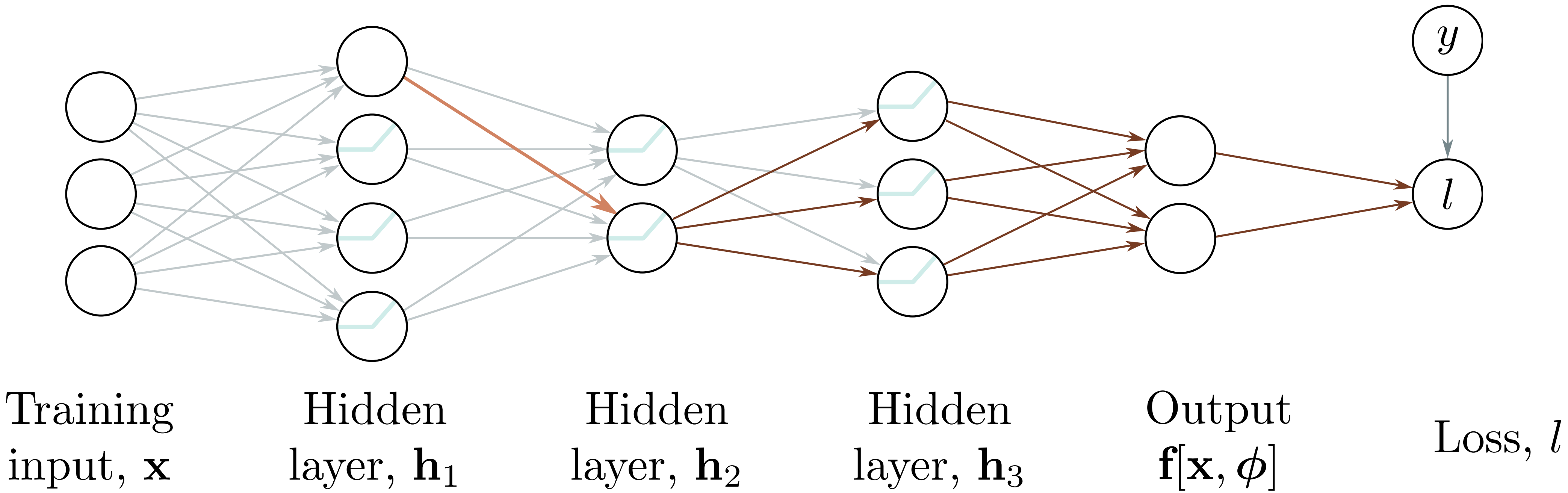
BackProp intuition #2: the backward pass



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

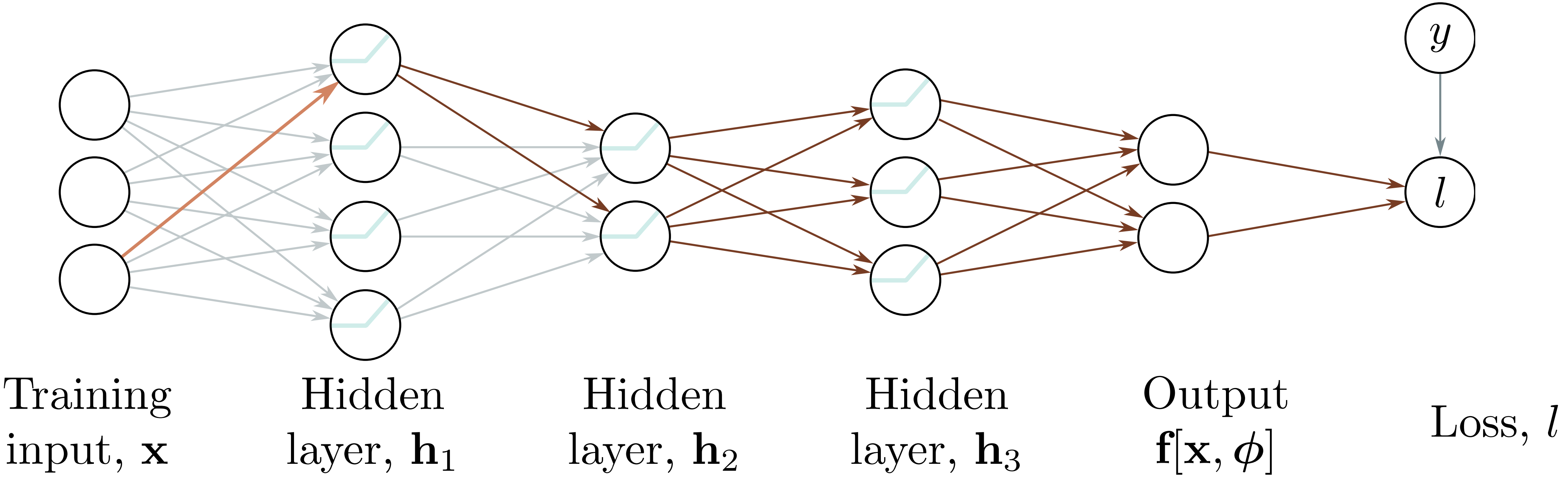


To calculate how a small change in a weight or bias feeding into hidden layer $\mathbf{h}_2$ modifies the loss, we need to know:

- 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

- Backpropagation intuition
- Toy model
- Matrix calculus
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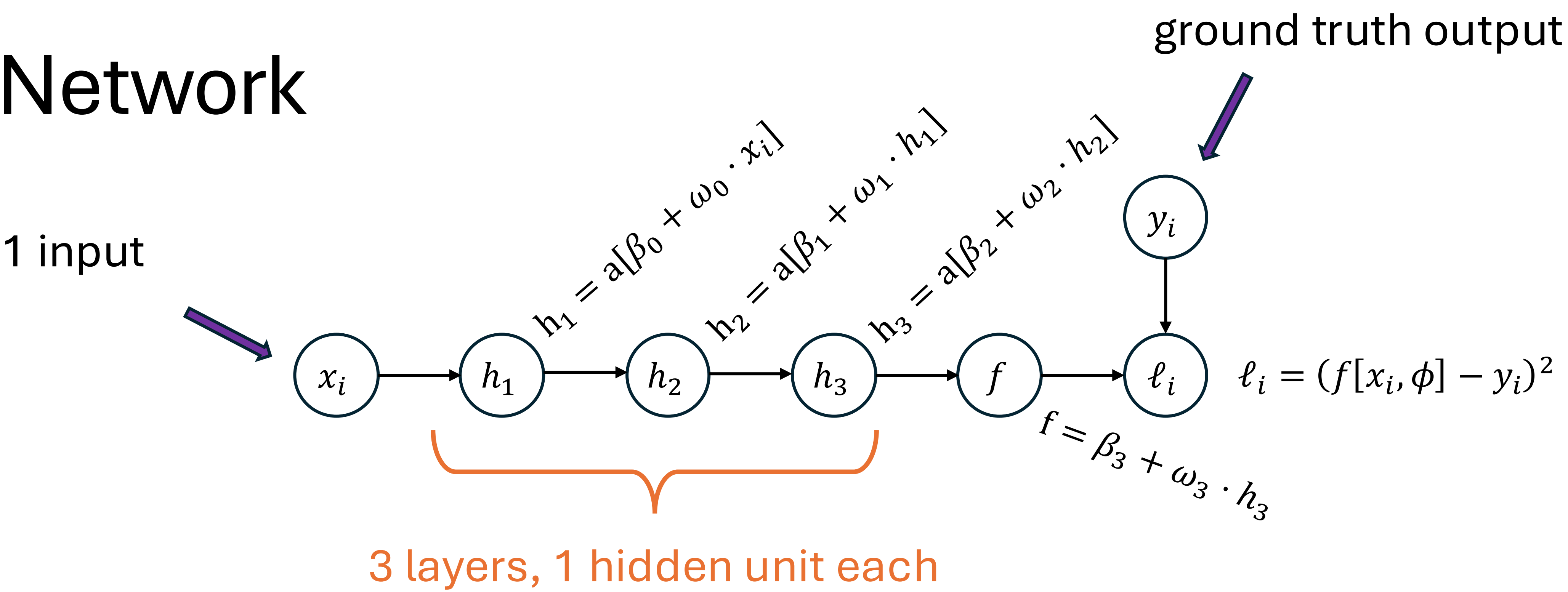
Toy Network



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

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

Gradients of toy function

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

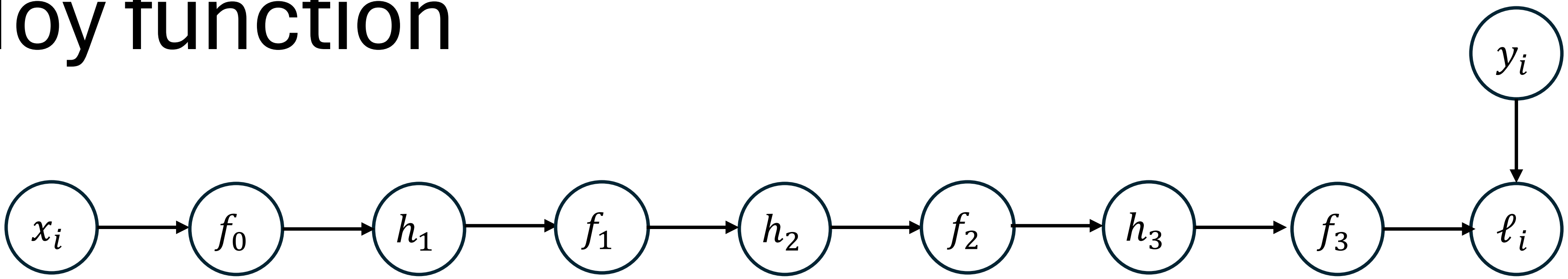
$$\ell_i = (f[x_i, \phi] - y_i)^2$$

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

We want to calculate each partial:

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

Toy function



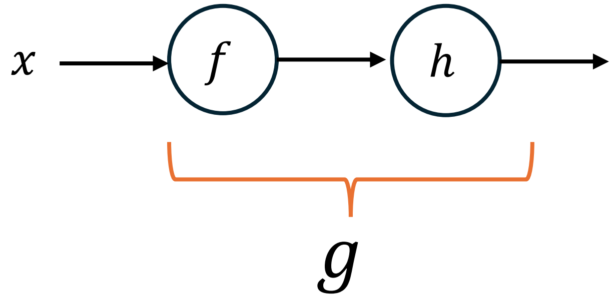
Pre-Activations

$$f_0 = \beta_0 + \omega_0 \cdot x$$
$$h_1 = \mathrm{a}[f_0]$$
$$f_1 = \beta_1 + \omega_1 \cdot h_1$$
$$h_2 = \mathrm{a}[f_1]$$

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

Intermediate values

Refresher: The Chain Rule



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

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

Lagrange's Notation

Or can be written equivalently as

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

Leibniz's Notation

Forward pass

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

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

1. Write this as a series of intermediate calculations

2. Compute these intermediate quantities

$$f_0 = \beta_0 + \omega_0 \cdot x_i$$
$$h_1 = \mathrm{a}[f_0]$$
$$f_1 = \beta_1 + \omega_1 \cdot h_1$$
$$h_2 = \mathrm{a}[f_1]$$

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

$$x_i \rightarrow f_0 \rightarrow h_1 \rightarrow f_1 \rightarrow h_2 \rightarrow f_2 \rightarrow h_3 \rightarrow f_3 \rightarrow \ell_i$$

Backward pass

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

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

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

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

$$x_i \rightarrow f_0 \rightarrow h_1 \rightarrow f_1 \rightarrow h_2 \rightarrow f_2 \rightarrow h_3 \rightarrow f_3 \rightarrow \ell_i$$

Backward pass

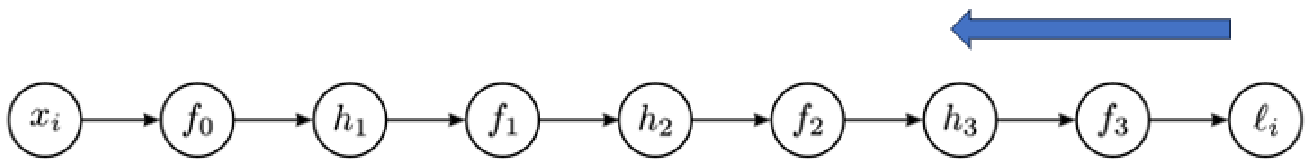
$$\mathrm{f}[x_i, \phi] = \beta_3 + \omega_3 \cdot \mathrm{a}\Big[\beta_2 + \omega_2 \cdot \mathrm{a}\big[\beta_1 + \omega_1 \cdot \mathrm{a}[\beta_0 + \omega_0 \cdot x_i]\big]\Big]$$

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

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.

$$f_0 = \beta_0 + \omega_0 \cdot x$$
$$h_1 = \mathrm{a}[f_0]$$
$$f_1 = \beta_1 + \omega_1 \cdot h_1$$
$$h_2 = \mathrm{a}[f_1]$$

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

- The first of these derivatives is trivial

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

Backward pass

$$x_i \rightarrow f_0 \rightarrow h_1 \rightarrow f_1 \rightarrow h_2 \rightarrow f_2 \rightarrow h_3 \rightarrow f_3 \rightarrow \ell_i$$

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

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

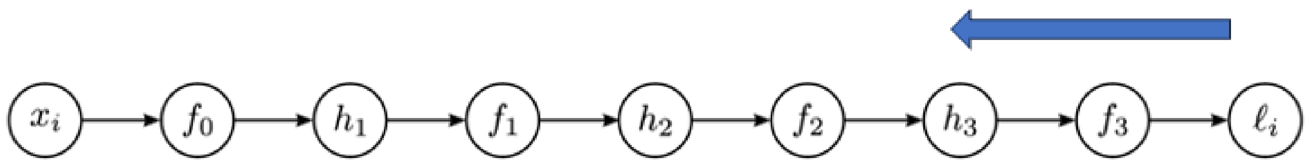
$$\begin{aligned}
f_2 &= \beta_2 + \omega_2 \cdot h_2 \\
h_3 &= \mathrm{a}[f_2] \\
f_3 &= \beta_3 + \omega_3 \cdot h_3 \\
\ell_i &= (y_i - f_3)^2
\end{aligned}$$

- 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 ℓ_i?

Backward pass



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

$$f_0 = \beta_0 + \omega_0 \cdot x$$
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- The second derivative is computed via the chain rule

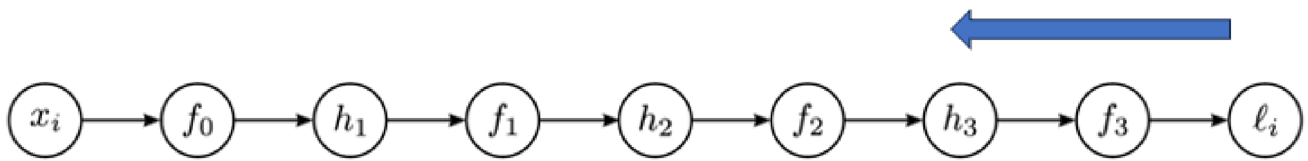
$$\frac{\partial \ell_i}{\partial h_3} = \frac{\partial f_3}{\partial h_3}\frac{\partial \ell_i}{\partial f_3}$$

How does a small change in f_3 change ℓ_i?

How does a small change in h_3 change ℓ_i?

How does a small change in h_3 change f_3?

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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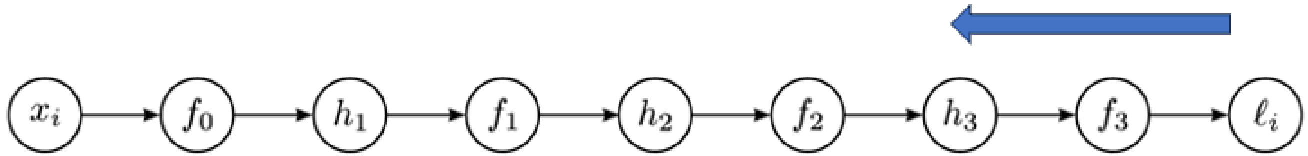
$$f_3 = \beta_3 + \omega_3 \cdot h_3$$
$$\ell_i = (y_i - f_3)^2$$

- 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!

Backward pass



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

- 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

$$x_i \rightarrow f_0 \rightarrow h_1 \rightarrow f_1 \rightarrow h_2 \rightarrow f_2 \rightarrow h_3 \rightarrow f_3 \rightarrow \ell_i$$

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

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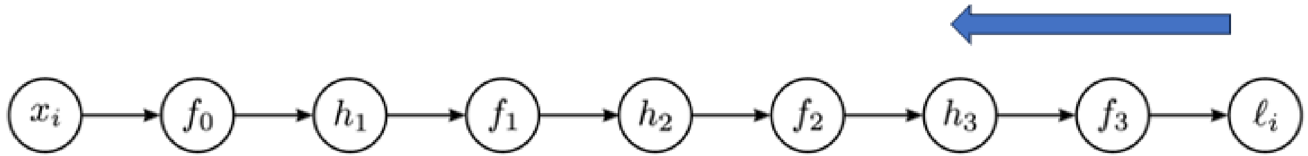
$$\frac{\partial \ell_i}{\partial f_2} = \frac{\partial h_3}{\partial f_2} \left(\frac{\partial f_3}{\partial h_3} \frac{\partial \ell_i}{\partial f_3} \right)$$

Already computed!

Backward pass



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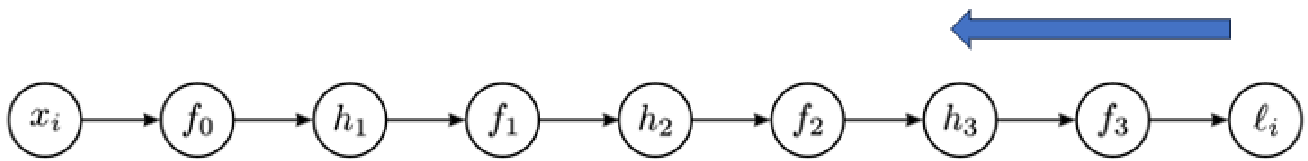
- The remaining derivatives also calculated by further use of chain rule

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

Backward pass



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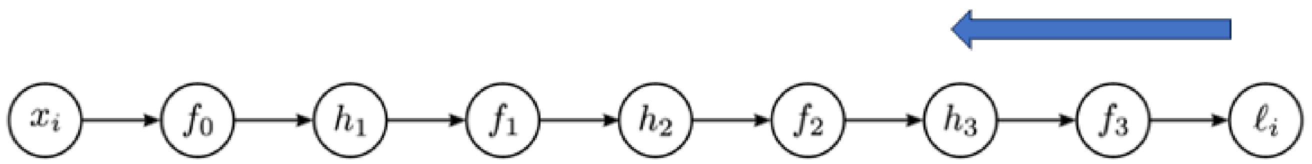
$$f_2 = \beta_2 + \omega_2 \cdot h_2$$
$$h_3 = \mathrm{a}[f_2]$$
$$f_3 = \beta_3 + \omega_3 \cdot h_3$$
$$\ell_i = (y_i - f_3)^2$$

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

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

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

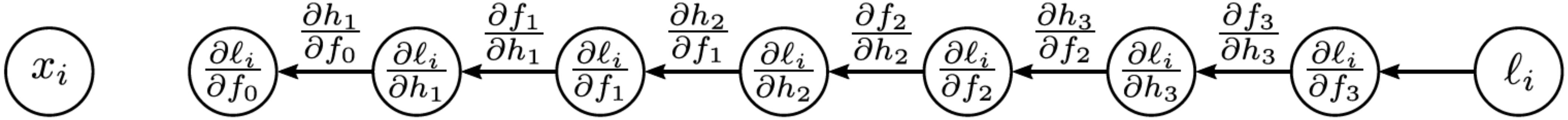
$$
\begin{aligned}
\frac{\partial \ell_i}{\partial f_3} &= 2(f_3 - y_i) \\
\frac{\partial \ell_i}{\partial h_3} &= \frac{\partial f_3}{\partial h_3}\frac{\partial \ell_i}{\partial f_3} \\
\frac{\partial \ell_i}{\partial f_2} &= \frac{\partial h_3}{\partial f_2}\left(\frac{\partial f_3}{\partial h_3}\frac{\partial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

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

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



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

Backward pass

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

$$f_0 = \beta_0 + \omega_0 \cdot x$$
$$h_1 = \mathrm{a}[f_0]$$
$$f_1 = \beta_1 + \omega_1 \cdot h_1$$
$$h_2 = \mathrm{a}[f_1]$$

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

- 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?

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.

$$f_0 = \beta_0 + \omega_0 \cdot x$$
$$h_1 = \mathrm{a}[f_0]$$
$$f_1 = \beta_1 + \omega_1 \cdot h_1$$
$$h_2 = \mathrm{a}[f_1]$$

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

- 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.

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

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

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

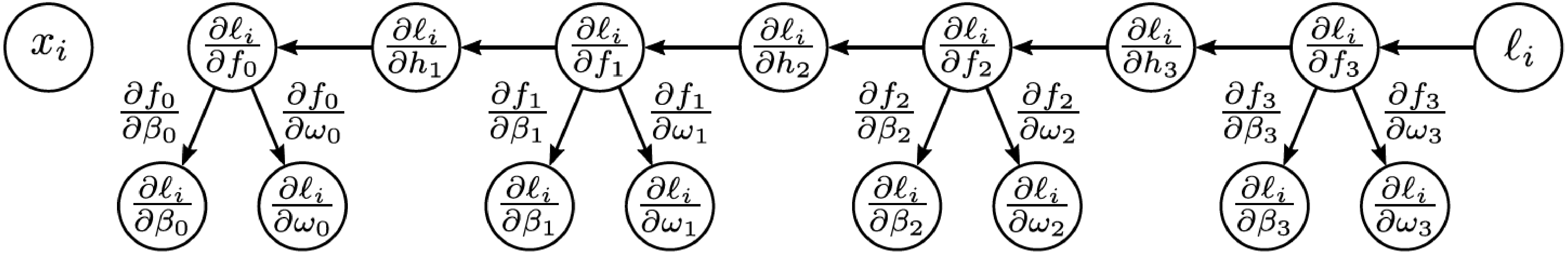
$$\frac{\partial \ell_i}{\partial \omega_k} = \frac{\partial f_k}{\partial \omega_k}\frac{\partial \ell_i}{\partial f_k}$$

$$\frac{\partial \ell_i}{\partial \beta_k} = \underbrace{\frac{\partial f_k}{\partial \beta_k}}_{1}\frac{\partial \ell_i}{\partial f_k}$$

Backward pass

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

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



Gradients

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

Matrix calculus

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

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

The derivative with respect to vector $\mathbf{a}$ is a vector of the same shape as $\mathbf{a}$.

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 with respect to matrix $\mathbf{A}$ is a matrix of the same shape as $\mathbf{A}$.

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

Rows are each variable element

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

Comparing vector and matrix

Scalar derivatives:

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

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

Comparing vector and matrix

Scalar derivatives:

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

Matrix derivatives:

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

Comparing vector and matrix

Scalar derivatives:

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

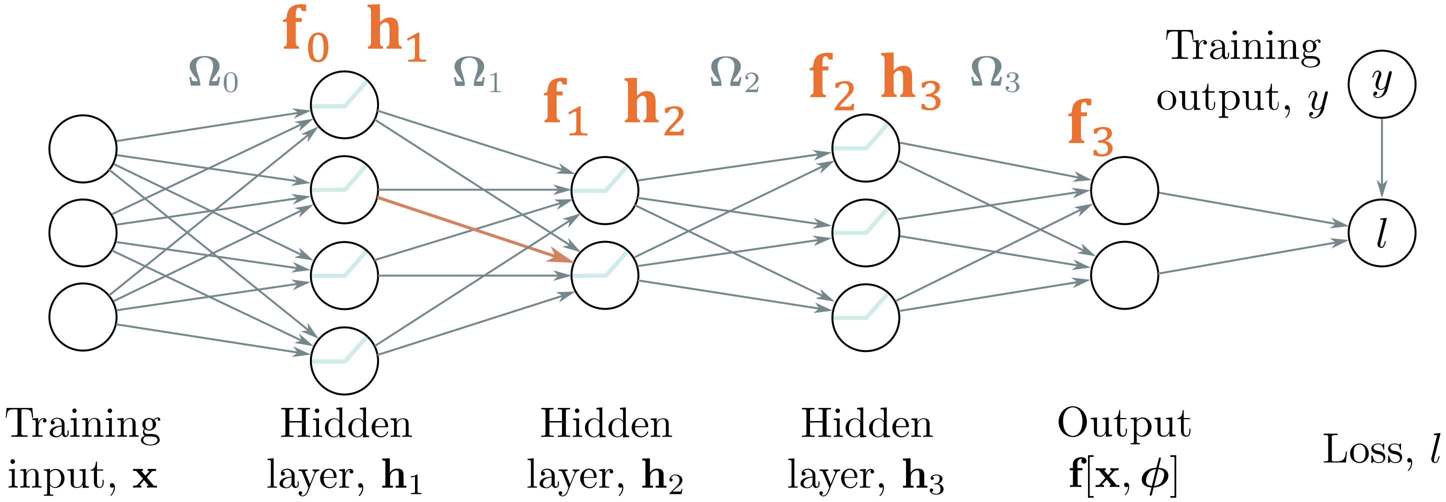
Matrix derivatives:

$$\mathbf{f}_3 = \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \qquad \frac{\partial \mathbf{f}_3}{\partial \boldsymbol{\beta}_3} = \frac{\partial}{\partial \beta_3}(\boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3) = \mathbf{I}$$

Gradients

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

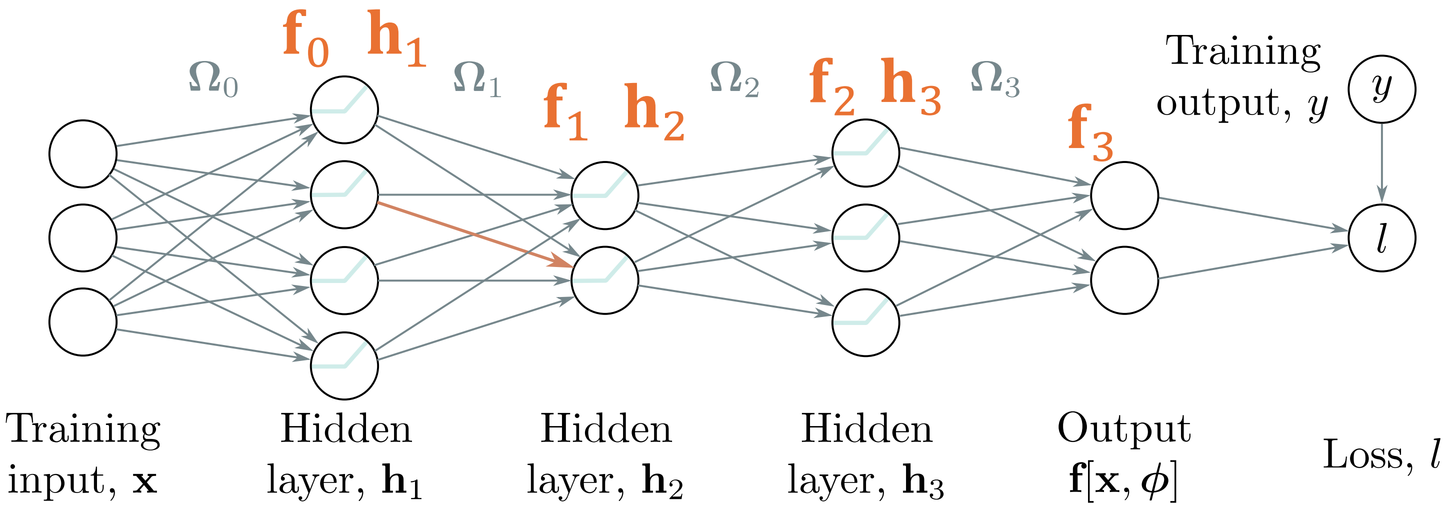
The forward pass



1. Write this as a series of intermediate calculations

$$
\begin{aligned}
\mathbf{f}_0 &= \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i \\
\mathbf{h}_1 &= \mathbf{a}[\mathbf{f}_0] \\
\mathbf{f}_1 &= \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1 \\
\mathbf{h}_2 &= \mathbf{a}[\mathbf{f}_1] \\
\mathbf{f}_2 &= \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2 \\
\mathbf{h}_3 &= \mathbf{a}[\mathbf{f}_2] \\
\mathbf{f}_3 &= \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \\
\ell_i &= \mathrm{l}[\mathbf{f}_3, y_i]
\end{aligned}
$$

The forward pass

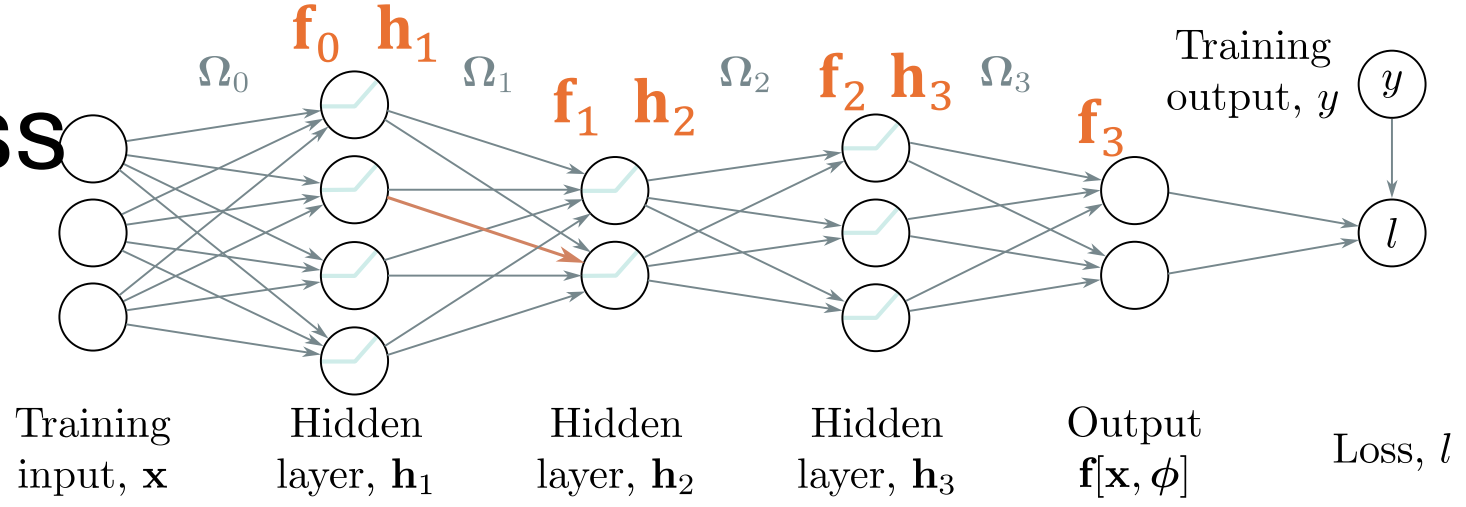


1. Write this as a series of intermediate calculations

2. Compute these intermediate quantities

$$
\begin{aligned}
\mathbf{f}_0 &= \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i \\
\mathbf{h}_1 &= \mathbf{a}[\mathbf{f}_0] \\
\mathbf{f}_1 &= \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1 \\
\mathbf{h}_2 &= \mathbf{a}[\mathbf{f}_1] \\
\mathbf{f}_2 &= \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2 \\
\mathbf{h}_3 &= \mathbf{a}[\mathbf{f}_2] \\
\mathbf{f}_3 &= \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \\
\ell_i &= \mathrm{l}[\mathbf{f}_3, y_i]
\end{aligned}
$$

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

$$
\begin{aligned}
\mathbf{f}_0 &= \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i \\
\mathbf{h}_1 &= \mathbf{a}[\mathbf{f}_0] \\
\mathbf{f}_1 &= \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1 \\
\mathbf{h}_2 &= \mathbf{a}[\mathbf{f}_1] \\
\mathbf{f}_2 &= \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2 \\
\mathbf{h}_3 &= \mathbf{a}[\mathbf{f}_2] \\
\mathbf{f}_3 &= \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \\
\ell_i &= \mathrm{l}[\mathbf{f}_3, y_i]
\end{aligned}
$$

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

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

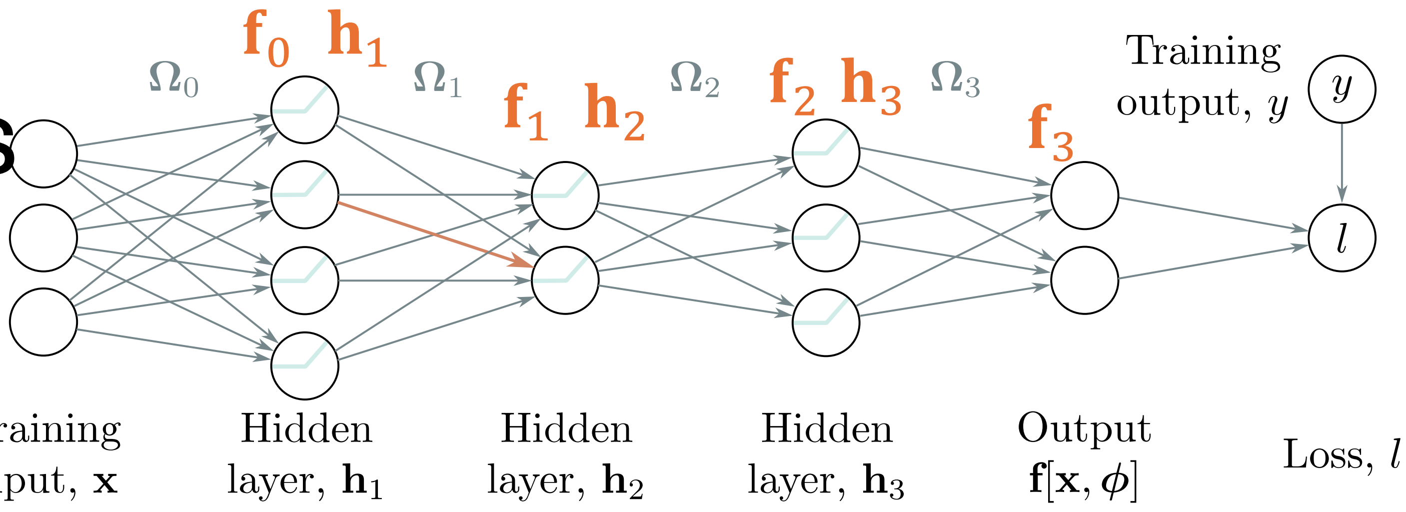
$$\frac{\partial \ell_i}{\partial \mathbf{f}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \left(\frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3}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

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

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

2. Compute these intermediate quantities

3. Take derivatives of output with respect to intermediate quantities

$$
\begin{aligned}
\mathbf{f}_0 &= \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i \\
\mathbf{h}_1 &= \mathbf{a}[\mathbf{f}_0] \\
\mathbf{f}_1 &= \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1 \\
\mathbf{h}_2 &= \mathbf{a}[\mathbf{f}_1] \\
\mathbf{f}_2 &= \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2 \\
\mathbf{h}_3 &= \mathbf{a}[\mathbf{f}_2] \\
\mathbf{f}_3 &= \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \\
\ell_i &= \mathrm{l}[\mathbf{f}_3, y_i]
\end{aligned}
$$

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

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

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

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

Yikes!

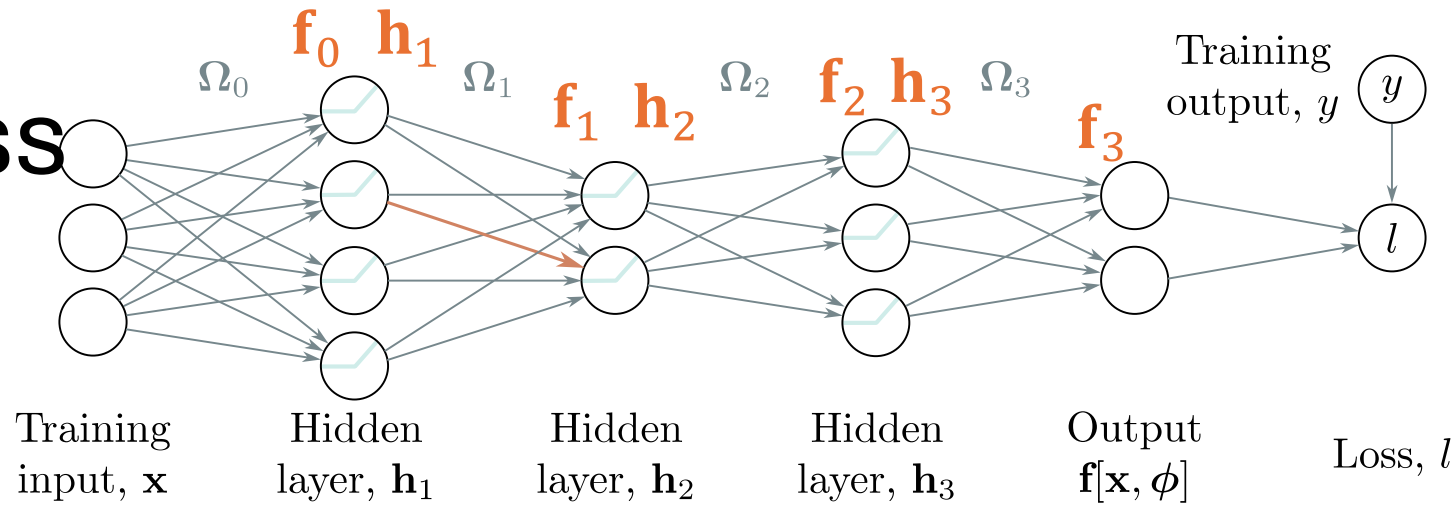
- But:

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

- Quite similar to:

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

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

$$
\begin{aligned}
\mathbf{f}_0 &= \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i \\
\mathbf{h}_1 &= \mathbf{a}[\mathbf{f}_0] \\
\mathbf{f}_1 &= \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1 \\
\mathbf{h}_2 &= \mathbf{a}[\mathbf{f}_1] \\
\mathbf{f}_2 &= \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2 \\
\mathbf{h}_3 &= \mathbf{a}[\mathbf{f}_2] \\
\mathbf{f}_3 &= \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \\
\ell_i &= \mathrm{l}[\mathbf{f}_3, y_i]
\end{aligned}
$$

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

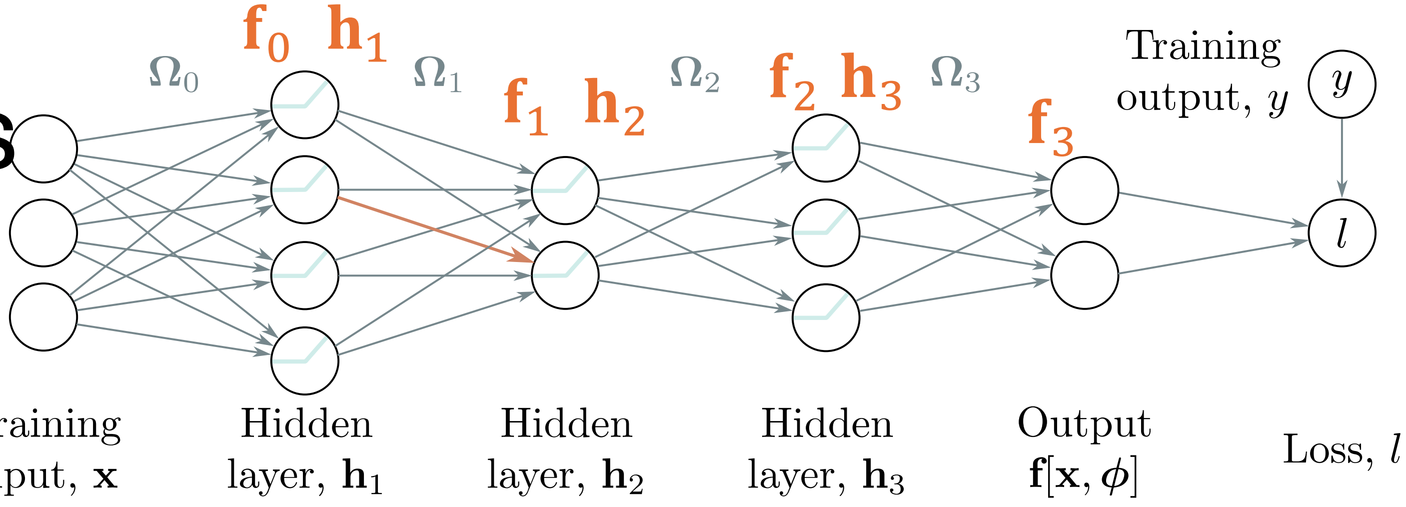
$$\frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

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

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

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

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

$$
\begin{aligned}
\mathbf{f}_0 &= \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i \\
\mathbf{h}_1 &= \mathbf{a}[\mathbf{f}_0] \\
\mathbf{f}_1 &= \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1 \\
\mathbf{h}_2 &= \mathbf{a}[\mathbf{f}_1] \\
\mathbf{f}_2 &= \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2 \\
\mathbf{h}_3 &= \mathbf{a}[\mathbf{f}_2] \\
\mathbf{f}_3 &= \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \\
\ell_i &= \mathrm{l}[\mathbf{f}_3, y_i]
\end{aligned}
$$

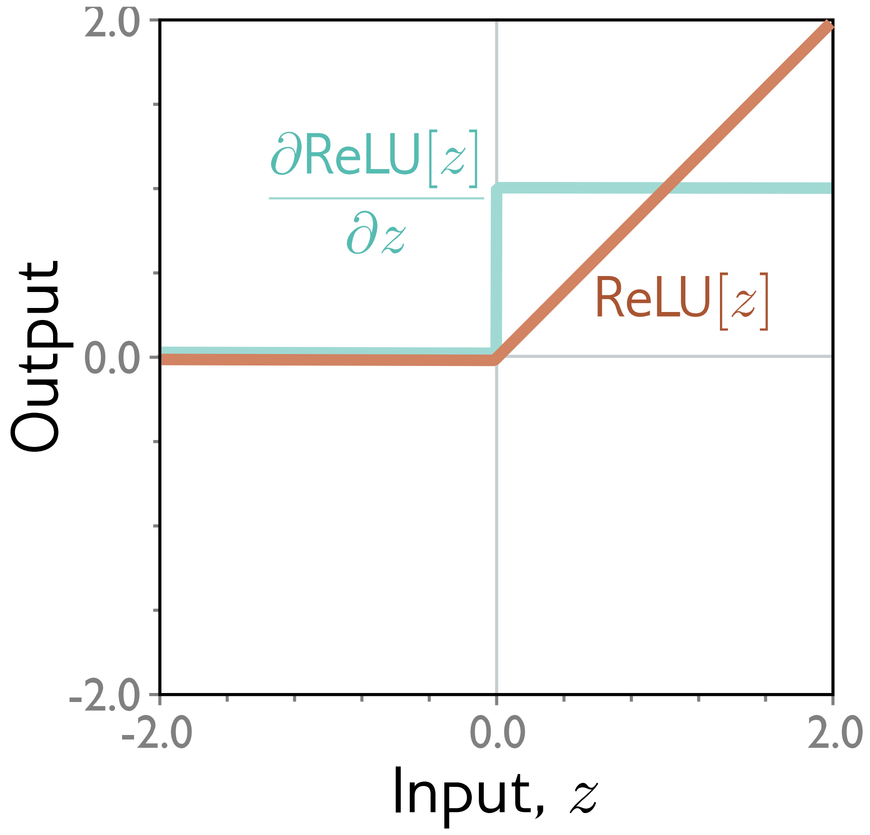
$$\frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

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

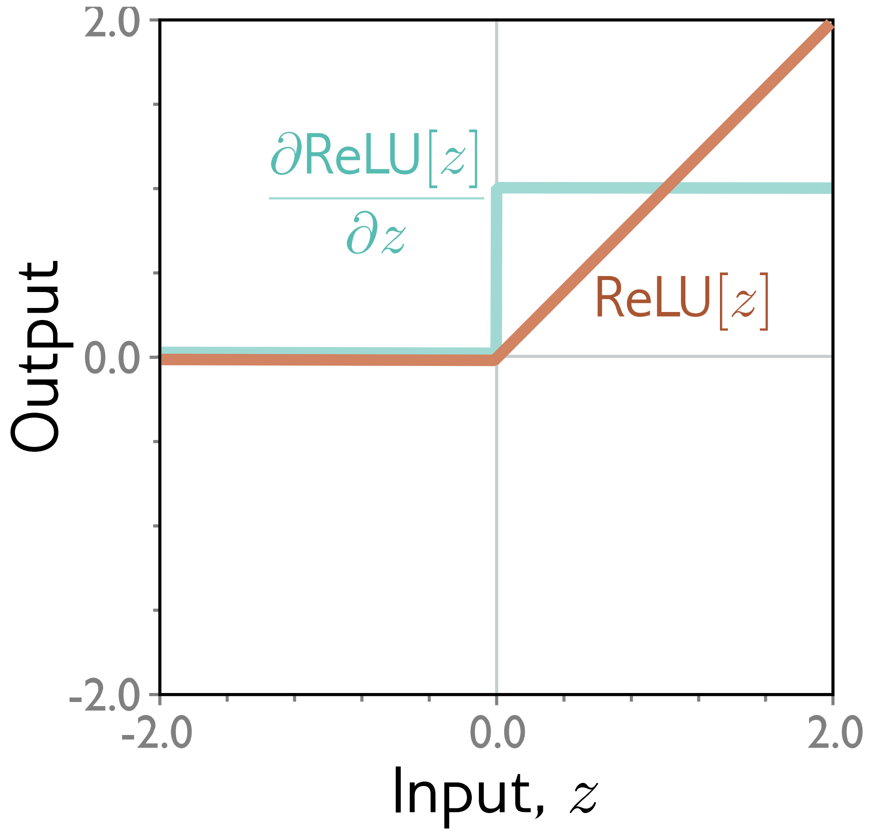
$$\frac{\partial \ell_i}{\partial \mathbf{f}_1} = \frac{\partial \mathbf{h}_2}{\partial \mathbf{f}_1} \frac{\partial \mathbf{f}_2}{\partial \mathbf{h}_2} \left(\frac{\partial \mathbf{h}_3}{\partial \mathbf{f}_2} \frac{\partial \mathbf{f}_3}{\partial \mathbf{h}_3} \frac{\partial \ell_i}{\partial \mathbf{f}_3}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

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

Derivative of ReLU



Derivative of ReLU



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

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

"Indicator function"

Derivative of ReLU

1. Consider:

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

where:

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

2. We could equivalently write:

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

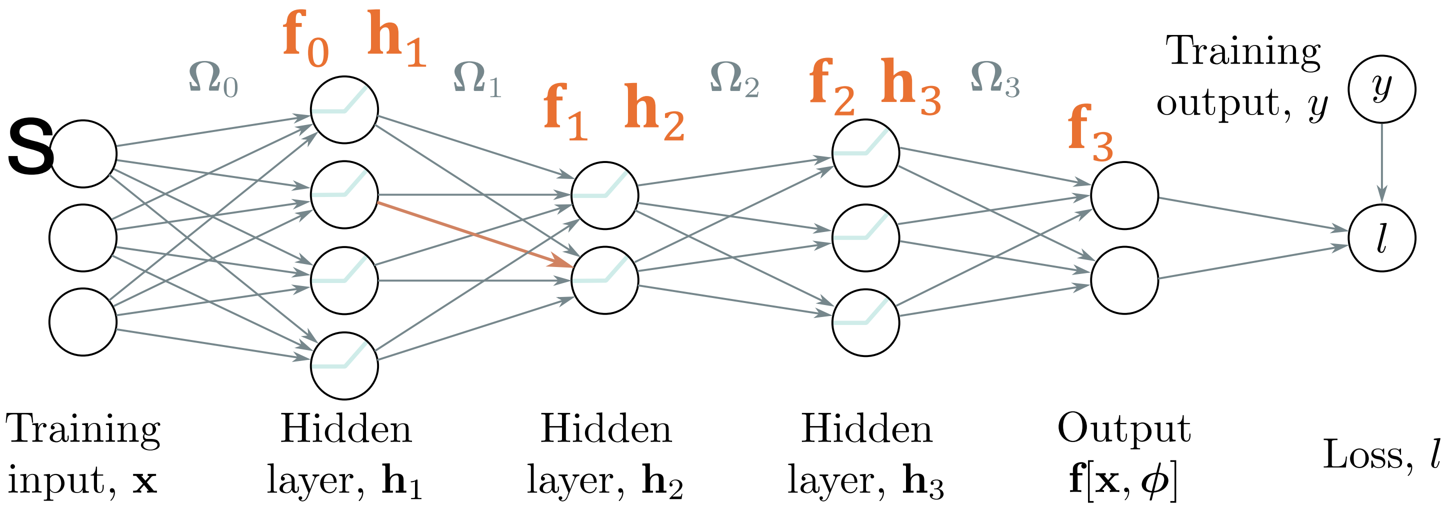
3. Taking the derivative

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

4. We can equivalently pointwise multiply by diagonal

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

The backward pass



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

1. Write this as a series of intermediate calculations

2. Compute these intermediate quantities

3. Take derivatives of output with respect to intermediate quantities

$$\begin{aligned}
\mathbf{f}_0 &= \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i \\
\mathbf{h}_1 &= \mathbf{a}[\mathbf{f}_0] \\
\mathbf{f}_1 &= \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1 \\
\mathbf{h}_2 &= \mathbf{a}[\mathbf{f}_1] \\
\mathbf{f}_2 &= \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2 \\
\mathbf{h}_3 &= \mathbf{a}[\mathbf{f}_2] \\
\mathbf{f}_3 &= \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \\
\ell_i &= \mathrm{l}[\mathbf{f}_3, y_i]
\end{aligned}$$

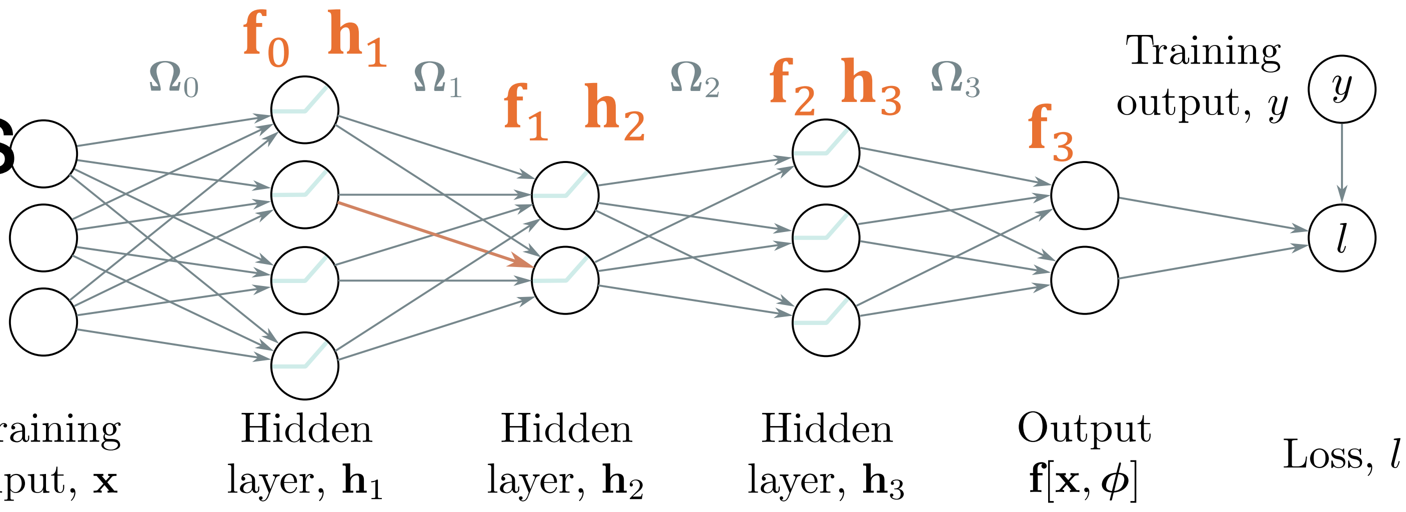
$$\frac{\partial \ell_i}{\partial \mathbf{f}_3}$$

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

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

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

The backward pass



1. Write this as a series of intermediate calculations

2. Compute these intermediate quantities

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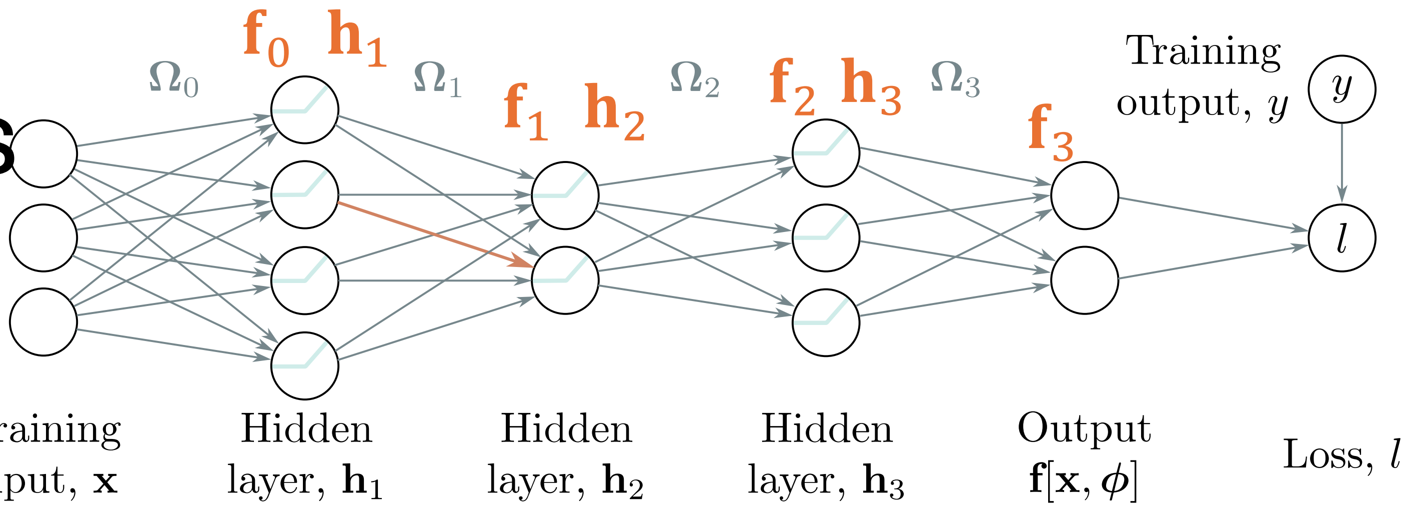
4. Take derivatives w.r.t. parameters

$$
\begin{aligned}
\mathbf{f}_0 &= \boldsymbol{\beta}_0 + \boldsymbol{\Omega}_0 \mathbf{x}_i \\
\mathbf{h}_1 &= \mathbf{a}[\mathbf{f}_0] \\
\mathbf{f}_1 &= \boldsymbol{\beta}_1 + \boldsymbol{\Omega}_1 \mathbf{h}_1 \\
\mathbf{h}_2 &= \mathbf{a}[\mathbf{f}_1] \\
\mathbf{f}_2 &= \boldsymbol{\beta}_2 + \boldsymbol{\Omega}_2 \mathbf{h}_2 \\
\mathbf{h}_3 &= \mathbf{a}[\mathbf{f}_2] \\
\mathbf{f}_3 &= \boldsymbol{\beta}_3 + \boldsymbol{\Omega}_3 \mathbf{h}_3 \\
\ell_i &= \mathrm{l}[\mathbf{f}_3, y_i]
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \ell_i}{\partial \boldsymbol{\beta}_k} &= \frac{\partial \mathbf{f}_k}{\partial \boldsymbol{\beta}_k} \frac{\partial \ell_i}{\partial \mathbf{f}_k} \\
&= \frac{\partial}{\partial \boldsymbol{\beta}_k} \left(\boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathbf{h}_k \right) \frac{\partial \ell_i}{\partial \mathbf{f}_k} \\
&= \frac{\partial \ell_i}{\partial \mathbf{f}_k},
\end{aligned}
$$

The backward pass



1. Write this as a series of intermediate calculations

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\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 &= \mathrm{l}[\mathbf{f}_3, y_i]
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \ell_i}{\partial \boldsymbol{\Omega}_k} &= \frac{\partial \mathbf{f}_k}{\partial \boldsymbol{\Omega}_k} \frac{\partial \ell_i}{\partial \mathbf{f}_k} \\
&= \frac{\partial}{\partial \boldsymbol{\Omega}_k} \left(\boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathbf{h}_k \right) \frac{\partial \ell_i}{\partial \mathbf{f}_k} \\
&= \frac{\partial \ell_i}{\partial \mathbf{f}_k} \mathbf{h}_k^T
\end{aligned}
$$

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.

Looking Ahead to Initialization

The chain rule tells us to multiply all these "local" partial derivatives together…

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

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

- What happens when most of those values are >2.0?
- What happens when most of those values are <0.5?

Our initialization will be setting the initial local partial derivatives.