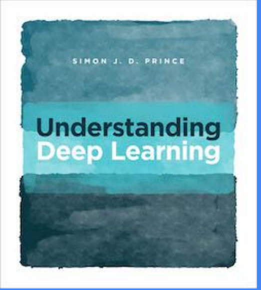
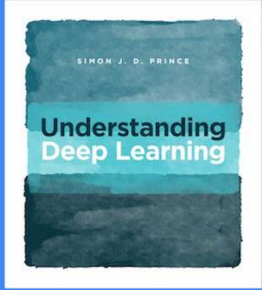
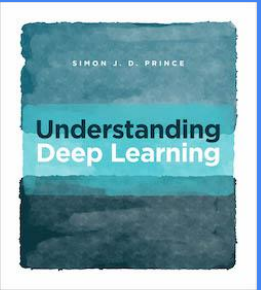
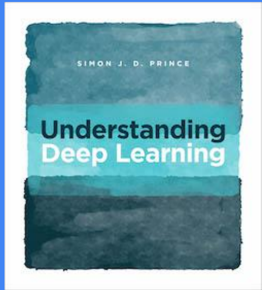


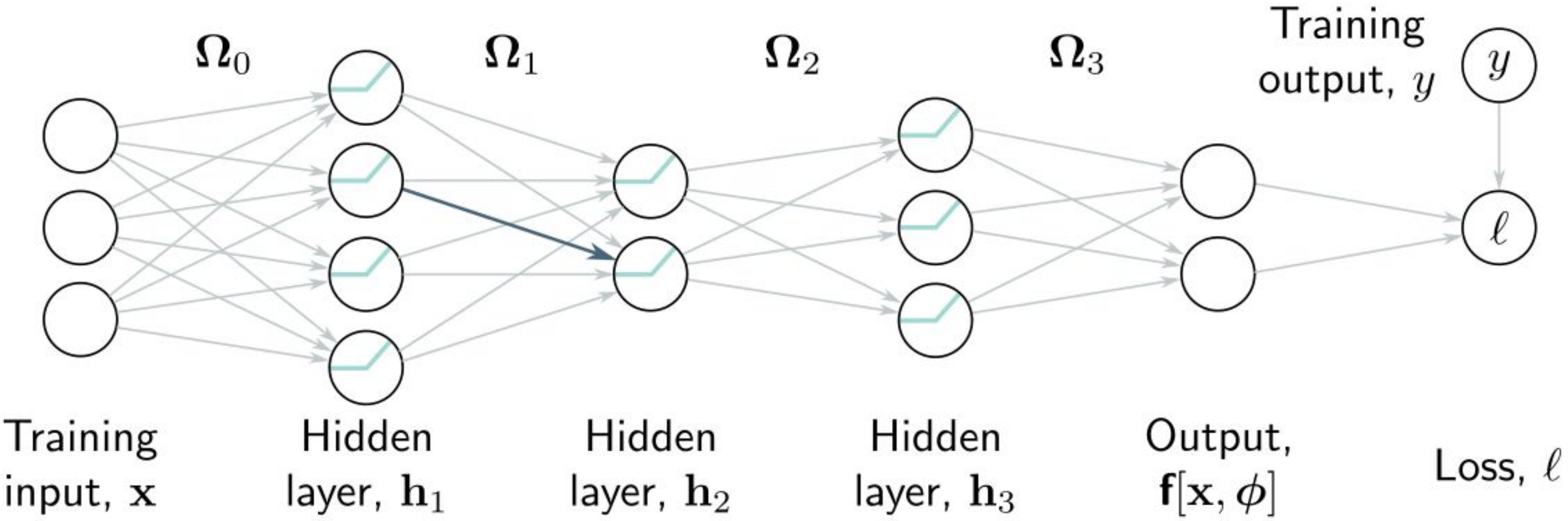


Gradients and initialization
Chapter 7





Goal: to compute the derivatives of the loss ℓ with respect to each of the weights (arrows) and biases (not shown)



Backpropagation forward pass

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

Figure 7.3 Backpropagation forward pass. We compute and store each of the intermediate variables in turn until we finally calculate the loss.

Backpropagation backward pass

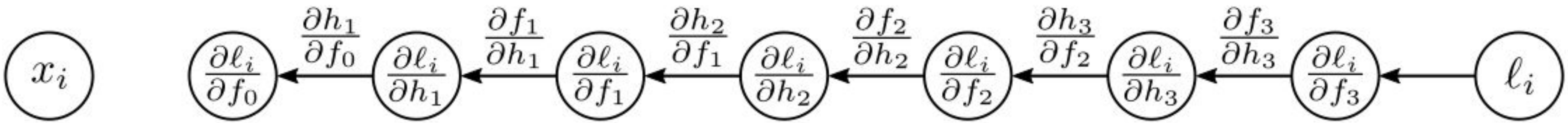
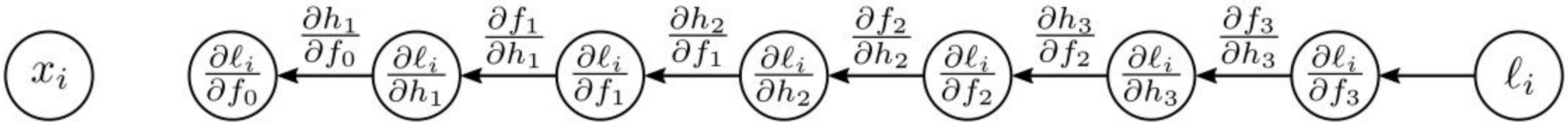
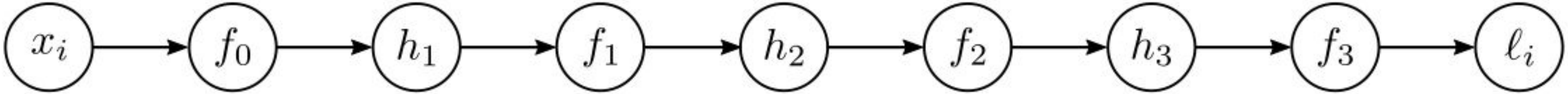


Figure 7.4 Backpropagation backward pass #1. We work backward from the end of the function computing the derivatives $\partial \ell_i / \partial f_\bullet$ and $\partial \ell_i / \partial h_\bullet$ of the loss with respect to the intermediate quantities. Each derivative is computed from the previous one by multiplying by terms of the form $\partial f_k / \partial h_k$ or $\partial h_k / \partial f_{k-1}$.

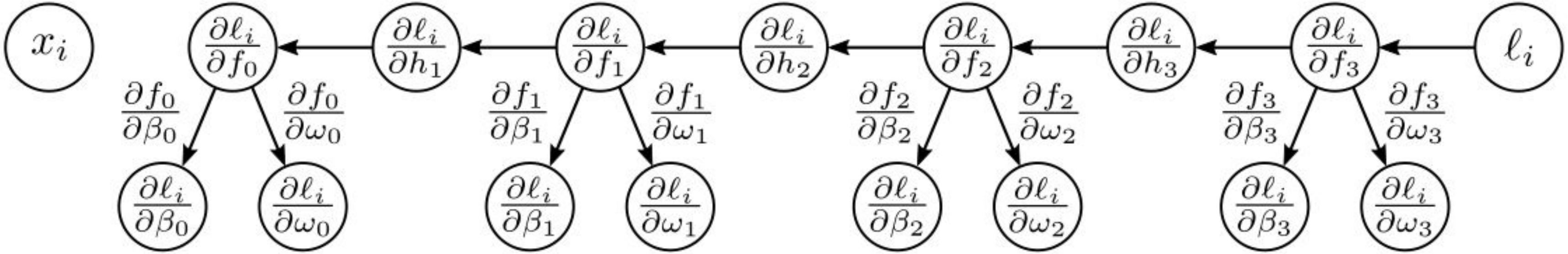


$$
\begin{aligned}
\frac{\partial \ell_i}{\partial f_2} &= \frac{\partial h_3}{\partial f_2}\left(\frac{\partial f_3}{\partial h_3}\frac{\partial \ell_i}{\partial f_3}\right)\\
\frac{\partial \ell_i}{\partial h_2} &= \frac{\partial f_2}{\partial h_2}\left(\frac{\partial h_3}{\partial f_2}\frac{\partial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



$$f_k = \beta_k + \omega_k \cdot h_k$$

$$\frac{\partial f_k}{\partial \beta_k} = 1 \qquad \text{and} \qquad \frac{\partial f_k}{\partial \omega_k} \quad = \quad h_k$$



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

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

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

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

$D_3 \times D_3, D_3 \times D_f,$ and $D_f \times 1$

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

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

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

$D_3 \times D_3, D_3 \times D_f,$ and $D_f \times 1$

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

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

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

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

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

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

The derivative $\partial \ell_i / \partial \mathbf{f}_3$ of the loss ℓ_i with respect to the network output $\mathbf{f}_3$ will depend on the loss function but usually has a simple form.

The derivative $\partial \mathbf{f}_3/\partial \mathbf{h}_3$ of the network output with respect to hidden layer $\mathbf{h}_3$ is:

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

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

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

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

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

$$
\begin{aligned}
\frac{\partial \ell_i}{\partial \boldsymbol{\beta}_0} &= \frac{\partial \ell_i}{\partial \mathbf{f}_0} \\
\frac{\partial \ell_i}{\partial \boldsymbol{\Omega}_0} &= \frac{\partial \ell_i}{\partial \mathbf{f}_0}\mathbf{x}_i^T
\end{aligned}
$$

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

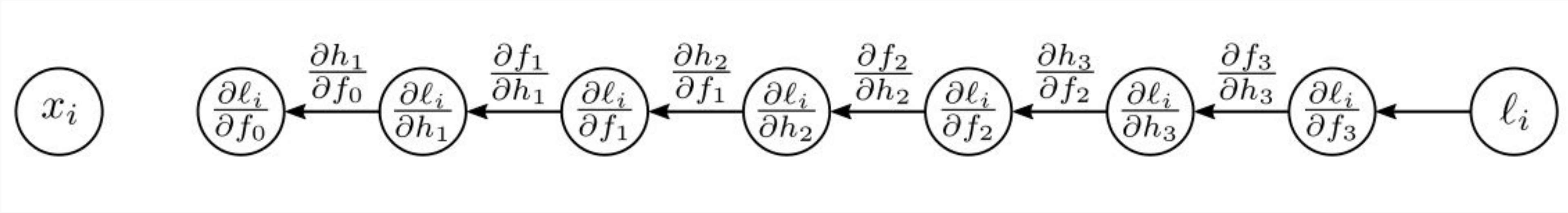
Forward pass

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

An example:

$$\begin{aligned}
f_0 &= \beta_0 + \omega_0 \cdot x_i \\
h_1 &= \sin[f_0] \\
f_1 &= \beta_1 + \omega_1 \cdot h_1 \\
h_2 &= \exp[f_1] \\
f_2 &= \beta_2 + \omega_2 \cdot h_2 \\
h_3 &= \cos[f_2] \\
f_3 &= \beta_3 + \omega_3 \cdot h_3 \\
\ell_i &= (f_3 - y_i)^2.
\end{aligned}$$

Backward pass



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

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

$$f_k = \beta_k + \omega_k . h_k$$

$$\frac{\partial f_k}{\partial \beta_k} = 1 \qquad \text{and} \qquad \frac{\partial f_k}{\partial \omega_k} = h_k$$

$$\frac{\partial f_0}{\partial \beta_0} = 1 \qquad \text{and} \qquad \frac{\partial f_0}{\partial \omega_0} = x_i$$

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

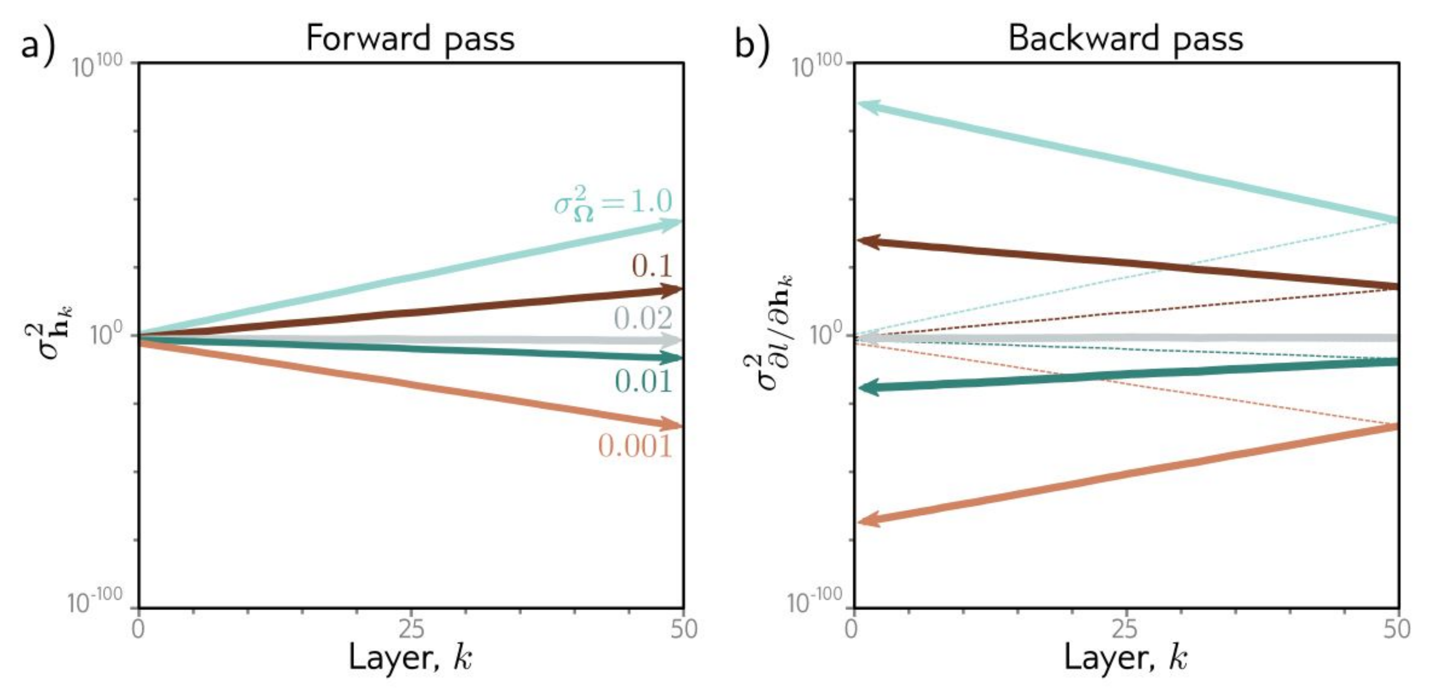
$$\frac{\partial \ell_i}{\partial h_3} = \frac{\partial f_3}{\partial h_3}\frac{\partial \ell_i}{\partial f_3}$$

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

Parameter initialization

$$
\begin{aligned}
\mathbf{f}_k &= \boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathbf{h}_k \\
&= \boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathrm{a}[\mathbf{f}_{k-1}]
\end{aligned}
$$

vanishing gradient problem & exploding gradient problem



$$
\begin{aligned}
\mathbb{E}[f_i'] &= \mathbb{E}\left[\beta_i + \sum_{j=1}^{D_h} \Omega_{ij} h_j\right] \\
&= \mathbb{E}\left[\beta_i\right] + \sum_{j=1}^{D_h} \mathbb{E}\left[\Omega_{ij} h_j\right] \\
&= \mathbb{E}\left[\beta_i\right] + \sum_{j=1}^{D_h} \mathbb{E}\left[\Omega_{ij}\right] \mathbb{E}\left[h_j\right] \\
&= 0 + \sum_{j=1}^{D_h} 0 \cdot \mathbb{E}\left[h_j\right] = 0,
\end{aligned}
$$

$$
\begin{aligned}
\sigma_{f'}^2 &= \mathbb{E}[f_i'^2] - \mathbb{E}[f_i']^2 \\
&= \mathbb{E}\left[\left(\beta_i + \sum_{j=1}^{D_h} \Omega_{ij} h_j\right)^2\right] - 0 \\
&= \mathbb{E}\left[\left(\sum_{j=1}^{D_h} \Omega_{ij} h_j\right)^2\right] \\
&= \sum_{j=1}^{D_h} \mathbb{E}\left[\Omega_{ij}^2\right] \mathbb{E}\left[h_j^2\right] \\
&= \sum_{j=1}^{D_h} \sigma_\Omega^2 \mathbb{E}\left[h_j^2\right] = \sigma_\Omega^2 \sum_{j=1}^{D_h} \mathbb{E}\left[h_j^2\right],
\end{aligned}
$$

$$
\sigma^2 = \mathbb{E}[(z - \mathbb{E}[z])^2] = \mathbb{E}[z^2] - \mathbb{E}[z]^2
$$

$$
\sigma_{f'}^2 = \sigma_\Omega^2 \sum_{j=1}^{D_h} \frac{\sigma_f^2}{2} = \frac{1}{2} D_h \sigma_\Omega^2 \sigma_f^2
$$

He initialization (Kaiming Initialization)

$$\sigma_\Omega^2 = \frac{2}{D_h}$$

$$\Uparrow$$

$$\sigma_{f'}^2 = \sigma_\Omega^2 \sum_{j=1}^{D_h} \frac{\sigma_f^2}{2} = \frac{1}{2} D_h \sigma_\Omega^2 \sigma_f^2$$

Initialization for both forward and backward pass

$$\sigma_{\Omega}^{2} = \frac{2}{D_{h'}}$$

Initialization for both forward and backward pass

$$\sigma_{\Omega}^2 = \frac{4}{D_h + D_{h'}}$$

Understanding Deep Learning

Chapter 8