Initialization

- Consider standard building block of NN in terms of *preactivations*:

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

- Set all the biases to 0

$$\boldsymbol{\beta}_k = \mathbf{0}$$

- Weights normally distributed
    - mean 0
    - variance σ_Ω^2

- What will happen as we move through the network if σ_Ω^2 is very small?
- What will happen as we move through the network if σ_Ω^2 is very large?

Backprop summary

Backward pass: We start with the derivative $\partial \ell_i / \partial \mathbf{f}_K$ of the loss function ℓ_i with respect to the network output $\mathbf{f}_K$ and work backward through the network:

$$
\begin{aligned}
\frac{\partial \ell_i}{\partial \boldsymbol{\beta}_k} &= \frac{\partial \ell_i}{\partial \mathbf{f}_k} & k \in \{K, K-1, \ldots 1\} \\
\frac{\partial \ell_i}{\partial \boldsymbol{\Omega}_k} &= \frac{\partial \ell_i}{\partial \mathbf{f}_k} \mathbf{h}_k^T & k \in \{K, K-1, \ldots 1\} \\
\frac{\partial \ell_i}{\partial \mathbf{f}_{k-1}} &= \mathbb{I}[\mathbf{f}_{k-1} > 0] \odot \left(\boldsymbol{\Omega}_k^T \frac{\partial \ell_i}{\partial \mathbf{f}_k} \right), & k \in \{K, K-1, \ldots 1\}
\end{aligned}
\tag{7.13}
$$

where $\odot$ denotes pointwise multiplication and $\mathbb{I}[\mathbf{f}_{k-1} > 0]$ is a vector containing ones where $\mathbf{f}_{k-1}$ is greater than zero and zeros elsewhere. Finally, we compute the derivatives with respect to the first set of biases and weights:

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

Initialization

- Need for initialization
- He initialization
- Interlude: Expectations
- Show that $\mathbb{E}[f'_i] = 0$
- Write variance of pre-activations *f'* in terms of activations *h* in previous layer

$$\sigma^2_{f'} = \sigma^2_{\Omega} \sum_{j=1}^{D_h} \mathbb{E}\left[h_j^2\right]$$

- Write variance of pre-activations f' in terms of pre-activations f in previous layer

$$\sigma^2_{f'} = \frac{D_h \sigma^2_{\Omega} \sigma^2_f}{2}$$

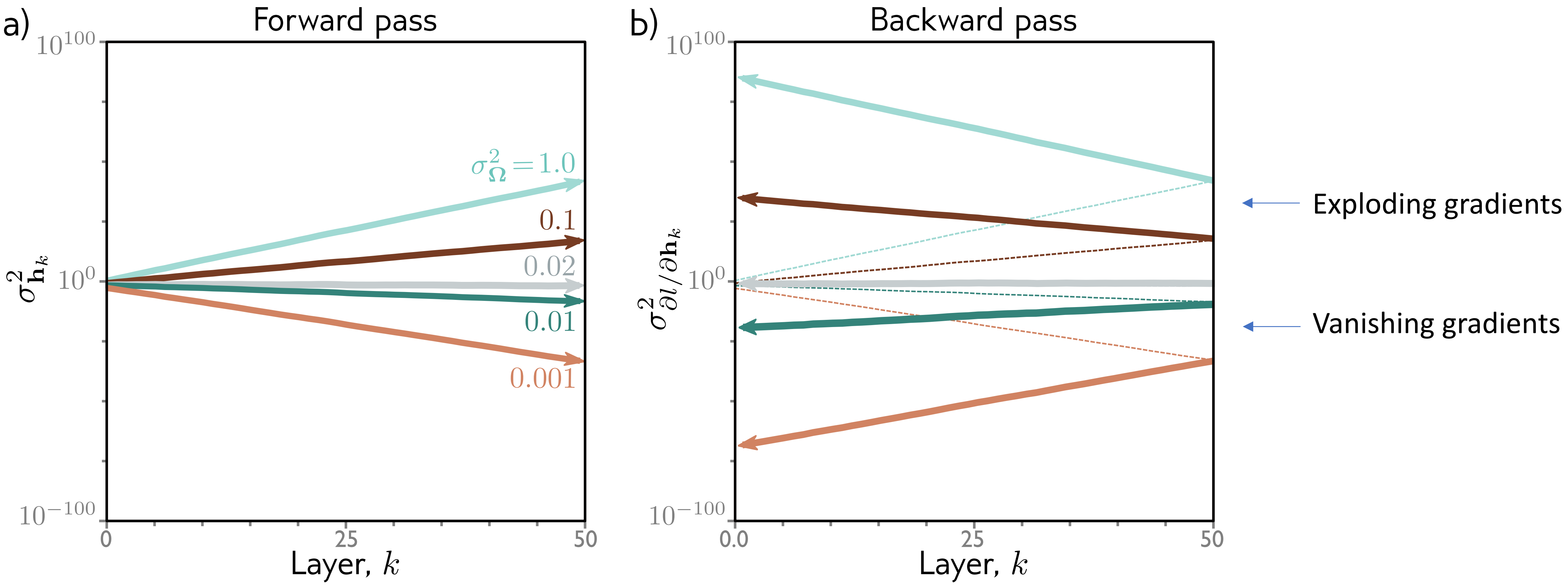


Figure 7.4 Weight initialization. Consider a deep network with 50 hidden layers and $D_h = 100$ hidden units per layer. The network has a 100 dimensional input $\mathbf{x}$ initialized with values from a standard normal distribution, a single output fixed at $y = 0$, and a least squares loss function. The bias vectors $\boldsymbol{\beta}_k$ are initialized to zero and the weight matrices $\boldsymbol{\Omega}_k$ are initialized with a normal distribution with mean zero and five different variances $\sigma^2_\Omega \in \{0.001, 0.01, 0.02, 0.1, 1.0\}$. a)

He initialization (assumes ReLU)

- Forward pass: want the variance of hidden unit activations in layer k+1 to be the same as variance of activations in layer k:

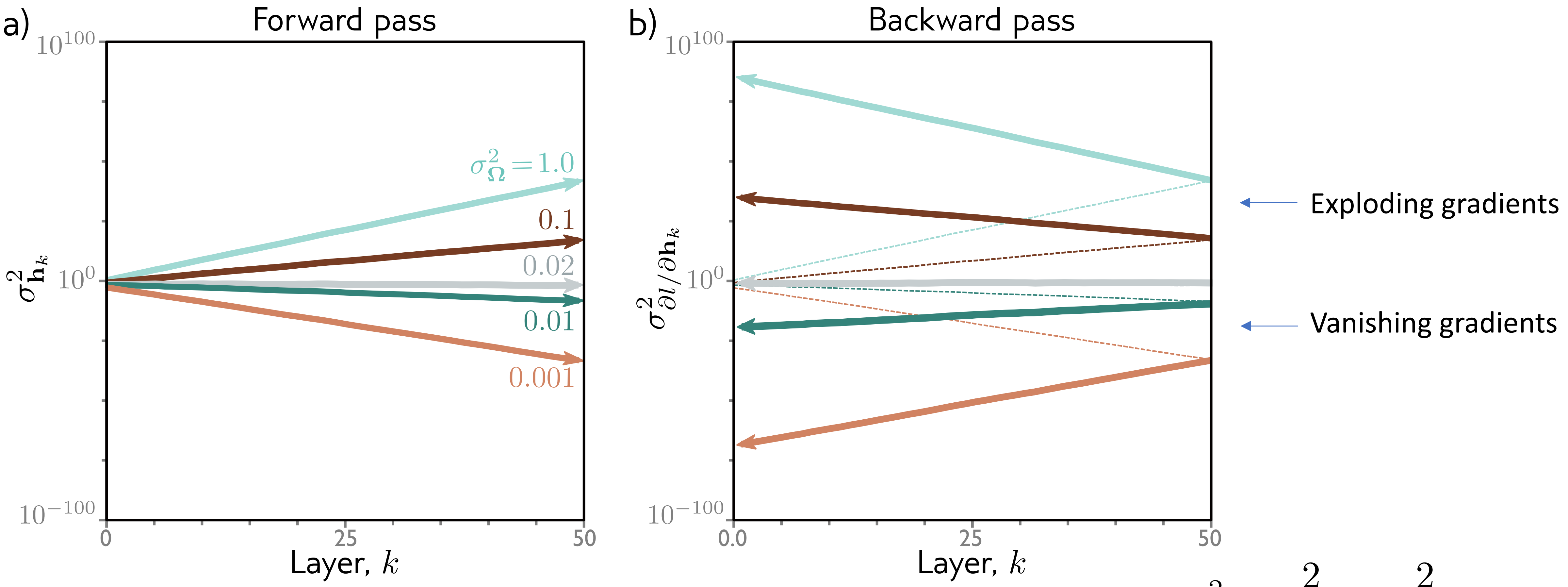
$$\sigma_\Omega^2 = \frac{2}{D_h}$$

Number of units at layer k

- Backward pass: want the variance of gradients at layer k to be the same as variance of gradient in layer k+1:

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

Number of units at layer k+1



$$\sigma_\Omega^2 = \frac{2}{D_h} = \frac{2}{100} = 0.02$$

Figure 7.4 Weight initialization. Consider a deep network with 50 hidden layers and $D_h = 100$ hidden units per layer. The network has a 100 dimensional input $\mathbf{x}$ initialized with values from a standard normal distribution, a single output fixed at $y = 0$, and a least squares loss function. The bias vectors $\boldsymbol{\beta}_k$ are initialized to zero and the weight matrices $\boldsymbol{\Omega}_k$ are initialized with a normal distribution with mean zero and five different variances $\sigma^2_{\boldsymbol{\Omega}} \in \{0.001, 0.01, 0.02, 0.1, 1.0\}$. a)

Expectations

Function g[•]	Expectation
x	mean, μ
x^k	kth moment about zero
$(x-\mu)^k$	kth moment about the mean
$(x-\mu)^2$	variance
$(x-\mu)^3$	skew
$(x-\mu)^4$	kurtosis

Table B.1 Special cases of expectation. For some functions $\mathrm{g}[x]$, the expectation $\mathbb{E}[\mathrm{g}[x]]$ is given a special name. Here we use the notation μ_x to represent the mean with respect to random variable x.

Rules for manipulating expectation

$$\mathbb{E}\Big[k\Big] = k$$

$$\mathbb{E}\Big[k \cdot \mathrm{g}[x]\Big] = k \cdot \mathbb{E}\Big[\mathrm{g}[x]\Big]$$

$$\mathbb{E}\Big[\mathrm{f}[x] + \mathrm{g}[x]\Big] = \mathbb{E}\Big[\mathrm{f}[x]\Big] + \mathbb{E}\Big[\mathrm{g}[x]\Big]$$

$$\mathbb{E}\Big[\mathrm{f}[x]g[y]\Big] = \mathbb{E}\Big[\mathrm{f}[x]\Big]\mathbb{E}\Big[\mathrm{g}[y]\Big] \qquad \text{if} \quad x, y \quad \text{independent}$$

Now let's prove:

$$\mathbb{E}\left[(x-\mu)^2\right] = \mathbb{E}[x^2] - \mathbb{E}[x]^2$$

Keeping in mind:

$$\mathbb{E}[x] = \mu$$

Rule 1: $\mathbb{E}\Big[k\Big] = k$

Rule 2: $\mathbb{E}\Big[k \cdot \mathrm{g}[x]\Big] = k \cdot \mathbb{E}\Big[\mathrm{g}[x]\Big]$

Rule 3: $\mathbb{E}\Big[\mathrm{f}[x] + \mathrm{g}[x]\Big] = \mathbb{E}\Big[\mathrm{f}[x]\Big] + \mathbb{E}\Big[\mathrm{g}[x]\Big]$

Def'n $\mathbb{E}[x] = \mu$

$$
\begin{aligned}
\mathbb{E}[(x-\mu^2)] &= \mathbb{E}[x^2 - 2x\mu + \mu^2] \\
&= \mathbb{E}[x^2] - \mathbb{E}[2x\mu] + \mathbb{E}[\mu^2] \\
&= \mathbb{E}[x^2] - 2\mu\mathbb{E}[x] + \mu^2 \\
&= \mathbb{E}[x^2] - 2\mu^2 + \mu^2 \\
&= \mathbb{E}[x^2] - \mu^2 \\
&= \mathbb{E}[x^2] - E[x]^2
\end{aligned}
$$

Initialization

- Need for initialization
- He initialization
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- Write variance of pre-activations *f'* in terms of activations *h* in previous layer

$$\sigma^2_{f'} = \sigma^2_{\Omega} \sum_{j=1}^{D_h} \mathbb{E}\left[h_j^2\right]$$

- Write variance of pre-activations f' in terms of pre-activations f in previous layer

$$\sigma^2_{f'} = \frac{D_h \sigma^2_{\Omega} \sigma^2_f}{2}$$

Initialization

- Consider standard building block of NN in terms of *preactivations*:

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

- Set all the biases to 0

$$\boldsymbol{\beta}_k = \mathbf{0}$$

- Weights normally distributed
  - mean 0
  - variance σ_Ω^2

- What will happen as we move through the network if σ_Ω^2 is very small?
- What will happen as we move through the network if σ_Ω^2 is very large?

Aim: keep variance same between two layers

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

Consider the mean of the pre-activations:

$$\mathbb{E}[f_i'] = \mathbb{E}\left[\beta_i + \sum_{j=1}^{D_h} \Omega_{ij} h_j\right]$$

Rule 1: $\mathbb{E}\Big[k\Big] = k$

Rule 2: $\mathbb{E}\Big[k \cdot \mathrm{g}[x]\Big] = k \cdot \mathbb{E}\Big[\mathrm{g}[x]\Big]$

Rule 3: $\mathbb{E}\Big[\mathrm{f}[x] + \mathrm{g}[x]\Big] = \mathbb{E}\Big[\mathrm{f}[x]\Big] + \mathbb{E}\Big[\mathrm{g}[x]\Big]$

Rule 4: $\mathbb{E}\Big[\mathrm{f}[x]g[y]\Big] = \mathbb{E}\Big[\mathrm{f}[x]\Big]\mathbb{E}\Big[\mathrm{g}[y]\Big] \quad \text{if} \quad x, y \quad \text{independent}$

$$\mathbb{E}[f_i'] = \mathbb{E}\left[\beta_i + \sum_{j=1}^{D_h} \Omega_{ij} h_j\right]$$

$$= \mathbb{E}\left[\beta_i\right] + \sum_{j=1}^{D_h} \mathbb{E}\left[\Omega_{ij} h_j\right]$$

Set all the biases to 0

$$= \mathbb{E}\left[\beta_i\right] + \sum_{j=1}^{D_h} \mathbb{E}\left[\Omega_{ij}\right]\mathbb{E}\left[h_j\right]$$

Weights normally distributed

mean 0

variance σ_Ω^2

$$= 0 + \sum_{j=1}^{D_h} 0 \cdot \mathbb{E}\left[h_j\right] = 0$$

Initialization

- Need for initialization
- He initialization
- Interlude: Expectations
- Show that $\mathbb{E}[f_i'] = 0$
- Write variance of pre-activations *f'* in terms of activations *h* in previous layer

$$\sigma^2_{f'} = \sigma^2_\Omega \sum_{j=1}^{D_h} \mathbb{E}\left[h_j^2\right]$$

- Write variance of pre-activations f' in terms of pre-activations f in previous layer

$$\sigma^2_{f'} = \frac{D_h \sigma^2_\Omega \sigma^2_f}{2}$$

Aim: keep variance same between two layers

$$\mathbf{f}' = \boldsymbol{\beta} + \boldsymbol{\Omega}\mathbf{h}$$
$$\mathbf{h} = \mathbf{a}[\mathbf{f}],$$

$$\sigma^2_{f'} = \mathbb{E}[f_i'^2] - \mathbb{E}[f_i']^2$$

$$\longrightarrow \quad \mathbb{E}\left[(x-\mu)^2\right] = \mathbb{E}[x^2] - \mathbb{E}[x]^2$$

Rule 1: $\mathbb{E}\Big[k\Big] = k$

Rule 2: $\mathbb{E}\Big[k \cdot \mathrm{g}[x]\Big] = k \cdot \mathbb{E}\Big[\mathrm{g}[x]\Big]$

Rule 3: $\mathbb{E}\Big[\mathrm{f}[x] + \mathrm{g}[x]\Big] = \mathbb{E}\Big[\mathrm{f}[x]\Big] + \mathbb{E}\Big[\mathrm{g}[x]\Big]$

Rule 4: $\mathbb{E}\Big[\mathrm{f}[x]g[y]\Big] = \mathbb{E}\Big[\mathrm{f}[x]\Big]\mathbb{E}\Big[\mathrm{g}[y]\Big] \quad \text{if} \quad x, y \quad \text{independent}$

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

Set all the biases to 0

Weights normally distributed
- mean 0
- variance σ_Ω^2

Initialization

- Need for initialization
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- Write variance of pre-activations f’ in terms of pre-activations f in previous layer

$$\sigma^2_{f'} = \frac{D_h \sigma^2_{\Omega} \sigma^2_f}{2}$$

$$
\begin{aligned}
\sigma^2_{f'} &= \sigma^2_\Omega \sum_{j=1}^{D_h} \mathbb{E}\left[h_j^2\right] \\
&= \sigma^2_\Omega \sum_{j=1}^{D_h} \mathbb{E}\left[\mathrm{ReLU}[f_j]^2\right] \\
&= \sigma^2_\Omega \sum_{j=1}^{D_h} \int_{-\infty}^{\infty} \mathrm{ReLU}[f_j]^2 Pr(f_j) df_j \\
&= \sigma^2_\Omega \sum_{j=1}^{D_h} \int_{-\infty}^{\infty} (\mathbb{I}[f_j > 0] f_j)^2 Pr(f_j) df_j \\
&= \sigma^2_\Omega \sum_{j=1}^{D_h} \int_{0}^{\infty} f_j^2 Pr(f_j) df_j \\
&= \sigma^2_\Omega \sum_{j=1}^{D_h} \frac{\sigma_f^2}{2} = \frac{D_h \sigma^2_\Omega \sigma^2_f}{2}
\end{aligned}
$$

Aim: keep variance same between two layers

$$\sigma^2_{f'} = \frac{D_h \sigma^2_\Omega \sigma^2_f}{2}$$

Should choose:

$$\sigma^2_\Omega = \frac{2}{D_h}$$

This is called He initialization.