BOSTON UNIVERSITY

Lecture 07b Initialization

DL4DS – Spring 2025

Where we are

=== Foundational Concepts ===

- ✓ 02 -- Supervised learning refresher
- ✓ 03 -- Shallow networks and their representation capacity
- ✓ 04 -- Deep networks and depth efficiency
- ✓ 05 -- Loss function in terms of maximizing likelihoods
- ✓ 06 – Fitting models with different optimizers
- ✓ 07a – Gradients on deep models and backpropagation
- 07b – Initialization to avoid vanishing and exploding weights & gradients
- 08 – Measuring performance, test sets, overfitting and double descent
- 09 – Regularization to improve fitting on test sets and unseen data

=== Network Architectures and Applications ===

- 10 – Convolutional Networks
- 11 – Residual Networks
- 12 – Transformers
- Large Language and other Foundational Models
- Generative Models
- Graph Neural Networks
- …

Agenda

- Finish Adam optimizer from lecture 06 – Fitting Models
- Quick tips on how to read a research paper
- Model Initialization

Model Initialization

- The need for weights initialization
- Expectations Refresher
- The He (Kaiming) Initialization

Initialization

- Consider standard building block of NN in terms of pre-activations:

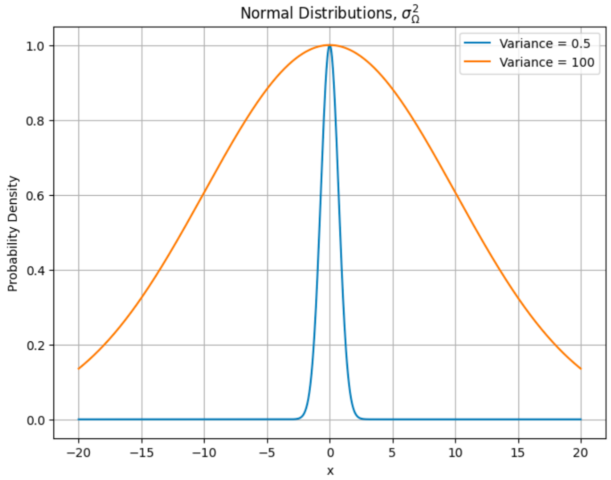
$$\begin{aligned}\mathbf{f}_k &= \boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathbf{h}_k \\ &= \boldsymbol{\beta}_k + \boldsymbol{\Omega}_k \mathrm{a}[\mathbf{f}_{k-1}]\end{aligned}$$

- How do we initialize the biases and weights?
- Equivalent to choosing starting point in our gradient descent searches

Forward Pass

- Consider standard building block of NN in terms of *pre-activations*:

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



- Set all the biases to 0

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

- Set weights to be normally distributed
  - mean 0
  - variance σ_Ω^2

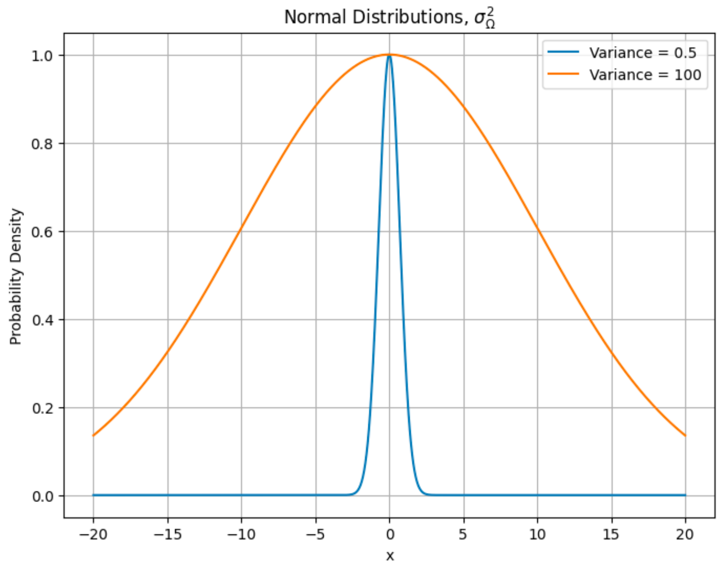
- What will happen as we move through the network if σ_Ω^2 is very small?
- What will happen as we move through the network if σ_Ω^2 is very large?

Backward Pass

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

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

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



Initialize weights to different variances

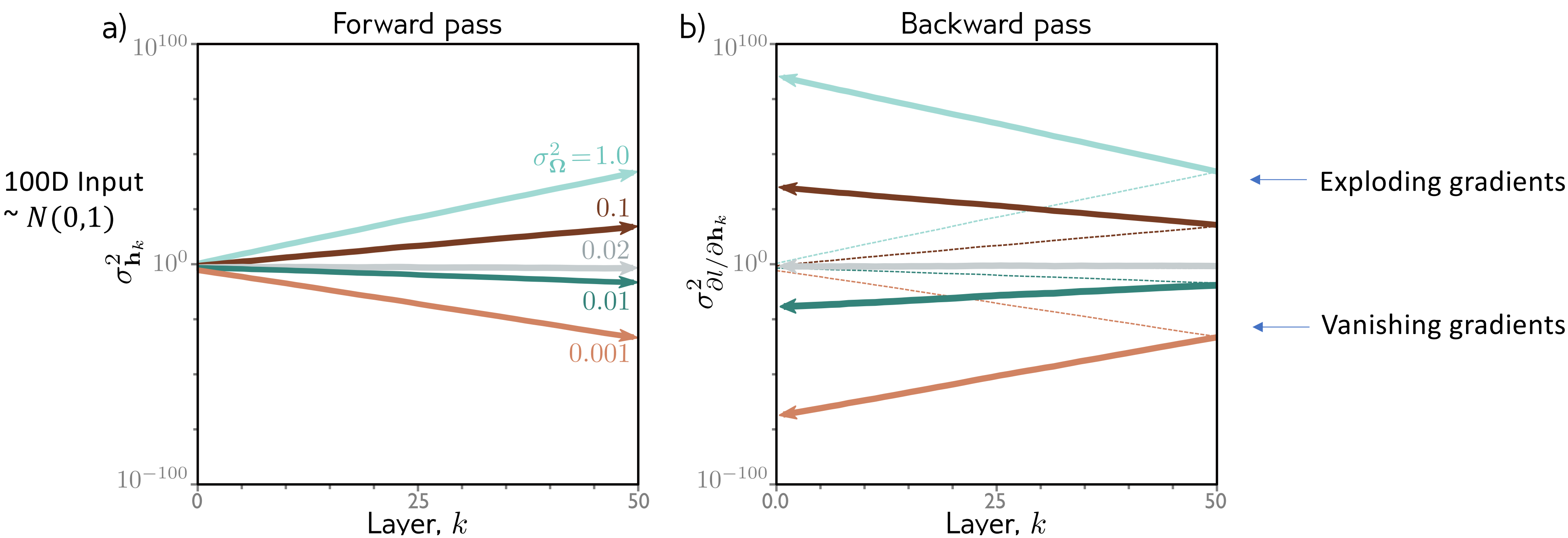


Figure 7.4 Weight initialization. Consider a deep network with 50 hidden layers and $D_h = 100$ hidden units per layer. The network has a 100 dimensional input $\mathbf{x}$ initialized with values from a standard normal distribution, a single output fixed at $y = 0$, and a least squares loss function. 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)

How do we initialize weights to keep variance stable across layers?

Aim: keep variance same between two layers

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

Definition of variance:

$$\sigma_{f'}^2 = \mathbb{E}[(f_i' - \mathbb{E}[f_i'])^2]$$

Agenda

- The need for weights initialization
- Expectations Refresher
- The He (Kaiming) Initialization

Expectations

$$\mathbb{E}\Big[\mathrm{g}[x]\Big] = \int \mathrm{g}[x] Pr(x) dx,$$

Interpretation: what is the average value of g[x] when taking into account the probability of x?

Consider discrete case and assume uniform probability so calculating g[x] reduces to taking average:

$$\mathbb{E}\Big[\mathrm{g}[x]\Big] \approx \frac{1}{N}\sum_{n=1}^{N} \mathrm{g}[x_n^*] \qquad \text{where} \qquad x_n^* \sim Pr(x)$$

Common Expectation Functions

Function $g[\bullet]$	**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 $g[x]$, the expectation $\mathbb{E}[g[x]$ 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

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

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

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

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

Agenda

- The need for weights initialization
- Expectations Refresher
- The He (Kaiming) Initialization

Aim: keep variance same between two layers

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

Definition of variance:

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

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

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

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

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

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

$$= \mathbb{E}[x^2] - \mathbb{E}[2x\mu] + \mathbb{E}[\mu^2]$$

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

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

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

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

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

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

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

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

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&= \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
\end{aligned}$$

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&= \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}
$$

Aim: keep variance same between two layers

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

$$\sigma_{f'}^2 = \mathbb{E}[(f_i' - \mathbb{E}[f_i'])^2]$$

$$\sigma_{f'}^2 = \mathbb{E}\left[f_i'^2\right] - \mathbb{E}[f_i']^2$$

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

Aim: keep variance same between two layers

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

$$\sigma_{f'}^2 = \mathbb{E}[(f_i' - \mathbb{E}[f_i'])^2]$$

$$\sigma_{f'}^2 = \mathbb{E}\left[f_i'^2\right] - \mathbb{E}[f_i']^2$$

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

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

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

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&= \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]
\end{aligned}
$$

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

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

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

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

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

Aim: keep variance same between two layers

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

$$\mathbf{h} = \mathbf{a}[\mathbf{f}],$$

$$\sigma_{f'}^2 = \mathbb{E}[(f_i' - \mathbb{E}[f_i'])^2]$$

$$\sigma_{f'}^2 = \mathbb{E}\left[f_i'^2\right] - \underbrace{\mathbb{E}[f_i']^2}_{0} = \mathbb{E}\left[f_i'^2\right]$$

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

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

Set all the biases to 0

Weights normally distributed

- mean 0
- variance σ^2_Ω

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

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

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\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]
\end{aligned}
$$

Set all the biases to 0

Weights normally distributed

mean 0

variance σ^2_Ω

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

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

For all the cross terms, $E[\Omega_{\mathrm{ij}}] = 0$ so only the squared terms are left, then use independence.

Set all the biases to 0

Weights normally distributed
mean 0
variance σ_Ω^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: $$\mathbb{E}\Big[\mathrm{f}[x]+\mathrm{g}[x]\Big] = \mathbb{E}\Big[\mathrm{f}[x]\Big]+\mathbb{E}\Big[\mathrm{g}[x]\Big]$$

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

Set all the biases to 0

Weights normally distributed
mean 0
variance σ_Ω^2

Because the Ω's are zero mean, this is the variance.

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

$$= \sigma^2_\Omega \sum_{j=1}^{D_h} \mathbb{E}\left[\text{ReLU}[f_j]^2\right]$$

$$= \sigma^2_\Omega \sum_{j=1}^{D_h} \int_{-\infty}^{\infty} \text{ReLU}[f_j]^2 Pr(f_j) df_j$$

From the definition of expectation.

$$= \sigma^2_\Omega \sum_{j=1}^{D_h} \int_{-\infty}^{\infty} (\mathbb{I}[f_j > 0] f_j)^2 Pr(f_j) df_j$$

$$= \sigma^2_\Omega \sum_{j=1}^{D_h} \int_{0}^{\infty} f_j^2 Pr(f_j) df_j$$

Only positive integral limits because of ReLU

$$= \sigma^2_\Omega \sum_{j=1}^{D_h} \frac{\sigma_f^2}{2} = \frac{D_h \sigma^2_\Omega \sigma^2_f}{2}$$

½ of the variance for zero mean distribution

Aim: keep variance same between two layers

Since:

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

Should choose:

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

To get:

$$\sigma_{f'}^2 = \sigma_f^2$$

This is called He initialization or Kaiming initialization.

K. He, X. Zhang, S. Ren, and J. Sun, "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification," Proc. IEEE International Conference on Computer Vision, 2015, pp. 1026–1034. Accessed: Feb. 11, 2024.

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

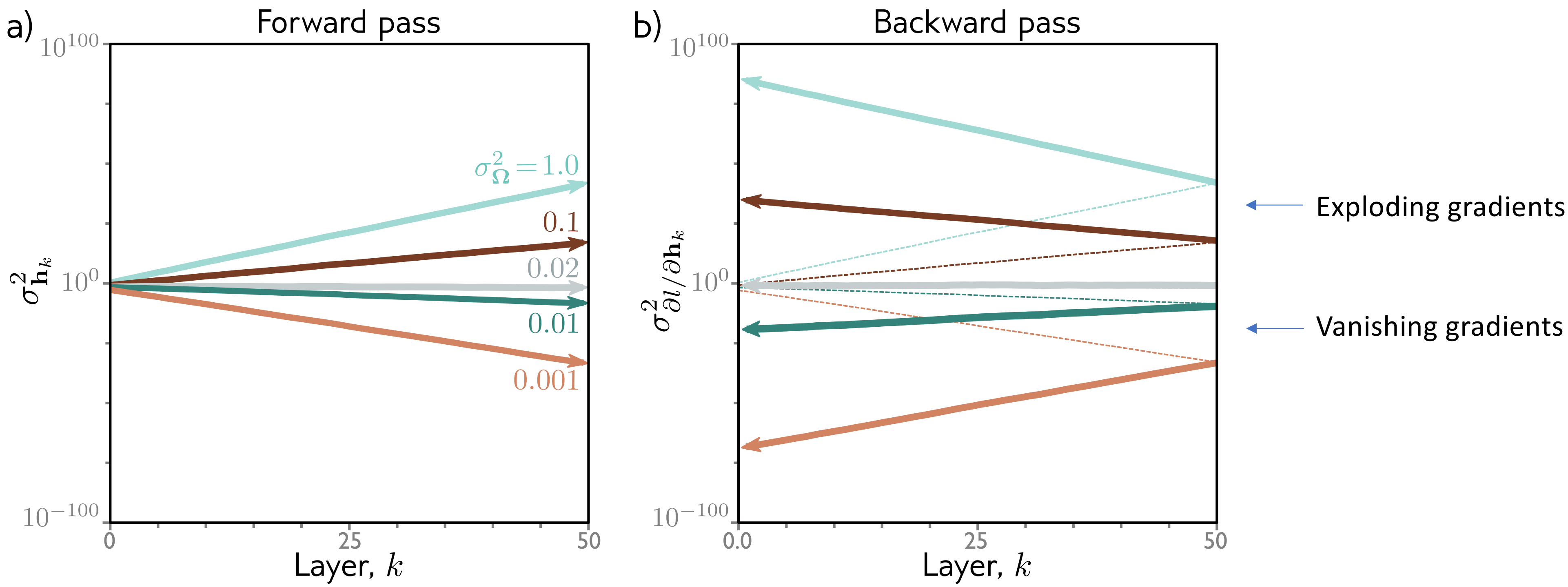

Figure 7.4 Weight initialization. Consider a deep network with 50 hidden layers and $D_h = 100$ hidden units per layer. The network has a 100 dimensional input $\mathbf{x}$ initialized with values from a standard normal distribution, a single output fixed at $y = 0$, and a least squares loss function. 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)

$$\boxed{\sigma^2_{\Omega} = \frac{2}{D_h} = \frac{2}{100} = 0.02}$$

Default Initialization in PyTorch

https://pytorch.org/docs/stable/nn.init.html#torch.nn.init.kaiming_uniform_

torch.nn.init.kaiming_uniform_(*tensor*, *a=0*, *mode='fan_in'*, *nonlinearity='leaky_relu'*, *generator=None*) [SOURCE]

Fill the input *Tensor* with values using a Kaiming uniform distribution.

The method is described in *Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification* - He, K. et al. (2015). The resulting tensor will have values sampled from $\mathcal{U}(-\text{bound}, \text{bound})$ where

$$\text{bound} = \text{gain} \times \sqrt{\frac{3}{\text{fan\_mode}}}$$

Also known as He initialization.

Feedback?

Link