CM20315 - Machine Learning

Prof. Simon Prince

7b Initialization

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

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

Initialization

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

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

- How do we initialize the biases and weights?
- Equivalent to choosing starting point in Gabor/Linear regression models

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:

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

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

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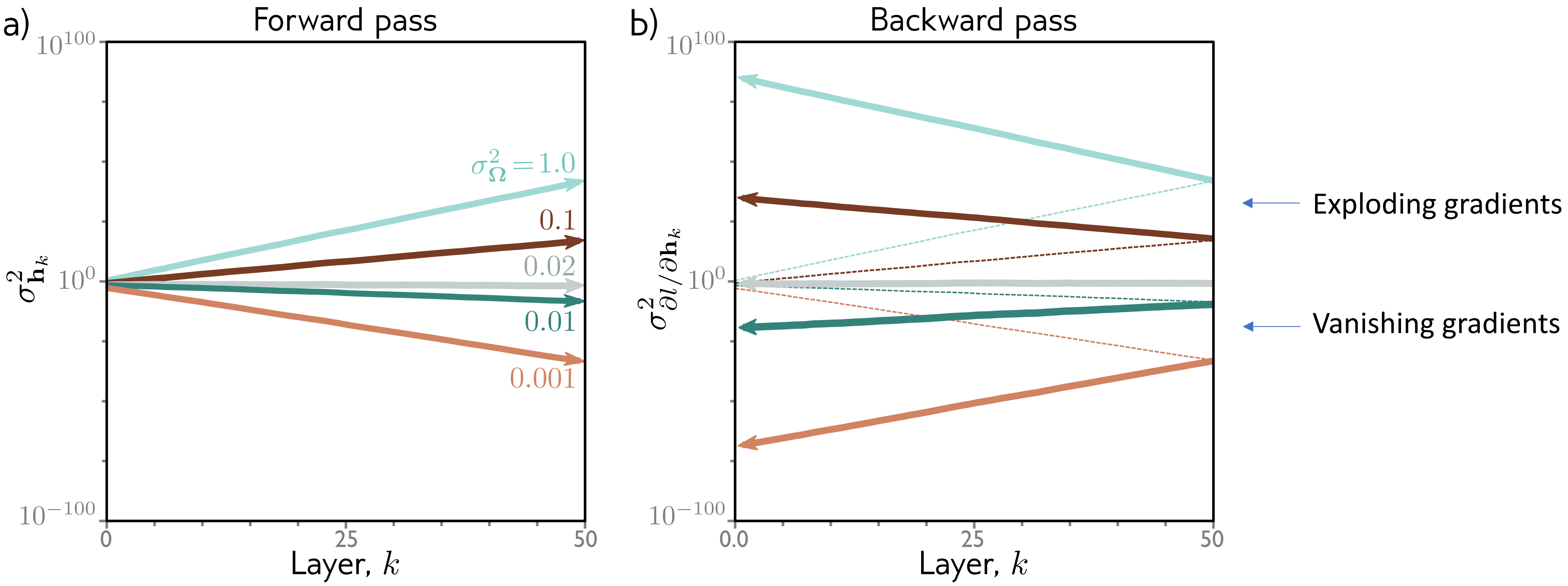


Figure 7.4 Weight initialization. Consider a deep network with 50 hidden layers and $D_h = 100$ hidden units per layer. The network has a 100 dimensional input $\mathbf{x}$ initialized with values from a standard normal distribution, a single output fixed at $y = 0$, and a least squares loss function.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

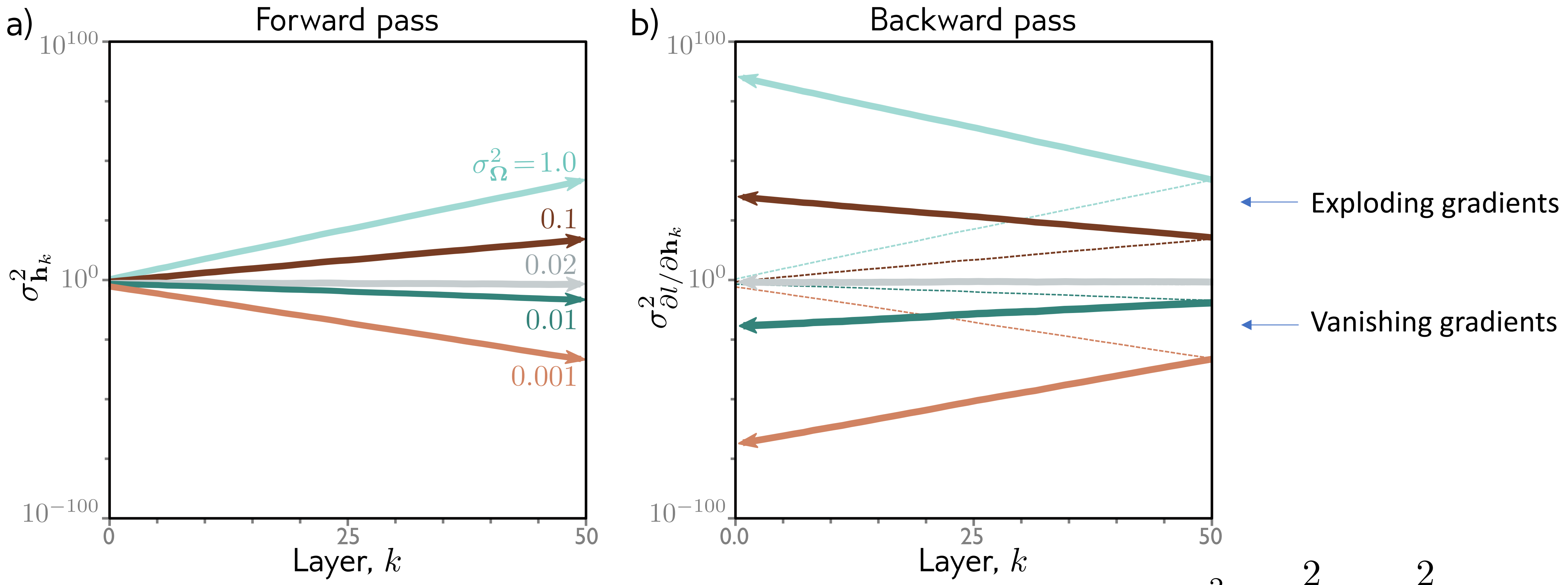
$$\sigma_{\Omega}^{2} = \frac{2}{D_h}$$

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



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

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)

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

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?

Could approximate, by sampling many values of x from the distribution, calculating g[x], and taking average:

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

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

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

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

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

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

Rule 1

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

$$\begin{aligned}\mathbb{E}\Big[\kappa\Big] &= \int \kappa Pr(x)dx \\ &= \kappa \int Pr(x)dx \\ &= \kappa.\end{aligned}$$

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

Rule 2

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

$$\begin{aligned}
\mathbb{E}\Big[\kappa \cdot \mathrm{g}[x]\Big] &= \int \kappa \cdot \mathrm{g}[x] Pr(x) dx \\
&= \kappa \cdot \int \mathrm{g}[x] Pr(x) dx \\
&= \kappa \cdot \mathbb{E}\Big[\mathrm{g}[x]\Big]
\end{aligned}$$

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

Rule 3

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

$$\begin{aligned}
\mathbb{E}\Big[\mathrm{f}[x] + \mathrm{g}[x]\Big] &= \int (\mathrm{f}[x] + \mathrm{g}[x]) Pr(x) dx \\
&= \int \left(\mathrm{f}[x] Pr(x) + \mathrm{g}[x] Pr(x)\right) dx \\
&= \int \mathrm{f}[x] Pr(x) dx + \int \mathrm{g}[x] Pr(x) dx \\
&= \mathbb{E}\Big[\mathrm{f}[x]\Big] + \mathbb{E}\Big[\mathrm{g}[x]\Big]
\end{aligned}$$

Rules for manipulating expectation

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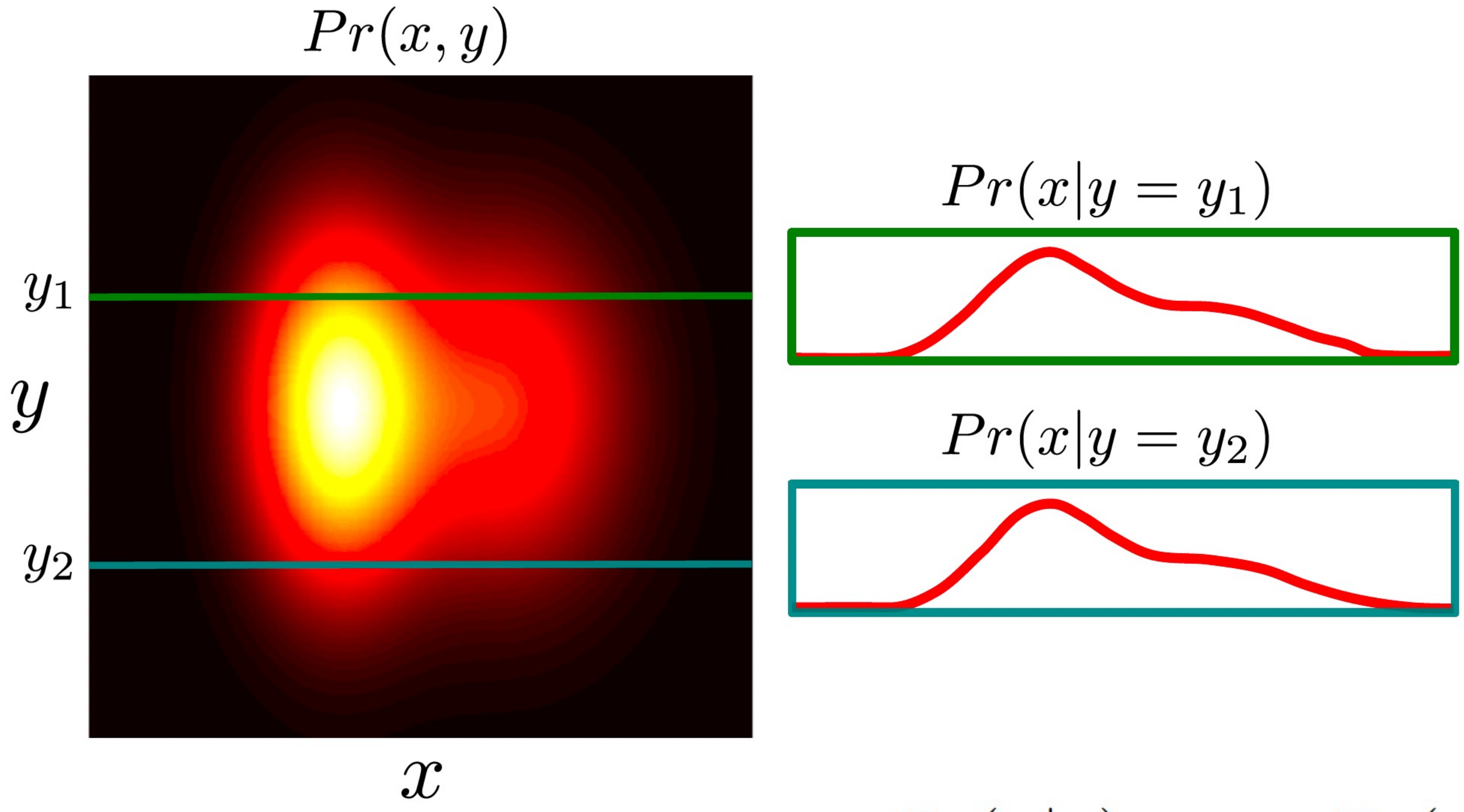
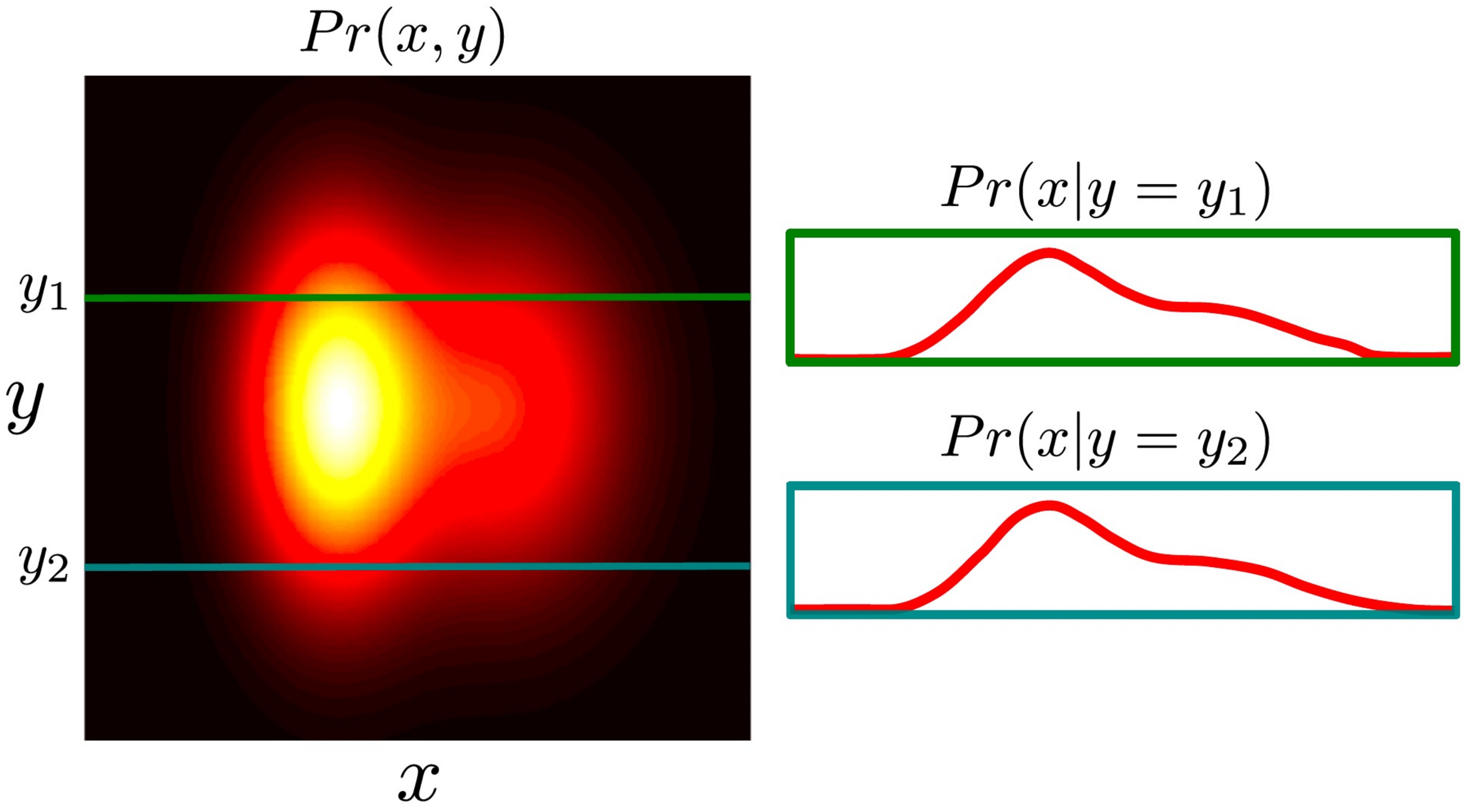
Independence



$$
\begin{aligned}
Pr(x|y) &= Pr(x) \\
Pr(y|x) &= Pr(y)
\end{aligned}
$$

Probability of x and y

Independence



$$Pr(x, y) = Pr(x)Pr(y)$$

Probability of x and y

Rule 4

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

$$\begin{aligned}
\mathbb{E}\Big[\mathrm{f}[x]\cdot\mathrm{g}[y]\Big] &= \int\int \mathrm{f}[x]\cdot\mathrm{g}[y] Pr(x,y) dx dy \\
&= \int\int \mathrm{f}[x]\cdot\mathrm{g}[y] Pr(x) Pr(y) dx dy \\
&= \int \mathrm{f}[x] Pr(x) dx \int \mathrm{g}[y] Pr(y) dy \\
&= \mathbb{E}\Big[\mathrm{f}[x]\Big]\mathbb{E}\Big[\mathrm{g}[y]\Big] \qquad \text{if} \quad x, y \quad \text{independent}
\end{aligned}$$

Because independent

Now let’s prove:

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

Keeping in mind:

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

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

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

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

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

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- Set all the biases to 0

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

- Weights normally distributed
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- What will happen as we move through the network if σ_Ω^2 is very small?
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Aim: keep variance same between two layers

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

Consider the mean of the pre-activations:

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

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

Set all the biases to 0

Weights normally distributed

mean 0

variance σ_Ω^2

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Aim: keep variance same between two layers

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

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

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

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

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

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variance σ^2_{Ω}

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

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

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

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

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
- 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

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

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

Aim: keep variance same between two layers

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

Should choose:

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

This is called He initialization.

Feedback