A Fully Rigorous Proof of the Derivation of Xavier and He’s Initialization for Deep ReLU Networks

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Abstract
A fully rigorous proof of the derivation of Xavier/He’s initialization for ReLU nets is given.

1 Introduction
Consider an $L$-layer ReLU network with layer widths $(n_l)_{l=0}^L$. Here, $n_0$ and $n_L$ denote the input and output dimension respectively, and the others are hidden layer widths. For simplicity, we assume that the network has a single output, i.e. $n_L = 1$. Let the feature map $f_l : \mathbb{R}^{n_l} \rightarrow \mathbb{R}^{n_l}$ be defined as

$$f_l(x) = \begin{cases} x & l = 0, \\ \sigma(W_l^{T}f_{l-1}) & l \in [L-1], \\ W_L^{T}f_{L-1} & l = L, \end{cases}$$

where $W_l \in \mathbb{R}^{n_{l-1} \times n_l}$, and $\sigma(x) = \max(0, x)$. Let $g_l : \mathbb{R}^{n_0} \rightarrow \mathbb{R}^{n_l}$ be the pre-activation feature map so that $f_l(x) = \sigma(g_l(x))$. Let us denote the backward derivative

$$\delta_{k,p}(x) = \frac{\partial f_L(x)}{\partial g_{k,p}(x)}, \quad \forall k \in [L-1], p \in [n_k].$$

Two quantities that are relevant for deriving Xavier and He’s initialization [1, 2] are the variance of the output of every neuron (forward pass), and the variance of the above derivative (backward pass). It is easy to see that for i.i.d weights at the initialization, we have $\text{var}(\delta_{k,p}(x)) = \text{var}(\delta_{k,q}(x))$ and $\text{var}(f_{k,p}(x)) = \text{var}(f_{k,q}(x))$, for every $p, q \in [n_k], x \in \mathbb{R}^{n_0}$. For this reason, in the following we will write $\delta_{k,p}(x)$ without mentioning the value of $p$. For every $k \in [L]$, let us also define

$$S_k = \frac{\|x\|_2}{\sqrt{2\pi}} \left( \prod_{l=1}^{k-1} \sqrt{\frac{n_l}{2}} \right) \left( \prod_{l=1}^{k} \beta_l \right).$$

In [2,1], the authors propose to initialize neural network weights in such a way that the following properties hold at the initialization:

1. All the neurons have the same variance:

$$\text{var}(f_{k,p}(x)) = \text{var}(f_{k-1,p}(x)), \quad \forall k \in [2, L]$$

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2. All the backward derivatives have the same variance for all the neurons:

\[ \text{var} (\delta_{k,p}(x)) = \text{var} (\delta_{k-1,p}(x)), \quad \forall k \in [2, L] \]  \hfill (5)

By using a heuristic derivation, they end up with the following initialization for ReLU networks:

\[ \beta_k = \frac{2}{n_k}, \quad \text{or} \quad \beta_k = \frac{2}{n_k}. \]  \hfill (5)

Here, the choice of \( \beta_k \) depends on which of the above two criteria is used.

## 2 Main Results

The following theorem provides a rigorous proof of the derivation of Xavier/He’s initialization schemes [1, 2].

**Theorem 2.1** Let \( S_k \) be defined as in (3). Then, we have:

1. Fix any \( \epsilon \in (0, 1) \). Suppose that \( \min_{l \in [k-1]} n_l \geq \Omega \left( \frac{k}{\log(1+\epsilon)} \right) \). Then, it holds:

\[ (\pi - (1 + \epsilon)^2) S_k^2 \leq \text{var}(f_{k,p}(x)) \leq (\pi - (1 - \epsilon)^2) S_k^2. \]  \hfill (6)

Moreover, \( S_k = S_{k-1} \) if and only if \( \beta_k^2 = \frac{2}{n_{k-1}}. \)

2. \( \text{var} (\delta_{k,p}(x)) = \text{var} (\delta_{k-1,p}(x)) \) if and only if \( \beta_k^2 = \frac{2}{n_k}. \)

Let us prove Theorem 2.1. The following inequalities will be useful.

**Lemma 2.2** Let us define

\[ A_n = \sum_{k=1}^{n} \left( \binom{n}{k} \sqrt{k-1}, \quad B_n = \sum_{k=1}^{n} \binom{n}{k} \sqrt{k+1}. \right. \]  \hfill (7)

Then it holds

\[ 2^n \sqrt{n} \left( 1 - \frac{3}{2n} - \frac{2}{n^2} \right) \leq A_n \leq B_n \leq 2^n \sqrt{n} - 1. \]

As a consequence, we have for \( n \geq \Omega(\epsilon^{-1}) \) that

\[ (1 - \epsilon) 2^n \sqrt{\frac{n}{2}} \leq A_n \leq B_n \leq (1 + \epsilon) 2^n \sqrt{\frac{n}{2}}. \]

**Proof:** Let \( X \sim B(n, 1/2) \) be a binomial random variable. For every \( t \geq 0 \), we have \( \sqrt{t} \geq \frac{3t-t^2}{2}. \)

Applying this inequality to \( X/(EX+1) \) and taking the expectation of both sides, we get

\[ \mathbb{E} \sqrt{X} \geq \sqrt{EX+1} \left( \frac{3EX}{2(EX+1)} - \frac{\mathbb{E}(X^2)}{2(EX+1)^2} \right). \]  \hfill (8)

Note that \( A_n = 2^n \mathbb{E} \sqrt{X} - 1. \) By applying (8) to the random variable \( X - 1 \), we obtain

\[ A_n \geq 2^n \sqrt{EX} \left( \frac{3(EX - 1)}{2EX} - \frac{EX - 2EX + 1}{2(EX)^2} \right). \]  \hfill (9)
Substituting $\mathbb{E}X = \frac{n}{2}$ and $\mathbb{E}(X^2) = \frac{n^2 + n}{4}$ gives the result. Finally, we have

$$B_n = 2^n \sqrt{\mathbb{E}X + 1} \leq 2^n \sqrt{\mathbb{E}X + 1} = 2^n \sqrt{\frac{n}{2} + 1}. \quad (10)$$

\[\square\]

Theorem 2.1 follows directly from the results of Theorem 2.3 and Theorem 2.4 presented below.

**Theorem 2.3 (Forward Pass)** Fix any $k \in [L]$, $p \in [n_k]$, $x \in \mathbb{R}^{n_k}$. Let $S_k$ be defined as in (3). Fix any $\epsilon \in (0, 1)$. Suppose that $\min_{l \in [k-1]} n_l \geq \Omega \left( \frac{k}{\log(1+\epsilon)} \right)$. Then, we have:

1. **First moment:** $(1 - \epsilon)S_k \leq \mathbb{E}[f_{k,p}(x)] \leq (1 + \epsilon)S_k$.

2. **Second moment:** $\mathbb{E}(f_{k,p}(x)^2) = \frac{\|x\|^2}{2} \left( \prod_{i=1}^{k-1} \frac{n_i}{n} \right) \left( \prod_{i=1}^{k} \beta_i^2 \right)$.

3. **Variance:** $(\pi - (1 + \epsilon)^2) S_k^2 \leq \text{var}(f_{k,p}(x)) \leq (\pi - (1 - \epsilon)^2) S_k^2$.

**Proof:**

1. Let $F_l = \{W_1, \ldots, W_l\}$. Below we omit the argument $x$ as it is clear from the context.

2. For convenience, let $f_{l}^{\otimes m}$ denote the $m$-times iterated integral $f_{l} \ldots f_{1}$. Let $v_j = \langle f_{k-1}, (W_k)_{j} \rangle$. Let $F_{k-2} = \{W_1, \ldots, W_{k-2}\}$. Conditioned on $F_{k-2}$, the variables $v_j$’s are independent Gaussian random variables: $v_j \sim \mathcal{N}(0, \beta_k^2 \|f_{k-1}\|_2^2)$. We have

$$\mathbb{E} \|f_{k-1}\|_2 = \mathbb{E} \left[ \left( \sum_{j=1}^{n_{k-1}} \sigma(v_j^2) \right)^{\frac{1}{2}} \right] = \mathbb{E} \left[ \left( \sum_{j=1}^{n_{k-1}} \sigma(v_j^2) dP(v_1 | F_{k-2}) \ldots dP(v_{n_{k-1}} | F_{k-2}) \right)^{\frac{1}{2}} \right]$$

$$= \mathbb{E} \left[ \left( \sum_{j=1}^{n_{k-1}} \sigma(v_j^2) dP(v_1 | F_{k-2}) \ldots dP(v_{n_{k-1}} | F_{k-2}) \right)^{\frac{1}{2}} \right]$$

$$= \sum_{i=1}^{n_{k-1}} \left( \frac{n_{k-1}}{i} \right)^{\otimes i} \int_{\mathbb{R}} \sum_{j=1}^{n_{k-1}} \sigma(v_j^2) dP(v_1 | F_{k-2}) \ldots dP(v_{n_{k-1}} | F_{k-2})$$

$$= \sum_{i=1}^{n_{k-1}} \left( \frac{n_{k-1}}{i} \right)^{\otimes i} \int_{\mathbb{R}} \sum_{j=1}^{n_{k-1}} \sigma(v_j^2) dP(v_1 | F_{k-2}) \ldots dP(v_{n_{k-1}} | F_{k-2})$$

$$= \sum_{i=1}^{n_{k-1}} \left( \frac{n_{k-1}}{i} \right)^{\otimes i} \int_{\mathbb{R}} \sum_{j=1}^{n_{k-1}} \sigma(v_j^2) dP(v_1 | F_{k-2}) \ldots dP(v_{n_{k-1}} | F_{k-2})$$

$$= \sum_{i=1}^{n_{k-1}} \left( \frac{n_{k-1}}{i} \right)^{\otimes i} \int_{\mathbb{R}} \sum_{j=1}^{n_{k-1}} \sigma(v_j^2) dP(v_1 | F_{k-2}) \ldots dP(v_{n_{k-1}} | F_{k-2})$$

$$= \left[ \beta_k \sum_{i=1}^{n_{k-1}} \left( \frac{n_{k-1}}{i} \right)^{\otimes i} \int_{\mathbb{R}} \sum_{j=1}^{n_{k-1}} \sigma(v_j^2) dP(v_1 | F_{k-2}) \ldots dP(v_{n_{k-1}} | F_{k-2}) \right] \mathbb{E} \|f_{k-2}\|_2.$$
Iterating this equality gives
\[
E[f_{k,p}] = \|x\|_2 \frac{\beta_k}{\sqrt{2\pi}} \prod_{l=1}^{k-1} \left[ \beta_l \sum_{i=1}^{n_l} \left( \frac{n_l}{i} \right)^{2-n_l} \sqrt{2\Gamma \left( \frac{i+1}{2} \right)} \right].
\]

By Gautschi’s inequality, we have
\[
\sqrt{\frac{i-1}{2}} \leq \sqrt{\frac{2\Gamma \left( \frac{i+1}{2} \right)}{\Gamma \left( \frac{i}{2} \right)}} \leq \sqrt{\frac{i+1}{2}}.
\]

This combined with Lemma 2.2 yields
\[
\frac{\|x\|_2}{\sqrt{2\pi}} \beta_k \prod_{l=1}^{k-1} \left[ \left( 1 - \frac{e}{k-1} \right) \beta_l \sqrt{\frac{n_l}{2}} \right] \leq E[f_{k,p}] \leq \frac{\|x\|_2}{\sqrt{2\pi}} \beta_k \prod_{l=1}^{k-1} \left[ \left( 1 + \frac{\log(1+e)}{k-1} \right) \beta_l \sqrt{\frac{n_l}{2}} \right].
\]

where we used twice our assumption in the corollary. Using the facts that \(1 + x \leq e^x\) and \(1 - \epsilon)^k \geq 1 - k\epsilon\) for \(\epsilon \in (0, 1)\), the final result follows.

2. We have \(f_{k,p}(x) = \sigma(\langle W_k, p, f_{k-1}(x) \rangle)\). Note that the distribution of the inner product is symmetric around 0, and thus taking the expectation over \(W_L\) yields
\[
E_{(W_k)}(f_{k,p}(x)^2) = \frac{\beta_k^2}{2} \|f_{k-1}(x)\|_2^2 = \frac{\beta_k^2}{2} \sum_{j=1}^{n_{k-1}} f_{k-1,j}(x)^2 = \frac{\beta_k^2}{2} \sum_{j=1}^{n_{k-1}} \sigma(\langle (W_{k-1})_j, f_{k-2}(x) \rangle)^2.
\]

Taking the expectation with respect to \(W_{L-1}\), and using the symmetry again, we obtain
\[
E_{(W_k, W_{k-1})}(f_{k,p}(x)^2) = \frac{\beta_k^2}{2} \beta_{k-1}^2 \sum_{j=1}^{n_{k-1}} \sigma(\langle (W_{k-1})_j, f_{k-2}(x) \rangle)^2.
\]

Iterating this equality leads to the result.

3. This follows from the first two statements.

The next lemma characterizes the second moments of the neurons and backward derivatives.

**Theorem 2.4 (Backward Pass)** Fix any \(k \in [L], p \in [n_k], x \in \mathbb{R}^{n_0}\). Then, we have:

1. First moment: \(E(\delta_{k,p}(x)) = 0\).

2. Second moment and Variance:
\[
\text{var}(\delta_{k,p}(x)) = E(\delta_{k,p}(x)^2) = \frac{1}{2} \left( \prod_{l=k+1}^{L-1} \frac{n_l}{2} \right) \left( \prod_{l=k+1}^{L} \beta_l^2 \right).
\]

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**Proof:** Let $v_r$ be the vector defined by

$$v_r^T = \sigma'(g_{k,p}(x)) (W_{k+1})^T \sigma_{k+1}(x) \left( \prod_{l=k+2}^{r} W_l \sigma_l(x) \right). \tag{14}$$

where $\Sigma_l(x) = \text{diag}([\sigma'(g_{l,j}(x))]_{j=1}^{n_l})$. By the chain rules, we have

$$\delta_{k,p}(x) = v_{L-1}^T W_L. \tag{15}$$

1. This follows directly from (15).

2. From (15), we have

$$\mathbb{E}_{\{W_L\}}(\delta_{k,p}(x)^2) = \beta_L^2 \|v_{L-1}\|^2. \tag{16}$$

By definition, we have $v_{L-1}^T = v_{L-2}^T W_{L-1} \Sigma_{L-1}(x)$, and thus it holds

$$\|v_{L-1}\|^2 = \sum_{j=1}^{n_{L-1}} \langle v_{L-2}, (W_{L-1})_{j} \rangle^2 \sigma'((W_{L-1})_{j}, f_{L-2}(x))).$$

Let $w$ be a copy of the random vector $(W_{L-1})_{1}$. Conditioned on $f_{L-2}(x)$, the RHS of the previous expression is a sum of i.i.d. terms, so we have

$$\mathbb{E}_{\{W_{L-1}\}} \|v_{L-1}\|^2 = n_{L-1} \mathbb{E}_{\{w\}} \langle v_{L-2}, w \rangle^2 \sigma'((w, f_{L-2}(x))) = \frac{n_{L-1} \beta_{L-1}^2}{2} \|v_{L-2}\|^2,$$

where the last equality follows from the fact that $w$ and $-w$ have the same distribution, and we used the identity $\sigma'(x) = 1 - \sigma'(x)$. Iterating this argument leads to the result.

□

**References**

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