Revisiting Initialization of Neural Networks

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Abstract

Good initialization of weights is crucial for effective training of deep neural networks. In this paper we discuss an initialization scheme based on rigorous estimation of the local curvature. The proposed approach is more systematic and recovers previous results for activations such as smooth functions, ReLU and drops.

1 Introduction

1.1 Initialization of neural networks

We look at a neural network as a chain of mappings

\[ z^{(k+1)} = f^{(k)} \left( w^{(k)} \cdot z^{(k)} + b^{(k)} \right) \]

which sequentially process the input \( z^0 = x \). We assume that \( z^{(k)} \) are real vectors of shape \( [d_k] \), weights \( w^{(k)} \) are matrices of shape \( [d_{k+1}, d_k] \), biases \( b^{(k)} \) are of shape \( [d_{k+1}] \), and \( f^{(k)} \) are (possibly non-linear) activation functions applied element-wise. The task is to minimize some cost function \( L(z, t) \) where \( z = z^n \) is the network output and \( t \) is ground truth, over the weights \( w^0, \ldots, w^{n-1} \).

Neural networks are optimized with variants of gradient descents and weights are initialized randomly. Too small weights make the learning process slow while too high may cause unstable updates and over-shooting issues. Good initialization schemes aim to find the right balance.

Initialization based on variance flow Glorot and Bengio [2] proposed a framework which estimates the variance at different layers in order to maintain the balance. In this approach we assume that activation functions are approximately like identity around zero, that is \( f(u) \approx u \) for small \( u \) (this can be easily generalized, see [4, 10]). Linearizing we obtain

\[ z_i^{(k+1)} \approx \sum_{j=1}^{d_k} w_{i,j}^{(k)} \cdot z_j^{(k)} + b_i^{(k)} \]  

(1)

In the forward pass, we require \( \text{Var}[z^{(k+1)}] \approx \text{Var}[z^{(k)}] \) to maintain the magnitude of inputs until the last layer. In the backward we compute the gradients by recursively applying the chain rule

\[ \partial_{z_i^{(k)}} L = \sum_{j=1}^{d_k} \partial_{z_j^{(k+1)}} L \cdot \partial_{z_j^{(k)}} z_j^{(k+1)} \approx \sum_{j=1}^{d_k+1} \partial_{z_j^{(k+1)}} L \cdot w_{j,i}^{(k)} \]  

(2)

and want to keep their magnitude, that is \( \text{Var}[\partial_{z^{(k-1)}} L] \approx \text{Var}[\partial_{z^{(k)}} L] \). Looking at Equation (1) and Equation (2) we see that the weights \( w^{(k)} \) act on the previous layer during forward pass and on the next layer during the backward pass. The first action is multiplying along the input dimension \( d_k \) and the second action is multiplying along the output dimension \( d_{k+1} \). One can prove that, in general, taking dot-product with an independent centered random matrix along the dimension \( d \) scales the variance by the factor \( d^2 \) [2, 10]. To balance the action during the forward and backward pass one therefore chooses \( w^{(k)} \) to be zero-mean, iid with standard deviation

\[ \sigma[w^{(k)}] = \sqrt{\frac{2}{d_k + d_{k+1}}} \]  

(3)
Criticism of variance flow analysis  We briefly discuss drawbacks of the variance analysis before presenting our framework

Ignored correlations Previous works [2, 4, 10, 5] less or more silently assumed the independence of weights across layers. To our knowledge we are first to point this is not true already in first pass, as backpropagated gradients depend on weights used during the forward pass and also on inputs. Consider regression with two layers and linear activation so that \( L = (z - t)^2, z = w_2w_1x \). Note that \( \partial_z L = 2(z - t) = -2(w_2w_1 - t) \) depends on both \( w_2 \) and \( w_1 \). To see correlations with inputs consider one-dimension regression \( L = (z - t)^2, z = wx \) from Eq. 5 in [2] we should have \( \text{Var}[\partial_w L] = \text{Var}[\partial_w z] \cdot \text{Var}[\partial_t L] \) for \( w \) with unit variance, but this gives \( \text{Var}[2(wx - t)x] = \text{Var}[x] \cdot \text{Var}[2(wx - t)] \). Not only two sides can be a factor away but also target \( t \) can be correlated to input \( x \).

Limited quantitative insights Except these flaws, the variance analysis provides only qualitative insights as it does not directly connect the variance estimation to the optimization problem. In fact, we cannot get more quantitative insights such as estimating the step size from the first order methods.

1.2 Our contribution

We propose to use the second order methods, more precisely to estimate the curvature at the initialization point. We discuss a framework that can be used to approximate and control the hessian norm under initialization. Besides theoretical results, we provide an implementation of our framework along with experiments. Under our framework, we are able to derives formulas very close to those proposed before.

1.2.1 Hessian-based framework

For training neural network one uses variants of gradient descent, which updates the model parameters \( w \) by a step towards the gradient \( g = D_wL \) of the loss function. In order to quantify the decrease we need the second-order approximation

\[
L(w - \gamma g) \approx L(w) - \gamma g^T g + \frac{\gamma^2}{2} g^T H g
\]

where \( \cdot \) stands for the matrix (or more generally: tensor) dot product. The maximal step size \( \gamma^* \) which guarantees a decrease equals \( \gamma^* = \| H \|^{-1} \) where \( \| H \| \) is the hessian norm, or equivalently: maximal eigenvalue. Turning this statement around: if we want to train with a constant step then we need to control the hessian. We propose the following paradigm

*Good initialization controls hessian:* we initialize so that \( \| H_w(k) \| \approx 1 \).

We make the following mild assumption about loss functions

*Admissible loss functions:* loss functions used satisfy \( f(0) = 0 \) and \( f''(0) = 0 \). This is the case of all standard functions: linear, sigmoid, tanh, relu.

Finally, our techniques aim to approximate the curvature up to leading terms. These approximations are accurate under the following mild assumption

*Relatively small inputs:* we have \( \| z^{(k)} \| \leq c \) for all layers \( k \) for some small constant \( c \), e.g. \( c = 0.1 \).

Note this is simply stability of the forward pass and is implicitly assumed in the variance flow analysis (which assumes linear regime).

Before presenting our results we need some more notation. Let \( F^{(k)} = z^{(k)} \) be the input of \( k \)-th layer. Let \( A^{(k)} = D_w(z^{(k+1)}) \) be the derivative of the forward activation at \( k \)-th layer, with respect to the output before activation \( u^{(k)} = w^{(k)} \cdot z^{(k)} + b^{(k)} \). Let \( B^{k+1} = D_{z^{(k+1)}} z^{(n)} \) be the output derivative backpropagated to the input of \( k + 1 \)-th layer. Let \( H_z = D_z^2L(z,t) \) be the loss hessian with respect to the predicted value \( z \). Let \( H_w = D^2L(z^{(n)}, t) \) be the loss hessian with respect to the weights.

\footnote{Visit \url{https://github.com/maciejskorski/nn_hessian_initialization/}}
Table 1: Relative error of our approximation in Theorem 1. The architecture is a 4-layer network for MNIST, with hidden layers each of 32 units and tanh activation.

Inputs are scaled by the factor $r$.

### 1.2.2 Approximating hessian chain rule

The hessian of the loss function on its domain is usually very simple and has nice properties. This however changes when a neural network reparametrizes the problem by a complicated dependency of the output $z$ on the weights $w$. We thus have to answer the following question: how the dependency of the network output on the weights changes the curvature? If general if $z = z(w)$ is a reparametrization then

$$
\frac{\partial^2}{\partial w \partial t} L(z(w), t) = \frac{\partial^2}{\partial z \partial t} L(z, t) \cdot \frac{\partial}{\partial w} z(w) \cdot \frac{\partial}{\partial t} z(w)
$$

where bullets are tensor dot-products along appropriate dimensions. This is more subtle than backpropagation of first derivatives, because both: first and second order effects have to be captured. The main contribution of this work is the following result, which basically says that the curvature effect is of smaller magnitude.

**Theorem 1** (Hessian chain rule for neural network). With notation as above, the loss hessian $H_w(z)$ with respect to the weights $w(k)$ satisfies, up to the leading term

$$
H_w(z)[g, g] \approx v^T \cdot H_z \cdot v, \quad v = B^{(k)} \cdot A^{(k)} \cdot g \cdot F^{(k)}
$$

where products are standard matrix products. More precisely, the approximation holds up to a third-order error term $f''' c^3 \cdot \|g\|^2$ where $f'''$ is the bound on the third derivative of activation functions and $c$ is the bound on inputs. The leading term is of order $c^2 \cdot \|g\|^2$.

We have two important properties.

**Remark 1** (Perfect approximation for relu). We have exact equality for activations satisfying $f'' = 0$ such as variants of relu.

**Remark 2** (Good approximation up to leading terms). Regardless of the activation function, the error term is of smaller order under our assumption of relatively small inputs.

We evaluate the approximation numerically.

### 1.2.3 Approximating hessian by layers jacobian products

We are left with the linearization effect and we can factor it further. This reduces the problem to controlling products of layer’s jacobians.

**Theorem 2** (Hessian factorized into jacobians). Up to third-order terms in $z^{(i)}$ we can factorize $v$ from Theorem 1 into

$$
v \approx J^{(n-1)} \cdot \ldots \cdot J^{(k+1)} \cdot A \cdot g \cdot J^{(k-1)} \cdot \ldots \cdot J^{(0)} \cdot z^{(0)}
$$

where $J^k = D_{z^{(k)}} z^{(k+1)}$ is the derivative of the output with respect to the input at $k$-th layer. In particular, the hessian biggest eigenvalue scales by a factor at most $\|v\|^2$ where

$$
\|v\| \leq \|J^{(n-1)} \cdot \ldots \cdot J^{(k+1)} \| \cdot \|A\| \cdot \|J^{(k-1)} \cdot \ldots \cdot J^{(0)}\| \cdot \|z^{(0)}\|
$$

3
The norm of the matrix product \( \|J_k \ldots J_1\| \) is computed as the maximum of the vector norm \( \|J_k \ldots J_1 \cdot v\| \) over vectors \( v \) with unit norm. Given this result, the good initialization aims to make the backward and forward products of norm roughly one.

**Remark 3** (Connection to products of random matrices). *Note that our problem closely resembles the problem of random matrix products [6]. This is because jacobians for smooth activations are simply random weight matrices.*

**Remark 4** (Connection to spectral norms). *It is possible to estimate the product of random matrices by the product of their spectral norms. In particular the spectral norm of random \( m \times n \) matrix with zero-mean and unit variance entries is \( \frac{1}{\sqrt{m+n}} \) on average [9]. For Gaussian case this can be computed more precisely by Wishart matrices [1]. This however is overly pessimistic for long products.*

### 1.2.4 Applications: initialization schemes

**Smooth activations** We need the following lemma

**Lemma 1** (Dot-product by random matrices). *Let \( w \) be a random matrix of shape \([n, m]\), with zero-mean entries of variance \( \sigma^2 \). Let \( z, z' \) be independent vectors of shape \([m] \) and \([n] \) respectively. Then

\[
\begin{align*}
\mathbb{E}\|w \cdot z\|^2 &= n\sigma^2 \cdot \mathbb{E}\|z\|^2 \\
\mathbb{E}\|z' \cdot w\|^2 &= m\sigma^2 \cdot \mathbb{E}\|z'\|^2.
\end{align*}
\]

Using this we can estimate the growth of jacobian products in Theorem 2 as follows

**Corollary 1** (Smooth activations [2]). *Consider activations such that \( f'(0) = 1 \). Then \( \mathbf{J}^{(k)} \approx w^{(k)} \) (up to leading terms) and the norm of the forward product is stable when

\[\operatorname{Var}[w^{(k)}] = \frac{1}{d_{k+1}}\]

and the norm of the backward product is stable when

\[\operatorname{Var}[w^{(k)}] = \frac{1}{d_k}\]

As a compromise we can choose

\[\operatorname{Var}[w^{(k)}] = \frac{2}{d_{k+1} + d_k}\]

**Dropout** Dropouts can be seen as a randomized function \( f_p \) which for a certain dropout probability \( p \) multiplies the input by \( B_{1-p} \cdot \frac{1}{1-p} \) where \( B_{1-p} \) is Bernoulli random variable with parameter \( 1-p \). The jacobian is precisely

\[
\mathbf{J} = w = \text{diag}(B_1, \ldots, B_d), \quad B_i \sim \text{Bern}(1-p)
\]

When multiplying from left or right, this scales the norm square by \((1-p)^{-2} \cdot \mathbb{E}[\text{Bern}(1-p)]^2 = 1 - p \). Thus we obtain

**Corollary 2** (Initialization for dropout). *Let \( 1-p \) be the keep rate of a dropout. Let \( \sigma^2 \) be the initialization variance without dropout, it should be corrected as

\[\sigma' = \sigma / \sqrt{1-p}\]

This corresponds to the analysis in [3], except that they suggest a different correction factor for backpropagation which appears to be a mistake.

**ReLU** Rectified Linear Unit [7] is a non-linear activation given by \( f(u) = \max(u, 0) \). Consider a layer such that \( z' = f(u) \), \( u = w \cdot z \) where \( w \) is zero-centered with variance \( \sigma^2 \) of shape \([n, m]\) and \( z \) is of shape \( m \). We have \( \mathbf{J} = D_z z' = \text{diag}(f'(u)) \cdot w \). For the forward product, we consider \( \mathbf{J} \cdot z = \text{diag}(f'(u)) \cdot u \). This scales the norm of \( u \) by \( \frac{1}{2} \) when \( u \) is symmetric and zero-centered, which is true when \( w \) is symmetric and zero-centered. The norm of \( z \) is thus changed by \( \frac{2\sigma}{\sqrt{m}} \). For the backward product we have to consider \( v \cdot \mathbf{J} \cdot \mathbf{J} \), where \( \mathbf{J} \) is the jacobian products for subsequent layers and possibly depends on \( u \). However if the next layer is initialized with IID, the output distribution only depends on the number of active neurons \( r = \# \{ i : u_i = 1 \} \). Conditioned on this information, next layers are independent from \( \mathbf{J} \). Given \( r \), the squared backward product norm changes by the factor \( r/n \cdot m\sigma^2 \). Since \( \mathbb{E}[r] = n/2 \) the scaling factor is \( \frac{m\sigma^2}{2} \).
Corollary 3 (ReLU initialization [4]). The initialization variance \( \sigma^2 \) in the presence of ReLU should be corrected as

\[
\sigma' = \frac{\sigma}{\sqrt{2}}
\]  

(14)

2 Preliminaries

Tensor derivatives For tensors \( y = y_{j_1,\ldots,j_p} \) of rank \( q \) and \( x = x_{i_1,\ldots,i_q} \) of rank \( q \) the derivative \( D = D_xy \) is a tensor of rank \( q+p \) with coordinates \( D_{j_1,\ldots,j_q,i_1,\ldots,i_p} = \frac{\partial y_{j_1,\ldots,j_q}}{\partial x_{i_1,\ldots,i_p}} \). If \( y = f(x) \) where \( x \) has shape \([n]\) and \( y \) has shape \([m]\) then \( D_xy \) is of shape \([m,n]\) and equals the total derivative of \( f \).

Tensor products Contraction sums over paired indices (axes), lowering rank by 2 (or more when more pairs are specified). For example, contracting positions \( a \) and \( b \) in \( x \) produces the tensor \( \sum_i x_{i_1,\ldots,i_a,i_{a+1},\ldots,i_p} \) with indices \( \{i_1,\ldots,i_a,i_{a+1},\ldots,i_p\} \). The dimensions of paired indices should match.

Full tensor product combines tensors \( x \) and \( y \) by cross-multiplications \( (x \otimes y)_{i_1,\ldots,i_p,j_1,\ldots,j_q} = x_{i_1,\ldots,i_p} \cdot y_{j_1,\ldots,j_q} \) producing a tensor of rank \( p+q \). Tensor dot-product is the full product followed by contraction of two compatible dimensions. For example, the standard matrix product of \( A_{i,j} \) and \( B_{k,l} \) is the tensor product followed by contraction of \( j \) and \( k \). We denote the dot-product by \( \bullet \), omitting the contracted axes when this is clear from context.

Chain and product rules Tensors obey similar chain and product rules as matrices. Namely we have \( D_x(A \bullet B) = D_xA \bullet B + A \bullet D_xB \). Also when \( B = f(A(x)) \) we have \( D_xB = D_A f \bullet D_xA \). The contraction is over all dimensions of \( A \) which match arguments of \( f \).

Spectral norm For any rectangular matrix \( A \) the singular eigenvalues are defined as square roots of eigenvalues of \( A^T A \) (which is square symmetric, hence positive definite). The spectral norm is the biggest singular eigenvalue.

3 Proof of Main Result

3.1 Hessian chain rule

Our goal is to compute the Hessian with respect to the parameters in the layer \( k \). By the chain rule

\[
D_{w^{(k)}} L = D_{z^{(n)}} L \bullet D_{w^{(k)}} z^{(n)}
\]  

(15)

Note that the second tensor is of shape \([d_1, d_{k+1}, d_k]\) (rank 3!), the contraction is over the dimension of \( z^{(n)} \). Again by the chain and product rules

\[
D^2_{w^{(k)}} L = D^2_{z^{(n)}} L \bullet D_{w^{(k)}} z^{(n)} \bullet D_{w^{(k)}} z^{(n)} + D_{z^{(n)}} L \bullet D^2_{w^{(k)}} z^{(n)}
\]  

(16)

In the component \( H_1 \) the dot-products contract indices \( z^{(n)} \) (note that \( D^2 \) is symmetric and the terms \( D \) are same, hence the order of pairing dimensions of \( w^{(k)} \) does not matter). As for the second component \( H_2 \), it is a product of tensors of rank 1 and 5. In order to further simplify, we are going to show that \( H_2 \) negligible compared to \( H_1 \), the intuition is as follows: in \( H_1 \) the contribution comes from gradients \( D_{w^{(k)}} \) while in \( H_2 \) from second-order derivatives \( D^2_{w^{(k)}} \); we consider activations such that \( f(u) = au + O(u^3) \) and therefore for small \( u \) second-derivatives are near zero but first derivatives are not, and their contributions dominate.

In the analysis below we assume that weights are sufficiently small, and biases are zero (or of much smaller variance compared to weights). Let \( u^{(k)} = w^{(k)} \cdot z^{(k)} + b^{(k)} \) be the output before activation at the \( k \)-th layer.

Due to Equation (16), our goal is to evaluate first and second derivatives of \( z^{(n)} \) with respect to weights \( w^{(k)} \), under the assumption that inputs \( z^{(i)} \) are sufficiently small. Consider how \( z^{(k+1)} \)
depends on \( w^{(k)} \). By the chain rules

\[
D_{w^{(k)}} z^{(k+1)} = D_{u^{(k)}} f(u^{(k)}) \bullet D_{w^{(k)}} u^{(k)} \tag{17}
\]
\[
D^2_{w^{(k)}} z^{(k+1)} = D^2_{u^{(k)}} f(u^{(k)}) \bullet D_{w^{(k)}} u^{(k)} \bullet D_{w^{(k)}} u^{(k)} \tag{18}
\]

Note that \( D_{u^{(k)}} f(u^{(k)}) \) and \( D^2_{u^{(k)}} f(u^{(k)}) \) are diagonal tensors because \( f \) is applied element-wise. More precisely

\[
\left[ D^2_{u^{(k)}} f(u^{(k)}) \right]_{i,j,j'} = \delta_{i,j} \delta_{i,j'} \cdot f'''(u_i^{(k)}) \tag{19}
\]

where \( \delta_{i,j} \) is the Kronecker delta which is one where indices match and zero otherwise. Moreover,

\[
\left[ D_{w^{(k)}} u^{(k)} \right]_{j,p,q} = \frac{\partial}{\partial w_{p,q}^{(k)}} (u_i^{(k)} \cdot z^{(k)} + b^{(k)})_j = \delta_{j,p} \cdot z_q^{(k)} \tag{20}
\]

Thus

\[
\left[ D^2_{w^{(k)}} z^{(k+1)} \right]_{i,p,q,p',q'} = \delta_{i,p} \delta_{i,p'} \cdot f'''(u_i^{(k)}) \cdot z_q^{(k)} \cdot z_{q'}^{(k)} \tag{21}
\]

When this tensor acts, as a bi-linear form, on a tensor \( g = g_{p,q} \) we therefore obtain

\[
\left[ D^2_{w^{(k)}} z^{(k+1)} \right] \bullet g \bullet g = f'''(u_i^{(k)}) \sum_{q,q'} z_q^{(k)} z_{q'}^{(k)} g_{i,q} g_{i,q'} \tag{22}
\]

\[
= f'''(u_i^{(k)}) \left( \sum_q z_q^{(k)} g_{i,q} \right)^2 \tag{23}
\]

Since our assumption on activations implies \( f'''(u) = O(f'' \cdot u) \) for real \( u \), we see this is of order \( O(f'' \| u^{(k)} \| \| z^{(k)} \|^2) \cdot \| g \|^2 \).

**Claim 1** (Magnitude of second derivative of weights).

\[
D^2_{w^{(k)}} z^{(k+1)} \bullet g \bullet g = O(f'' \| u^{(k)} \| \| z^{(k)} \|^2) \cdot \| g \|^2 \tag{24}
\]

which is of order \( O(f'' \cdot c^3) \) where \( c \) is the constant from our 'relatively small inputs' assumption.

Next, observe that the roles of \( z^{(k)} \) and \( u^{(k)} \) in \( u^{(k)} \) are symmetric. Thus we have a similar result with respect to \( z^{(k)} \).

**Claim 2** (Magnitude of second derivative of inputs).

\[
D^2_{z^{(k)}} z^{(k+1)} \bullet g \bullet g = O(f'' \| u^{(k)} \| \| w^{(k)} \|^2) \cdot \| g \|^2 \tag{25}
\]

which is of order \( O(f'' \cdot c) \) where \( c \) is the constant from our 'relatively small inputs' assumption.

We need to prove that this propagates to higher-level outputs \( z^{(i)} \), where \( i > k \). This is intuitive, considering now that \( z^{(i)} \) is a function of \( z^{(k+1)} \) with no dependencies on \( u^{(k)} \). To prove it formally look at the second-order chain rule

\[
D^2_{w^{(k)}} z^{(i)} = D^2_{z^{(k+1)}} z^{(i)} \bullet D_{w^{(k)}} z^{(k+1)} \bullet D_{w^{(k)}} w^{(k)} \bullet D_{w^{(k)}} w^{(k)} \tag{26}
\]

Now the second term is clearly \( O(f''' c^3) \) by the first claim. As for the first term, the first tensor is of order \( O(f'' c) \) while the two others are \( O(f c) \). The dot-product gives the bound \( O(f''' c^3) \).

**Claim 3.** For every \( i > k \) it holds \( D^2_{w^{(k)}} z^{(i)} = O(f'' c^3) \).

Summing up, we can ignore second-derivatives with respect to weights, and this is accurate except third-order terms in the magnitude of \( z^{(i)} \). In particular, we can ignore the effect of \( H_2 \).
3.2 Factorizing hessian quadratic form

Consider any potential update vector \( g \) for weights \( w^{(k)} \), it has to be of same shape as \( D_{w^{(k)}}L \) or equivalently \( w^{(k)} \), that is \([d_{k+1}, d_k] \). Our goal is to evaluate the hessian quadratic form on \( g \). Ignoring the smaller part \( H_2 \) we are left with \( H_1 \) which gives

\[
D^2_{w^{(k)}}L \cdot g \cdot g = D^2_{z^{(n)}}L \cdot D_{w^{(k)}}z^{(n)} \cdot D_{w^{(k)}}z^{(n)} \cdot g \cdot g
\]

(27)

where \( g \) is contracted on all indices together with \( w^{(k)} \). To emphasize this we can regroup, obtaining

**Claim 4** (Hessian quadratic form). The hessian quadratic form for an update \( g \) equals

\[
D^2_{w^{(k)}}L \cdot g \cdot g = D^2_{z^{(n)}}L \cdot \left(D_{w^{(k)}}z^{(n)} \cdot g \right) \cdot \left(D_{w^{(k)}}z^{(n)} \cdot g \right)
\]

(28)

We work further to simplify rank-3 tensors. By the chain rule

\[
D_{w^{(k)}}z^{(n)} \cdot g = D_{z^{(k+1)}}z^{(n)} \cdot D_{w^{(k)}}z^{(k+1)} \cdot g
\]

(29)

Let \( u^{(k)} = w^{(k)} \cdot z^{(k)} + b^{(k)} \) be the output before activation. By the chain rule

\[
D_{w^{(k)}}z^{(k+1)} = D_{u^{(k)}}z^{(k+1)} \cdot D_{w^{(k)}}u^{(k)}
\]

(30)

Note that \( D_{w^{(k)}}u^{(k)} \) is a third-order tensor of shape \([d_{k+1}, d_{k+1}, d_k] \). Denote its elements by \( M_{i',i,j} \). We have

\[
\left[D_{w^{(k)}}u^{(k)}\right]_{i',i,j} = [i' = i] \cdot z_j^{(k)}
\]

(31)

and we compute the dot product

\[
\left[D_{w^{(k)}}u^{(k)} \cdot g\right]_{i'} = \sum_{i,j} \left[D_{w^{(k)}}u^{(k)}\right]_{i',i,j} g_{i,j} = \sum_j z_j^{(k)} g_{i',j}
\]

(32)

which can be expressed compactly in matrix products as

\[
D_{w^{(k)}}u^{(k)} \cdot g = g \cdot z^{(k)}
\]

(33)

which is a vector of shape \([d_{k+1}] \). Using this in Equation (30) we obtain, in terms of matrix products

\[
D_{w^{(k)}}z^{(k+1)} \cdot g = D_{u^{(k)}}z^{(k+1)} \cdot \left(D_{w^{(k)}}z^{(k+1)} \cdot g\right) = D_{u^{(k)}}z^{(k+1)} \cdot g \cdot z^{(k)}
\]

(34)

Now, in terms of matrix products, Equation (29) becomes

\[
D_{w^{(k)}}z^{(n)} \cdot g = D_{z^{(k+1)}}z^{(n)} \cdot D_{w^{(k)}}z^{(k+1)} \cdot g \cdot z^{(k)}
\]

(35)

which is a vector of shape \([d_n] \). Finally note that \( H \cdot v \cdot v = v^T \cdot H \cdot v \) where \( H \) is a symmetric matrix and \( v \) is vector. This proves

**Claim 5** (Approximated hessian form). For sufficiently small inputs, the hessian quadratic form can be approximated as

\[
H_{w^{(k)}}[g, g] \approx v^T \cdot H_z \cdot v
\]

(36)

where

\[
v = D_{z^{(k+1)}}z^{(n)} \cdot D_{w^{(k)}}z^{(k+1)} \cdot g \cdot z^{(k)}.
\]

(37)

This claim implies the first part of Theorem. The error estimate follows by follows by the discussion in the previous subsection.

3.3 Further factorization

We have seen that the quadratic effects of \( w^{(k)} \) can be ignored, thus it is enough to consider the simplified recursion

\[
z^{(k+1)} \approx a \cdot (w^{(k)} \cdot z^{(k)} + b^{(k)})
\]

(38)

for a diagonal matrix \( a \) (which captures first-derivatives of activations), or equivalently
Claim 6 (Second-order recursion for small inputs). For relatively small inputs the hessian can be computed under the simplified recursion

\[ z^{(k+1)} \approx J^k \cdot z^{(k)} \]  

(39)

where \( J^k = D_{z^{(k)}} z^{(k+1)} \). In particular the term \( H_2 \) can be ignored.

We now proceed to further factorize \( v \). By linearization we obtain

\[ z^{(k)} \approx D_{z^{(k-1)}} z^{(k)} \cdot z^{(k-1)} = \ldots = D_{z^{(k-1)}} z^{(k)} \]  

(40)

Moreover, by the chain rule, output gradient factorizes as

\[ D_{z^{(k+1)}} z^{(n)} = D_{z^{(n-1)}} z^{(n)} \cdot z^{(k-1)} \cdot D_{z^{(n-2)}} z^{(n-1)} \cdot \ldots \cdot D_{z^{(k+1)}} z^{(k-1)} \cdot D_{z^{(k+1)}} z^{(k)} \]  

(41)

regardless of linearizing assumptions. Combining these two observations gives

Claim 7 (Factorizing under linearization). Up to terms linear in \( z^{(i)} \) for \( i = k - 1, \ldots, 1 \) we have

\[ v \approx D_{z^{(n-1)}} z^{(n)} \cdot D_{z^{(n-2)}} z^{(n-1)} \cdot \ldots \cdot D_{z^{(k+1)}} z^{(k+2)} \cdot A \cdot g \]

\[ \cdot D_{z^{(k-1)}} z^{(k)} \cdot \ldots \cdot D_{z^{(0)}} z^{(0)} \cdot z^{(0)} \]  

(42)

This proves Equation (6).

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