# Enhancing the trainability and expressivity of deep MLPs with globally orthogonal initialization

## Abstract

Multilayer Perceptrons (MLPs) defines a fundamental model class that forms the backbone of many modern deep learning architectures. Despite their universality guarantees, practical training via stochastic gradient descent often struggles to attain theoretical error bounds due to issues including (but not limited to) frequency bias, vanishing gradients, and stiff gradient flows. In this work we postulate that many of such issues find origins in the initialization of the network's parameters. While the initialization schemes proposed by Glorot *et al.* and He *et al.* have become the de-facto choices among practitioners, their goal to preserve the variance of forward- and backward-propagated signals is mainly achieved by assumptions on linearity, while the presence of nonlinear activation functions may partially destroy these efforts. Here, we revisit the initialization of MLPs from a dynamical systems viewpoint, and propose a novel initialization scheme that promotes orthogonality in the features of the last hidden layer, ultimately leading to more diverse representations. Our results demonstrate that network initialization alone can be sufficient in mitigating frequency bias and yields competitive results for high-frequency function approximation and image regression tasks, without any additional modifications to the network architecture or activation functions.

## 1 Introduction

It is now well understood that frequency bias [1, 2, 3] can prevent MLPs from approximating multi-scale target functions, such as the ones that routinely arise when modeling physical and engineering systems governed by differential equations [4, 5]. While many novel architectures such as residual networks [6], Fourier feature networks [7, 8], and SIREN networks [9] have been proposed to enhance the trainability and expressivity of MLPs, less attention has been placed on the importance of network initialization, epsecially in the context of frequency bias. Previous studies from He *et al.* and Sitzmann *et al.* [9, 10] have focused on studying how the input signal variance can be preserved from one layer to another, and deduce initialization schemes for the network weights to achieve so. In this work, we propose to model the initialization of deep MLPs as a discrete dynamical system, study its stability, and deduce a novel initialization scheme that prevents vanishing information flow and collapsed outputs.

## 2 Variance flow as a dynamical system

Consider a linear layer $Y = XW$, where $X$ is the input vector, $Y$ is the output vector, and $W$ is the weight matrix. W assume that the entries of $W$ are independent and identically distributed (i.i.d) with zero mean and standard deviation $c/\sqrt{d_{in}}$, where $d_{in}$ is the input dimension, while any bias parameters are initialized to zero. In the following text, $c$ will be denoted as a "variance offset" or the

(a)            (b)            (c)

Figure 1: The evolution of $s_i$ at Glorot initialization. The vertical dashed line labeled as "SIREN Var" is the standard deviation of the post-activation output proposed by *Sitzmann et al.* [9] that is invariant when $s_i = \sqrt{0.5}$ under some scaling conditions. (a) Eq. (2.1) for different activation functions $f_i$s. (b) The derivative of Eq. (2.1) for different activation functions $f_i$s. (c) The standard deviation of the post-activation hidden layer outputs for hyperbolic tangent networks, assuming zero mean and unit variance input.

35    "scale" of the initialization of $W$. Then the output variance of the linear layer then takes the form
36    $\text{Var}(X_i \cdot W_{j,i}) = c^2 \mathbb{E}(X_i^2)/d_{in}$, while the mean is $\mathbb{E}(X_i \cdot W_{j,i}) = 0$. Moreover, the inner product
37    $Y_k = \langle X, W_{\cdot,k} \rangle = \sum_{i=1}^{d_{in}} X_i W_{i,k}$ converges in distribution to a normal distribution with zero mean
38    and variance $c^2 \mathbb{E}(X_i^2)$ as $d_{in} \to \infty$, by the Lindeberg–Lévy Central Limit Theorem [11], if $\mathbb{E}(X_i^2)$
39    is finite. Consequently, we can use a normal distribution to approximate pre-activation distribution,
40    and estimate the corresponding post-activation second moment as

$$s_{i+1} = \sqrt{\mathbb{E}(f_i(cs_i\mathcal{N}(0,1))^2)}, \tag{2.1}$$

41    where $f_i$ is the activation function, and $s_i$ is the square root of the second moment of the post
42    activation, of the $i^{\text{th}}$ layer. The system described by Eq. 2.1 can be simulated numerically for common
43    choices of activation functions, as well as back-propagation (see Appendix A). Fig. 1 confirms the
44    known behavior of vanishing second moment for hyperbolic tangent and ReLU activation functions,
45    when $c = 1$ as the conventional Glorot scheme [12] initializes, eventually leading to collapsed outputs
46    especially for deeper MLPs (see Fig. 1(c)). It also confirms the preservation of the second moment in
47    ReLU networks initialized by the He scheme [10] where $c = \sqrt{2}$.

48    To further illustrate the effect of the variance offset $c$, we analyze the fixed points of Eq. (2.1) for
49    hyperbolic tangent networks, since the symmetry of $\tanh$ activation allows us to replace the second
50    moment in Eq. (2.1) with variance, and also replace
51    $s_i$ with standard deviation. As illustrated in Fig. 2(a),
52    our numerical results suggest that a bifurcation occurs
53    when varying the variance offset $c$. We numerically
54    locate the new fixed point and estimate its stability,
55    and Fig. 2(b) shows that the larger variance offset
56    $c$ leads to two fixed points, and the only stable one
57    is the positive fixed point, to which the variance of
58    the hidden layer output with slightly larger variance
59    offset converges (see Fig. 1(c)). Clearly, an interven-
60    tion that controls the onset of this bifurcation could
61    lead to a drastic change to the network's behavior and
62    help prevent vanishing information flows that leads
63    to collapsed outputs. In the next section we propose

(a)        (b)

Figure 2: Bifurcation of Eq. (2.1) at different variance offset values. (a) The fixed point of Eq. (2.1) at different variance offset. (b) The derivatives of Eq. (2.1) at the two fixed points.

64    an initialization procedure that automatically tunes the layer-wise variance offset and bias, ensuring a
65    diverse set of features in the network's last layer prior to the training.

## 3   Globally Orthogonal (GO) initialization of MLPs

67    We propose to use orthogonality in the last layer features as a measure to quantify the expressivity of
68    an MLP representation. Specifically, given a MLP $f_w$, with $m$ hidden layers, and weights $w$, we use
69    $\boldsymbol{g}_w$ to denote the post-activation outputs of the last hidden layer with $d$ features. Letting $\boldsymbol{g}_w^j$ denote

(a)

(b)

Figure 3: Neural network prediction at initialization with increasing depth (from left to right). (a) Glorot initialization. (b) Globally Orthogonal (GO) initialization.

the $j^{\text{th}}$ feature, the cosine of the angle $\theta^{i,j}$ between $\boldsymbol{g}_w^i, \boldsymbol{g}_w^j$ is defined as

$$\cos\theta^{i,j} := \frac{\langle \boldsymbol{g}_w^i, \boldsymbol{g}_w^j \rangle}{||\boldsymbol{g}_w^i||_2 ||\boldsymbol{g}_w^j||_2}. \tag{3.1}$$

In practice, given input data $X = (x_1, ..., x_N)$, the inner product $\langle \cdot, \cdot \rangle$ is evaluated with respect to the empirical data distribution $p(x) = \frac{1}{N}\sum_{i=1}^{N}\delta(x - x_i)$, with Dirac delta function $\delta$. Angles between the last layer features functions are then transformed to a loss objective, by which the initialization variances and the biases of the each layer except the last layer can be calibrated. Specifically, let the entries of the weight matrix of each layer be initialized with standard deviation $c_j/\sqrt{d_{in}^j}, j = 1, ..., m$, and let the bias of each layer be initialized as $b_j \mathbb{1}, j = 1, ..., m$, we proceed by optimizing $\{\boldsymbol{c}, \boldsymbol{b}\}$ by minimizing the following regularized loss

$$\min_{\boldsymbol{c},\boldsymbol{b}} -\frac{\sum_{i\neq j}\log(1 - (\cos\theta^{i,j})^2)}{d(d-1)} + \lambda||\boldsymbol{c}||_2^2. \tag{3.2}$$

Intuitively, this orthogonality objective aims to reduce the correlation between the gradients of the parameters at different locations and therefore drastically changes the expressiveness of an MLP at initialization, as shown in Fig. 3. As opposed to previous studies that focus on the parameters orthogonality [13, 14], we directly optimize the orthogonality of the features in the function space, and therefore name it as global orthogonality objective. As expected from the dynamical system of Eq. (2.1), while an MLP without proper initialization is collapsing to near zero outputs as the number of hidden layers is increased, the proposed Globally Orthogonal (GO) initialization scheme on the contrary leads to richer and increasingly localized features. This observation can also be confirmed by inspecting the limiting Neural Tangent Kernel (NTK) which is invariant under some conditions during training [15, 16, 17]. The NTK can be computed for a given batch of inputs $\{x_i\}_{i=1}^{N}$ as

$$\boldsymbol{K}_{i,j} = \nabla_w f_w(x_i) \cdot \nabla_w f_w(x_j), \tag{3.3}$$

where $\nabla_w$ denotes the gradient with respect to the parameter $w$. A visualization of the resulting NTK matrix reveals the correlation between the predicted MLP outputs corresponding to different input locations when responding to a small perturbation in the network's parameters. Fig. 4 shows the NTK matrices evaluated at an ordered grid of points for a wide and deep neural network initialized using Glorot initialization, and the proposed GO initialization, respectively. Each matrix is normalized by its Frobenius norm so that the color of each entry represents a proportion of the total energy. It is evident that by reducing the strength of the regularization parameter $\lambda$, the GO initialization yields increasingly more complex MLP features with localized spatial correlations, implying that the convergences of the MLP to data points are more independent and uniform.

## 4   Results

**Synthetic data:** In this example we demonstrate the effectiveness of GO initialization in mitigating frequency bias and enabling the approximation of synthetic high frequency functions in two dimen-

(a)             (b)             (c)

Figure 4: Absolute values of the normalized NTK matrices for various $\lambda$. The entries are normalized by the Frobenius norm of the entire matrix. (a) Glorot initialization. (b) GO initialization, $\lambda = 0.01$. (c) GO initialization, $\lambda = 0.0001$.

Figure 5: The median training errors (left), the median test errors (middle) on the same target function for different data sizes, and both errors in the same plot (right). The shaded region is the $80\%$ intervals.

sions. Training and testing errors associated with data-sets of various sizes are reported in Fig. 5, suggesting that the GO initialization yields significantly more accurate and robust results compared to the Glorot scheme which suffers from frequency bias.

**Image regression:** In this example, we will use a high definition RGB colored image. The sample image contains rich details of a city landscape. A continuous representation of the image is recovered by fitting $25\%$ of the pixels with total variation regularization. As shown in Fig. 6, an MLP with GO initialization is able to improve the SNR from $16.8$ dB to $20.0$ dB from the Glorot scheme, and recovers visually sharper details on light, shadow and texture that are on the contrary heavily distorted and smudged together in the representation trained from Glorot scheme. A comparison of SNRs for different sampling ratios and different competing approaches can be found in Appendix B.5.

## 5 Summary

By deriving a simplified discrete dynamical system to quantify information flow through MLPs at initialization, we identify and analyze vanishing output pathologies of conventional initialization schemes that hamper the trainability of deep fully-connected architectures. Motivated by these observations, we propose a novel initialization procedure that is designed to promote global orthogonality in the last layer's features, and demonstrate that such initialization leads to rich and localized feature representations. Our numerical results confirm that the proposed GO initialization can greatly enhance the trainability of deep MLPs and effectively mitigate frequency bias, without requiring any elaborate changes to the network architecture or activation functions.

Figure 6: Training results. (From left to right) Original image, sampling mask, result from Glorot initialization, and result from the GO initialization.

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# Appendix

## A Back-propagation as a dynamical system

We analyze the backward pass of an MLP [18] as a dynamical system to show that the increased variance offset discussed in section 2 will not lead to vanishing gradients in MLPs activated with hyperbolic tangent activations. To this end, a linear layer followed by a hyperbolic tangent activation can be expressed as $Y = \tanh(XW)$, where $X \in \mathbb{R}^{N \times m_0}$ is the input of the hidden layer, and $W \in \mathbb{R}^{m_0 \times m_1}$ is the weight matrix. Let $dY = \frac{\partial l}{\partial Y}$, i.e., the back propagated gradient with respect to the objective $l$. We again assume that the entries of $dY$ is distributed i.i.d. Then the gradient of the weight matrix is

$$dW = \frac{\partial l}{\partial W} = X^{\mathsf{T}} \tanh'(dY),\tag{A.1}$$

and the further back-propagated gradient is

$$dX = \frac{\partial l}{\partial X} = \tanh'(dY)W^{\mathsf{T}}.\tag{A.2}$$

To study the impact of the variance offset $c$ on the back-propagated gradients $dX$, we choose to trace the square root of second moment of $T_X = \tanh'(dX)$. Let $s_X^T = \sqrt{\mathbb{E}(T_X^2)}$, $T_Y = \tanh'(T_X W^{\mathsf{T}})$, and $s_Y^T = \sqrt{\mathbb{E}(T_Y^2)}$. Then, similarly, as $m_0 = m_1 \to \infty$, with the offset $c$, the distribution of $dX$ is approximately normal with zero mean and standard deviation $cs_X^T$. Therefore, we can write a discrete dynamical system for back-propagated gradients as

$$s_X^T = \sqrt{\mathbb{E}(\tanh'(cs_Y^T \mathcal{N}(0,1))^2)}.\tag{A.3}$$

Again, considering the difficulty in obtaining the analytic form of the integration, we resort to the law of large numbers to estimate the expectation. Furthermore, given that $\tanh'(x) = 1 - \tanh(x)^2$ which is an even function with monotonically decreasing component on $\mathbb{R}_+$, we have that

$$\tanh'(\sigma_{dX}^0 x)^2 < \tanh'(\sigma_{dX}^1 x)^2,\tag{A.4}$$

for all fixed $x$, if $\sigma_{dX}^0 > \sigma_{dX}^1 \geq 0$. Then since $\tanh'(x)$ is bounded (and therefore integrable), the right hand side of (A.3) decreases monotonically for positive $s_Y^T$. And since $\sqrt{\mathbb{E}(\tanh'(0\mathcal{N}(0,1))^2)} = 1$, the only fixed point of the system is positive. Fig. 7 shows the evolution of (A.3) at different variance offset value $c$s.

As before, we use a bisection method to roughly identify the fixed points given different variance offsets, and observe their stability. As shown in Fig. 7(b), our numerical results suggest that for a fixed variance offset at reasonable range, the only positive fixed point for the back-propagated gradient is stable. Moreover, although the second moment shrinks for larger variance offset, it does not vanish.

## B Experimental setup

All numerical experiments presented in this work were performed in Python using the JAX library [19]. Unless otherwise specified, the optimizer is Adam with default settings [20]. The input and output of the data are normalized to zero mean and unit variance. In the following we provide the necessary details for reproducing the main results and conclusions presented in the manuscript.

### B.1 Variance flow as a dynamical system

For Fig. 1(a,b), Eq. (2.1) and its derivative are approximated with 4096 draws from the unit normal distribution. For Fig. 1(c), the neural network consists of 32 layers, each with 1024 neurons, and a hyperbolic tangent activation function. Moreover, the function and its derivative shown in Fig. 2 are evaluated the same as that of Fig. 1. The fixed point is obtained by bisection method.

(a)

(b)

Figure 7: (a) The fixed point of Eq. (A.3) (left) and the its derivative at the root (right) for different variance offset values. (b) Positive fixed point (left), and its derivatives (right) of Eq. (A.3) for varying variance offset.

## B.2 Globally Orthogonal (GO) initialization of MLPs

For the visualization of the function behavior at initialization depicted in Fig. 3, we choose $2^{16}$ data points selected uniformly from the square region $[-1, 1] \times [-1, 1]$ and apply normalization for both dimension. The width of the MLP network is set to be $256$. The visualization of the outputs is on a $200 \times 200$ grid. The GO initialization scheme was applied using the Adam optimizer with a fixed learning rate of $0.005$. The orthogonality loss objective is regularized with $\lambda = 10^{-4}$, and $10,000$ stochastic gradient descent steps were performed.

The results presented in Fig.4 are obtained using an MLP network with $16$ layers, each with $256$ neurons activated with the hyperbolic tangent function. The GO initialization is trained on $2048$ of uniformly distributed points with zero mean and unit variance. The regularizer $\lambda = 10^{-3}$ and the learning rate is fixed at $0.005$. The GO initialization is trained for $10,000$ iterations. The NTK is calculated on $256$ evenly spaced points with zero mean and unit variance.

## B.3 Synthetic benchmark

The results presented in Fig.5 correspond to a regression task using target function with the following form

$$
\begin{aligned}
f(x,y) &= \sum_{i=1}^{4} A_{i,0} \sin(2\pi\nu_{i,0}x)\cos(2\pi\nu_{i,1}y) + A_{i,1}\sin(2\pi\nu_{i,2}x)\sin(2\pi\nu_{i,3}y), \\
&\nu_{i,j} \sim U(0,M), i = 1,...,4, j = 0,1,2,3 \\
&A_{i,j} \sim U(0,2), i = 1,...,4, j = 0,1.
\end{aligned} \tag{B.1}
$$

where $M = 18$ is the maximum frequency. Fig. 8 shows the target function that is used for data generation.

Here we have considered an MLP network with $16$ layers, each with $256$ neurons activated by the hyperbolic tangent. For the GO initialization, $2^{16}$ data points are generated uniformly randomly in the square $[-1, 1] \times [-1, 1]$. They are then normalized in each dimension. The GO initialization is trained with $\lambda = 10^{-4}$ and a learning rate of $0.005$. For each iteration, $2,048$ data points are selected uniformly from the pre-drawn points. The initialization is trained for $20,000$ iterations.

Figure 8: Target function used for the synthetic benchmark in section 4.

Once the model is initialized with proceed with solving the regression task, and $2048$ data points are chosen per batch uniformly and randomly from the data-set with given size. The MLP is then trained using the Adam optimizer with a learning rate of $5e-4$ and a decay rate of $0.99$ every $400$ iterations, for a total of $\sim 100,000$ iterations. We have performed a total of $32$ independent trials with parameters initialized from both schemes (i.e. Glorot and GO), and use the ensemble to estimate the $80\%$ probability interval. The testing error is computed on $200 \times 200$ regular grid, normalized by the training data normalization.

## B.4   Image regression benchmark

The benchmark presented in Fig.6 involves a real RGB image with a resolution of $960 \times 960 \times 3$. We use $25\%$ of the pixels as the training data-set, and the signal-to-noise ratio (SNR) is evaluated on the entire image including the training data. The MLP network we employed consists of $8$ layers with a width of $512$, and a hyperbolic tangent activation function. The GO initialization is trained using the same exact settings is in the synthetic example discussed above, using a batch size of $512$.

Once the model is initialized we proceed to solve the regression task, using the MSE loss objective and a total variation ($TV$) regularization on the Frobenius norm of the MLP Jacobian matrix

$$L(w|(X^1, Y^1), X^2) = \frac{1}{N_1} \sum_{j=1}^{N_1} ||f_w(X_j^1) - Y_j^1||_2^2 + \frac{\lambda_r}{N_2} \sum_{i=1}^{N_2} ||J_{f_w}(X_i^2)||_2^2, \qquad \text{(B.2)}$$

where $X^1$ is a batch of normalized indices, $Y^1$ is a batch of corresponding RGB value vectors, $X^2$ is a batch of points for evaluating the total variation regularization, $\lambda_r$ is the regularization coefficient, and $N_1, N_2$ are the corresponding batch sizes. In this case $X^1$ is drawn uniformly randomly from the sampled normalized indices, $X^2$ is sampled uniformly randomly in the normalized domain, $N_1 = N_2 = 512$, and $\lambda_r = 0.01$. The number of training iterations is $400,000$. The optimizer learning rate starts from $10^{-4}$, and decays with a rate of $0.99$ per $1,000$ steps.

## B.5   Comparison against SIREN

For a comparison against state-of-the-art methods for image regression, we report the results obtained by an MLP with GO initialization versus a scaled SIREN model [9]. The weight matrices of the SIREN network are initialized in accordance with [9], without using any heuristics on the first layer variance offset, and the architecture stays the same, except for the periodic activation function used in the SIREN case. Table 1 shows the SNRs for different configurations. Interestingly, the proposed GO initialization can achieve comparable image reconstructions to the SIREN network, suggesting that the proposed GO initialization alone can be sufficient in mitigating frequency bias, without any additional modifications to the network architecture or activation functions.

| Sample ratio | Init. Scheme | $\lambda_r = 0$ | $\lambda_r = 0.01$ | $\lambda_r = 1$ |
|---|---|---|---|---|
| 10% | Xavier | 16.1 | 16.1 | 16.1 |
| | GO | 16.8 | 17.0 | 17.4 |
| | SIREN | 16.9 | 17.2 | 17.4 |
| 25% | Xavier | 16.7 | 16.8 | 16.7 |
| | GO | 19.9 | 20.0 | 19.7 |
| | SIREN | 19.8 | 20.1 | 20.0 |
| 99% | Xavier | 16.9 | 16.9 | 16.9 |
| | GO | 22.4 | 22.4 | 21.0 |
| | SIREN | 25.1 | 25.0 | 22.0 |

Table 1: SNRs in decibel of different initialization schemes with sample ratio $0.1, 0.25, 0.99$ and total variation regularization coefficient $\lambda_r = 0, 0.01, 1$ on the colored landscape image. The Xavier and GO refer to MLP initialized with corresponding scheme, while SIREN is sine activated MLP with the recommended initialization scheme from the original paper [9].