NEURAL NETWORKS WITH TRAINABLE MATRIX ACTIVATION FUNCTIONS

Zhengqi Liu,1 Shuhao Cao,2 Yuwen Li,3 & Ludmil Zikatanov4,*

1 Department of Mathematics, The Pennsylvania State University, University Park, PA 16802, USA
2 School of Science and Engineering, University of Missouri–Kansas City, Kansas City, MO 64110, USA
3 School of Mathematical Sciences, Zhejiang University, Hangzhou, Zhejiang 310058, China
4 National Science Foundation, Alexandria, VA 22314, USA

*Address all correspondence to: Ludmil Zikatanov, National Science Foundation, Alexandria, VA, USA, E-mail: lzikatan@nsf.gov

The training process of neural networks usually optimizes weights and bias parameters of linear transformations, while nonlinear activation functions are prespecified and fixed. This work develops a systematic approach to constructing matrix-valued activation functions whose entries are generalized from rectified linear unit (ReLU). The activation is based on matrix-vector multiplications using only scalar multiplications and comparisons. The proposed activation functions depend on parameters that are trained along with the weights and bias vectors. Neural networks based on this approach are simple and efficient and are shown to be robust in numerical experiments.

KEY WORDS: machine learning, ReLU, ParaReLU, trainable activation

1. INTRODUCTION

In recent decades, deep neural networks (DNNs) have achieved significant success in many fields such as computer vision and natural language processing (Otter et al., 2018; Voulodimos et al., 2018). The DNN surrogate model is constructed using recursive composition of linear transformations and nonlinear activation functions. The nonlinear activation functions are essential in providing universal approximation, and problem-appropriate choices of them are vital to the model’s performance.

In the original universal approximation (Cybenko, 1989; Funahashi, 1989), sigmoid is used due to its property converging to 1 and 0 as the input goes to ±∞ and continuously changing within. However, in the modern application where the neural network layers are composed to be deeper and deeper while the whole community shifted from fp64 to fp32, sigmoid activation suffers from the “vanishing gradient” (Kolen and Kremer, 2001) during the training process, as the chain rule multiplies multiple small gradients resulting from sigmoid and eventually causes numerical underflow (You et al., 2017).

In practice, the rectified linear unit (ReLU) is one of the most popular activation functions due to its simplicity and efficiency. Moreover, it resolves the vanishing gradient problem completely, allowing a large DNN stacked with up to hundreds of layers such as the ones in He...
et al. (2015a). Nevertheless, a key drawback of ReLU is the “dying ReLU” problem (Lu et al., 2020) where, if during training a neuron’s ReLU activation becomes 0, then under certain circumstances it may never get activated again to output a nonzero value.

Several simple modifications have been proposed to address this problem and have achieved a certain level of success, e.g., the simple leaky ReLU, and piecewise linear unit (PLU) ( Nicolae, 2018), Softplus ( Glorot et al., 2011), exponential linear unit (ELU) ( Clevert et al., 2016), scaled exponential linear unit (SELU) ( Klambauer et al., 2017), and Gaussian error linear unit (GELU) ( Hendrycks and Gimpel, 2016).

Although the aforementioned activation functions are shown to be competitive in benchmark tests, they are still fixed nonlinear functions. In a DNN structure, it is often hard to determine \textit{a priori} the optimal activation function for a specific application. Empirically, there has been a community effort in search for a better activation ( Ramachandran et al., 2017), and currently the consensus is that GELU works well in large models such as GPT ( Radford et al., 2019) as it avoids the vanishing gradient, dying ReLU, and the shattered gradient problem ( Balduzzi et al., 2017). In general, GELU-like activations provide a gradient in the negative regime to stop neurons “dying” while bounding how far into the negative regime activations are able to have an effect, and this allows for a better cross-layer training procedure.

However, all the activations mentioned above are \textit{pointwise}, where this pointwiseness refers to the fact that the activations are scalar functions that only use a single componentwise value to determine its output, given a tensorial input. In this paper, we shall generalize these activation functions and introduce a mechanism to create matrix-valued activation functions, which is trainable to control the gradient magnitude in a data-adaptive fashion. The effectiveness of the proposed method is validated using function approximation examples and well-known benchmark functions and introduce a mechanism to create matrix-valued activation functions, which is trainable to control the gradient magnitude in a data-adaptive fashion. The effectiveness of the proposed method is validated using function approximation examples and well-known benchmark functions such as \textsc{MNIST} and \textsc{CIFAR-10}. There are a few classical works on adaptively tuning parameters in the training process, e.g., the parametric ReLU ( He et al., 2015b). However, our adaptive matrix-valued activation functions are shown to be competitive and more robust in those experiments.

1.1 Preliminaries

For the simplicity of presentation, we consider a simple model data-fitting problem, given a training set containing \( \{(x_n, f_n)\}_{n=1}^N \) where the coordinates \( \{x_n\}_{n=1}^N \subset \mathbb{R}^d \) are the inputs and \( \{f_n\}_{n=1}^N \subset \mathbb{R}^J \) are the outputs. They are implicitly related via an unknown target function \( f: \mathbb{R}^d \rightarrow \mathbb{R}^J \) with the assumption that \( f_n = f(x_n) \). The ReLU activation function is a piecewise linear function given by

\[
\sigma(t) = \max\{t, 0\}, \quad \text{for } t \in \mathbb{R}.
\]

In the literature \( \sigma \) is acting componentwise on an input vector. In a DNN, let \( L \) be the number of layers and \( n_\ell \) denote the number of neurons at the \( \ell \)-th layer for \( 0 \leq \ell \leq L \) with \( n_0 = d \) and \( n_L = J \). Let \( W = (W_1, W_2, \ldots, W_L) \in \prod_{\ell=1}^L \mathbb{R}^{n_\ell \times n_{\ell-1}} \) denote the tuple of admissible weight matrices and \( B = (b_1, b_2, \ldots, b_L) \in \prod_{\ell=1}^L \mathbb{R}^{n_\ell} \) the tuple of admissible bias vectors. The ReLU DNN approximation to \( f \) at the \( \ell \)-th layer is recursively defined as

\[
\eta_\ell(x) := \sigma(W_\ell \eta_{\ell-1}(x) + b_\ell) \in \mathbb{R}^{n_\ell}, \quad \eta_0(x) = x \in \mathbb{R}^d.
\]  

The traditional training process for such a DNN is to find optimal \( W_* \in \prod_{\ell=1}^L \mathbb{R}^{n_\ell \times n_{\ell-1}}, B_* \in \prod_{\ell=1}^L \mathbb{R}^{n_\ell} \) (and thus optimal \( \eta_L = \eta_{L, W_*, B_*} \)) such that
(W_*, B_*) = \arg \min_{W,B} E(W, B), \quad \text{where} \quad E(W, B) = \sum_{n=1}^{N} |f_n - \eta_{L,W,B}(x_n)|^2. \quad (2)

In other words, \( \eta_{L,W,B} \) best fits the data with respect to the discrete \( \ell^2 \)-norm within the function class \( \{\eta_{L,W,B}\} \). In practice, the sum of squares norm in \( E \) could be replaced with more convenient norms.

2. TRAINABLE MATRIX-VALUED ACTIVATION FUNCTION

Having a closer look at ReLU \( \sigma \), we have a simple but quite useful observation that the activation \( \sigma(\xi_\ell(x)) \) with \( \xi_\ell := W_\ell \eta_{\ell-1} + b_\ell \) could be written as a matrix-vector multiplication \( \sigma(\xi_\ell(x)) = D_\ell(\xi_\ell(x)) \xi_\ell(x) \), where \( D_\ell \) is a diagonal matrix-valued function mapping from \( \mathbb{R}^{n_\ell} \) to \( \mathbb{R}^{n_\ell \times n_\ell} \) with diagonal being \( 1_{\{(0,\infty)\}}(s) \), thus taking values from the discrete set \( \{0,1\} \).

There is no reason to restrict on \( \{0,1\} \) and we thus look for a larger set of values over which the diagonal entries of \( D_\ell \) are running or sampled. With a slight abuse of notation, our new DNN approximation to \( f \) is calculated using the following recurrence relation:

\[
\eta_0(x) = x \in \mathbb{R}^d, \quad \xi_\ell(x) = W_\ell \eta_{\ell-1}(x) + b_\ell, \quad \eta_\ell = (D_\ell \circ \xi_\ell) \xi_\ell, \quad \ell = 1, \ldots, L. \quad (3)
\]

Here each \( D_\ell \) is diagonal and is of the form

\[
D_\ell(y) = \text{diag}(\alpha_{\ell,1}(y_1), \alpha_{\ell,2}(y_2), \ldots, \alpha_{\ell,n_\ell}(y_{n_\ell})), \quad y \in \mathbb{R}^{n_\ell},
\]

where \( \alpha_{\ell,i}(y_i) \) is a nonlinear function to be determined. Since piecewise constant functions can approximate a continuous function within arbitrarily high accuracy, we specify \( \alpha_{\ell,i} \) with \( 1 \leq i \leq n_\ell \) as

\[
\alpha_{\ell,i}(s) = \begin{cases} 
  t_{\ell,i,0}, & s \in (-\infty, s_{\ell,i,1}], \\
  t_{\ell,i,1}, & s \in (s_{\ell,i,1}, s_{\ell,i,2}], \\
  \vdots & \\
  t_{\ell,i,m_{\ell,i}-1}, & s \in (s_{\ell,i,m_{\ell,i}-1}, s_{\ell,i,m_{\ell,i}}], \\
  t_{\ell,i,m_{\ell,i}}, & s \in (s_{\ell,i,m_{\ell,i}}, \infty), 
\end{cases}
\]

where \( m_{\ell,i} \) is a positive integer and \( \{t_{\ell,i,j}\}_{j=0}^{m_{\ell,i}} \) and \( \{s_{\ell,i,j}\}_{j=1}^{m_{\ell,i}} \) are constants. We may suppress the indices \( \ell, i \) in \( \alpha_{\ell,i}, m_{\ell,i}, t_{\ell,i,j}, s_{\ell,i,j} \) and write them as \( \alpha, m, t, s \) when those quantities are uniform across layers and neurons. If \( m = 1, s_1 = 0, t_0 = 0, t_1 = 1 \), then the DNN [Eq. (3)] is exactly the ReLU DNN. If \( m = 2, s_1 = 0, s_2 = 1, t_0 = t_2 = 0, t_1 = 1 \), then \( \alpha = \alpha_{\ell,i} \) actually represents a discontinuous activation function.

In our case, we shall fix some parameters from \( \bigcup_{\ell=1}^{L} \bigcup_{i=1}^{n_\ell} \{t_{\ell,i,j}\}_{j=0}^{m_{\ell,i}} \) and \( \bigcup_{\ell=1}^{L} \bigcup_{i=1}^{n_\ell} \{s_{\ell,i,j}\}_{j=1}^{m_{\ell,i}} \) and let the rest of them vary in the training process. When the diagonal cutoffs are fixed while making the slopes learnable, this replicates the layerwise adaptive rate scaling in You et al. (2017). Heuristically speaking, the activation functions among different layers in the resulting DNN may adapt to the target function \( f \). Since the nonparametric ReLU and a 1-parameter leaky ReLU are special cases of the new activation functions, the proposed DNN with the new activations theoretically should bear at least the same approximation property. If the optimization
problem is solved exactly, in practice the training error should be no worse than before. In the following, the activation function in Eq. (5) with trainable parameters in Eq. (3) is named as the “trainable matrix-valued activation function (TMAF).”

Starting from the diagonal activation $D_\ell$, one can step further to construct more general activation matrices. First we note that $D_\ell$ could be viewed as a nonlinear operator $T_\ell : [C(\mathbb{R}^d)]^{n_\ell} \rightarrow [C(\mathbb{R}^d)]^{n_\ell}$, where

$$
[T_\ell(g)](x) = D_\ell(g(x))g(x), \quad g \in [C(\mathbb{R}^d)]^{n_\ell}, \quad x \in \mathbb{R}^d.
$$

With this observation, one can parametrize a trainable nonlinear activation operator determined by more general matrices, e.g., the following tridiagonal operator:

$$
[T_\ell(g)](x) = \begin{pmatrix}
\alpha_{\ell,1} & \beta_{\ell,2} & 0 & \cdots & 0 \\
\gamma_{\ell,1} & \alpha_{\ell,2} & \beta_{\ell,3} & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \cdots & \alpha_{\ell,n_\ell-1} & \beta_{\ell,n_\ell} \\
0 & 0 & \cdots & \gamma_{\ell,n_\ell-1} & \alpha_{\ell,n_\ell}
\end{pmatrix} g(x), \quad x \in \mathbb{R}^d. \tag{6}
$$

The diagonal $\{\alpha_{\ell,i}\}$ is given in Eq. (5) while the off-diagonals $\beta_{\ell,i}$, $\gamma_{\ell,i}$ are piecewise constant functions in the $i$th coordinate $y_i$ of $y \in \mathbb{R}^{n_\ell}$ defined in a fashion similar to $\alpha_{\ell,i}$. Theoretically speaking, even trainable full matrix activation is possible despite potentially increased training cost. In summary, the corresponding DNN based on trainable nonlinear activation operators $\{T_\ell\}_{\ell=1}^L$ reads

$$
\eta_0(x) = x \in \mathbb{R}^d, \quad \xi_\ell(x) = W_\ell \eta_{\ell-1}(x) + b_\ell, \quad \eta_\ell := T_\ell(\xi_\ell), \quad \ell = 1, \ldots, L. \tag{7}
$$

The evaluations of $D_\ell$ and $T_\ell$ are cheap because they require only scalar multiplications and comparisons. When calling a general-purpose package such as PyTorch in the training process, it is observed that the computational time of $D_\ell$ and $T_\ell$ is comparable to the classical ReLU.

**Remark 1.** Our observation also applies to an activation function $\sigma$ other than ReLU. For example, we may rescale $\sigma(x)$ to obtain $\sigma(\omega_{\ell,i}x)$ for constants $\{\omega_{\ell,i}\}$ varying layer by layer and neuron by neuron. Then $\sigma(\omega_{\ell,i}x)$ are used to form a matrix activation function and a TMAF DNN, where $\{\omega_{\ell,i}\}$ are trained according to given data and are adapted to the target function. This observation may be useful for specific applications.

**Remark 2.** We also note that the diagonal activation with a fixed bandwidth bears similarity with the piecewise-linear activation after the convolution layer in a so-called alternating direction method of multipliers (ADMM)-net (Yang et al., 2017), yet is designed with a fundamentally different philosophy. In Yang et al. (2017), an activation matrix with the size of the filter is composed of the convolution operation. If one views the convolution operation as a diagonal matrix-valued operator, for a $p \times p$ convolution filter, the activation is a $n^2 \times n^2$ diagonal matrix with the bandwidth being $p^2$. The nonlinearity in ADMM couples neighboring pixels in an image, while here TMAF performs a nonlinear mixing in the channel dimension.

3. NUMERICAL RESULTS

In this section, we demonstrate the feasibility and efficiency of TMAF by comparing it with the traditional ReLU-type activation functions. In principle, all parameters in Eq. (5) are allowed to
be trained while we shall fix the intervals in Eq. (5) and only let function values \( \{t_j\} \) vary for simplicity in the following. In each experiment, we use the same neural network structure, as well as the same learning rates, stochastic gradient descent (SGD) optimization, and number of epochs (NE) (SGD iterations). In particular, the learning rate 1e–4 is used for epochs 1 to NE/2 and 1e–5 is used for epochs NE/2 + 1 to NE.

### 3.1 Function Approximation (Regression) Problem

For the first class of examples we use the \( \ell^2 \)-loss function as defined in Eq. (2). For the classification problems we consider the cross-entropy that is widely used as a loss function in classification models. The cross-entropy is defined using a training set which consists of \( p \) images, each with \( N \) pixels. Thus, we have a matrix \( Z \in \mathbb{R}^{N \times p} \) and each column corresponds to an image with \( N \) pixels. Each image belongs to a fixed class \( c_j \) from the set of image classes \( \{c_k\}_{k=1}^p \), where \( c_j \in \{1, \ldots, M\} \). The network structure maps \( Z \in \mathbb{R}^{N \times p} \) to \( X \in \mathbb{R}^{M \times p} \), and each column \( x_j \) of \( X \) is an output of the network evaluation at the corresponding column \( z_j \) of \( Z \). More precisely,

\[
Z = (z_1, \ldots, z_p), \quad X = (x_1, \ldots, x_p), \quad c_j = \text{class}(z_j),
\]

\[
x_j := \eta_{L,W,B}(z_j), \quad x_j \in \mathbb{R}^M, \quad z_j \in \mathbb{R}^N, \quad j = 1, \ldots, p.
\]

The cross-entropy loss function then is defined by

\[
C(W, B) = \sum_{k=1}^p -\log \left( \frac{\exp(x_{ck,k})}{\sum_{j=1}^M \exp(x_{j,k})} \right),
\]

\[
(W_*, B_*) = \arg \min_{W,B} C(W, B).
\]

To evaluate the loss function at a given image \( z \in \mathbb{R}^N \), we first evaluate the network at \( z \) with the given \( (W, B) = (W_*, B_*) \). We then define the class \( c(z) \) of \( z \) and the loss \( \text{loss}(z) \) at \( z \) as follows:

\[
c(z) = \arg \min_{1 \leq j \leq M} \{\exp(a_j)\}, \quad \text{where} \quad a = \eta_{L,W,B}(z),
\]

\[
\text{loss}(z) = -\log \left( \frac{\exp(a_{c(z)})}{\sum_{j=1}^M \exp(a_j)} \right).
\]

#### 3.1.1 Approximation of a Smooth Function

As our first example, we use neural networks to approximate

\[
f(x_1, \ldots, x_n) = \sin(\pi x_1 + \cdots + \pi x_n), \quad x_k \in [-2, 2], \quad k = 1, \ldots, n.
\]

The training datasets are 20,000 input-output data pairs where the input data are randomly sampled from the hypercube \([-2, 2]^n\). The networks [Eqs. (1) and (3)] have single or double hidden layers with 20 neurons per layer. For TMAF \( D_\ell \) in Eq. (4), the function \( \alpha = \alpha_{\ell,i} \) in Eq. (5) uses intervals \((-\infty, -5), (-5 + k, -4 + k), (5, \infty), 0 \leq k \leq 9 \). The approximation results are shown in Table 1 and Figs. 1–3. It is observed that TMAF is the most accurate activation approach. Moreover, the parametric ReLU does not approximate \( \sin(\pi x_1 + \cdots + \pi x_6) \) well; see Fig. 3(b).
TABLE 1: Approximation errors for $\sin(\pi x_1 + \cdots + \pi x_n)$ by neural networks

| Approximation Error | Single Hidden Layer | Two Hidden Layers |
|---------------------|---------------------|-------------------|
|                     | ReLU                | TMAF              |
| $n$                 | 1                   | 2                 | 3                 | 4                 | 5                 | 6                 | 7                 | 8                 |
| ReLU                | 0.089               | 0.34              | 0.39              | 0.41              | 0.14              | 0.21              | 0.25              | 0.31              |
| TMAF                | 0.015               | 0.016             | 0.13              | 0.18              | 0.07              | 0.105             | 0.153             | 0.17              |

FIG. 1: Training errors for $\sin(\pi x_1 + \cdots + \pi x_n)$, single hidden layer: (a) $n = 1$ and (b) $n = 2$

FIG. 2: Neural network approximations to $\sin(\pi x)$, single hidden layer: (a) ReLU and (b) TMAF

3.1.2 Approximation of an Oscillatory Multifrequency Function

The next example is of approximating the following function having high- and low-frequency components

$$f(x) = \sin(100\pi x) + \cos(50\pi x) + \sin(\pi x),$$

see Fig. 4 for an illustration. The function in Eq. (8) is notoriously difficult to capture by numerical methods in scientific computing. In the context of approximation using NNs, it is observed
FIG. 3: Training errors for \( \sin(\pi x_1 + \cdots + \pi x_n) \), two hidden layers: (a) \( n = 5 \) and (b) \( n = 6 \)

FIG. 4: (a) Plot of \( f(x) = \sin(100\pi x) + \cos(50\pi x) + \sin(\pi x) \), exact oscillating function, and (b) training loss comparison

in Hong et al. (2022) that ReLU-based NN cannot resolve the high-frequency oscillatory feature of this function at all. The training datasets are 20,000 input-output data pairs where the input data are randomly sampled from the interval \([-1, 1]\). We test the diagonal TMAF [Eq. (4)] and the function \( \alpha = \alpha_{t,i} \) [Eq. (5)] uses intervals \((-\infty, -5), (-5 + kh, -5 + (k + 1)h), (5, \infty)\) with \( h = 0.1, 0 \leq k \leq 99 \). We also consider the tridiagonal TMAF [Eq. (6)], where \( \{\alpha_{t,i}\} \) is the same as the diagonal TMAF, \( \{\beta_{t,i}\} \) and \( \{\gamma_{t,i}\} \) are all piecewise constants based on intervals \((-\infty, -5 + \frac{h}{2}), (-5 + kh + \frac{h}{2}, -5 + (k + 1)h + \frac{h}{2}), (5 + \frac{h}{2}, \infty)\) and \((-\infty, -5 + 2\frac{h}{3}), (-5 + kh + 2\frac{h}{3}, -5 + (k + 1)h + 2\frac{h}{3}), (5 + 2\frac{h}{3}, \infty)\) with \( \frac{h}{3} = 0.1/3, 0 \leq k \leq 99 \), respectively. Numerical results can be found in Figs. 4 and 5 and Table 2.

For this challenging problem, we note that the diagonal TMAF and tridiagonal TMAF produce high-quality approximations while ReLU and parametric ReLU are not able to approximate the highly oscillating function within reasonable accuracy. It is observed from Fig. 5 that ReLU actually approximates the low-frequency part of Eq. (8). To capture the high-frequency part, ReLU clearly has to use more neurons and thus much more weight and bias parameters. On the other hand, increasing the number of intervals in TMAF only leads to a few more training parameters.
3.2 Classification Problem of MNIST and CIFAR-10 Datasets

We now test TMAF by classifying images in the MNIST and CIFAR-10 datasets. For TMAF $D_i$ in Eq. (4), the function $\alpha = \alpha_{\ell,j}$ [Eq. (5)] uses intervals $(-\infty, -5), (-5+k, -4+k], (5, \infty)$ with $0 \leq k \leq 9$.

For the MNIST set, we implement single and double layer fully connected networks [Eqs. (1) and (3)] with 10 neurons per layer (except at the first layer $n_0 = 764$), and ReLU or diagonal TMAF [Eq. (4)] activation. Numerical results are shown in Figs. 6 and 7 and Table 3. We note...
that the TMAF with a single hidden layer ensures higher evaluation accuracy than ReLU; see Table 3.

For the CIFAR-10 dataset, we use the ResNet18 network structure with 18 layers and number of neurons provided by He et al. (2015a). The activation functions are still ReLU and the diagonal TMAF [Eq. (4)]. Numerical results are presented in Fig. 8 and Table 3. Those
parameters given in Paszke et al. (2017) are already tuned well with respect to ReLU. Nevertheless, TMAF still produces smaller errors in the training process and returns better classification results in the evaluation stage.

It is possible to improve the performance of TMAF applied to those benchmark datasets. The key point is to select suitable intervals in $\alpha_{\ell,i}$ to optimize the performance. A simple strategy is to let those intervals in Eq. (5) be varying and adjusted in the training process, which will be investigated in our future research.

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