Locally adaptive activation functions with slope recovery term for deep and physics-informed neural networks

Ameya D. Jagtap¹, Kenji Kawaguchi² and George Em Karniadakis¹,³,

¹Division of Applied Mathematics, Brown University, 182 George Street, Providence, RI 02912, USA.
²Massachusetts Institute of Technology, 77 Massachusetts Ave, Cambridge, MA 02139, USA.
³Pacific Northwest National Laboratory, Richland, WA 99354, USA.

Abstract
We propose two approaches of locally adaptive activation functions namely, layer-wise and neuron-wise locally adaptive activation functions, which improve the performance of deep and physics-informed neural networks. The local adaptation of activation function is achieved by introducing scalable hyper-parameters in each layer (layer-wise) and for every neuron separately (neuron-wise), and then optimizing it using the stochastic gradient descent algorithm. Introduction of neuron-wise activation function acts like a vector activation function in each hidden-layer as opposed to the traditional scalar activation function given by fixed, global and layer-wise activations. In order to further increase the training speed, an activation slope based slope recovery term is added in the loss function, which further accelerate convergence, thereby reducing the training cost. For numerical experiments, a nonlinear discontinuous function is approximated using a deep neural network with layer-wise and neuron-wise locally adaptive activation functions with and without the slope recovery term and compared with its global counterpart. Moreover, solution of the nonlinear Burgers equation, which exhibits steep gradients, is also obtained using the proposed methods. On the theoretical side, we prove that in the proposed method the gradient descent algorithms are not attracted to sub-optimal critical points or local minima under practical conditions on the initialization and learning rate. Furthermore, the proposed adaptive activation functions with the slope recovery are shown to accelerate the training process in standard deep learning benchmarks using CIFAR-10, CIFAR-100, SVHN, MNIST, KMNIST, Fashion-MNIST, and Semeion data sets with and without data augmentation.

Keywords: Machine learning, bad minima, stochastic gradients, accelerated training, PINN, deep learning benchmarks.

1. Introduction

In recent years, research on neural networks (NNs) has intensified around the world due to their successful applications in many diverse fields such as speech recognition [13], computer vision [16], natural language translation [25], etc. NNs have also been used to solve partial differential equations (PDEs) due to their ability to effectively approximate complex functions arising in diverse scientific disciplines (cf., Physics-informed Neural Networks (PINNs) by Raissi et al. [17]). PINNs can accurately solve both forward problems, where the approximate solutions of governing equations are obtained, as well as inverse problems, where parameters involved in the governing equation are inferred from the training data. In the PINN algorithm, along with the contribution from the neural network the loss function is enriched by the addition of the residual term from the governing equation, which act as a penalizing term constraining the space of admissible solutions. In general, the PINN algorithm relies on both training data obtained from the initial/boundary conditions, experiments etc, as well as the underlying physical process governed by the PDEs.
Highly efficient and adaptable algorithms are important to design the most effective NN which not only increases the accuracy of the solution but also reduces the training cost. Various architectures of NN like Dropout NN [18] are proposed in the literature, which can improve the efficiency of the algorithm for specific applications. Activation function plays an important role in the training process of NN. There is no rule of thumb for the choice of activation function, and in fact it solely depends on the problem at hand. Therefore, in this work, we are particularly focusing on adaptive activation functions, which adapt automatically such that the network can be trained faster. Various methods are proposed in the literature for adaptive activation function, like the adaptive sigmoidal activation function proposed by Yu et al [27] for multilayer feedforward NNs, while Qian et al [21] focuses on learning activation functions in convolutional NNs by combining basic activation functions in a data-driven way. Multiple activation functions per neuron are proposed by Dushkoff and Ptucha [7], where individual neurons select between a multitude of activation functions. Li et al [12] proposed a tunable activation function, where only a single hidden layer is used and the activation function is tuned. Shen et al [22], used a similar idea of tunable activation function but with multiple outputs. Recently, Kunc and Klén [14] proposed a transformative adaptive activation functions for gene expression inference, see [6] by introducing scalable hyper-parameter in the activation function, which can be optimized. Mathematically, it changes the slope of activation function thereby increasing the learning process, especially during the initial training period. Due to single scalar hyper-parameter, we call such adaptive activation functions globally adaptive activations, meaning that it gives an optimized slope for the entire network. One can think of doing such optimization at the local level, where the scalable hyper-parameter are introduced hidden layer-wise or even for each neuron in the network. Such local adaptation can further improve the performance of the network. Figure 1 shows a sketch of a neuron-wise locally adaptive activation function based physics-informed neural network (LAAF-PINN), where both the NN part along with the physics-informed part can be seen. In this architecture, along with the output of NN and the residual term from the governing equation, the activation slopes from every neuron are also contributing to the loss function in the form of slope recovery term. In every neuron, a scalable hyper-parameter is introduced, which can be optimized to lead to a quick and efficient training process in NN.

The rest of the paper is organized as follows. Section 2 presents the methodology of the proposed layer-wise and neuron-wise locally adaptive activations in detail. This also includes a discussion on the expansion of parametric space due to layer-wise and neuron-wise introduction of hyper-parameters, the slope recovery term, and a theoretical
result for gradient decent algorithms. In section 3, we perform various numerical experiments, where we approximate a nonlinear discontinuous function using deep NN by the proposed approaches. We also solve the Burgers equation using the PINN algorithm and present various comparisons with fixed and global activation functions. Section 4 presents numerical results with various standard deep learning benchmarks using CIFAR-10, CIFAR-100, SVHN, MNIST, KMNIST, Fashion-MNIST, and Semeion data sets. Finally, in section 5, we summarize the conclusions of our work.

2. Methodology

We use a NN of depth $D$ corresponding to a network with an input layer, $D - 1$ hidden-layers and an output layer. In the $k^{th}$ hidden-layer, $N_k$ number of neurons are present. Each hidden-layer of the network receives an output $z^{k-1} \in \mathbb{R}^{N_{k-1}}$ from the previous layer, where an affine transformation of the form

$$L_k(z^{k-1}) \triangleq w^k z^{k-1} + b^k$$

is performed. The network weights $w^k \in \mathbb{R}^{N_k \times N_{k-1}}$ and bias term $b^k \in \mathbb{R}^{N_k}$ associated with the $k^{th}$ layer are chosen from independent and identically distributed sampling. The nonlinear-activation function $\sigma(\cdot)$ is applied to each component of the transformed vector before sending it as an input to the next layer. The activation function is an identity function after an output layer. Thus, the final neural network representation is given by the composition

$$u_\Theta(z) = (L_D \circ \sigma \circ L_{D-1} \circ \ldots \circ \sigma \circ L_1)(z),$$

where the operator $\circ$ is the composition operator, $\Theta = [w^k, b^k]_{k=1}^D$ represents the trainable parameters in the network, $u$ is the output and $z^0 = z$ is the input.

In supervised learning of solution of PDEs, the training data is important to train the neural network, which can be obtained from the exact solution (if available) or from high-resolution numerical solution given by efficient numerical schemes and it can be even obtained from carefully performed experiments, which may yield both high- and low-fidelity data sets.

We aim to find the optimal weights for which the suitably defined loss function is minimized. In PINN the loss function is defined as

$$J(\Theta) = MS E_F + MS E_u,$$

where the mean squared error (MSE) is given by

$$MS E_F = \frac{1}{N_f} \sum_{i=1}^{N_f} |F(x_i, t_i)|^2,$$

$$MS E_u = \frac{1}{N_u} \sum_{i=1}^{N_u} |u_i - u(x_i, t_i)|^2.$$

Here $\{(x_i, t_i)\}^{N_f}_{i=1}$ represents the residual training points in space-time domain, while $\{(x_i, t_i)\}^{N_u}_{i=1}$ represents the boundary/initial training data. The neural network solution must satisfy the governing equation given by residue $F$ at randomly chosen residual points in the domain, which constitutes the physics-informed part of neural network given by first term, whereas the second term includes the known boundary/initial conditions, which must be satisfied by the neural network solution. The resulting optimization problem leads to finding the minimum of a loss function by optimizing the parameters like, weights and biases, i.e., we seek to find $w^*, b^* = \arg \min_{w,b} (J(w, b))$. One can approximate the solutions to this minimization problem iteratively by one of the forms of gradient descent algorithm.

The stochastic gradient descent (SGD) algorithm is widely used in machine learning community see, [20] for a complete survey. In SGD the weights are updated as $w^{m+1} = w^m - \eta_t \nabla w J_m(w)$, where $\eta_t > 0$ is the learning rate. SGD methods can be initialized with some starting value $w^0$. In this work, the ADAM optimizer $\Pi$, which is a variant of the SGD method is used.

A deep network is required to solve complex problems, which on the other hand is difficult to train. In most cases, a suitable architecture is selected based on the researcher’s experience. One can also think of tuning the network to
get the best performance out of it. In this regard, we propose the following two approaches to optimize the activation function.

1. Layer-wise locally adaptive activation functions (L-LAAF)
   Instead of globally defining the hyper-parameter $a$ for the adaptive activation function, let us define this parameter hidden layer-wise as
   $$\sigma(a_k^L(z^{k-1})), \ k = 1, 2, \cdots, D - 1.$$ 
   This gives additional $D - 1$ hyper-parameters to be optimized along with weights and biases. Here, every hidden-layer has its own slope for the activation function.

2. Neuron-wise locally adaptive activation functions (N-LAAF)
   One can also define such activation function at the neuron level as
   $$\sigma(a_k^i L_k(z^k - 1)), \ k = 1, 2, \cdots, D - 1, \ i = 1, 2, \cdots, N_k.$$ 
   This gives additional $\sum_{k=1}^{D-1} N_k$ hyper-parameters to be optimized. Neuron-wise activation function acts as a vector activation function in each hidden-layer as opposed to scalar activation function given by L-LAAF and global adaptive activation function (GAAF) approaches, where every neuron has its own slope for the activation function.

```python
def initialize_NN(self, layers):
    weights = []
    biases = []
    acti_param = [] # Neuron-wise activation slopes
    num_layers = len(layers)
    for l in range(0, num_layers - 1):
        W = self.xavier_init(size=[layers[l], layers[l+1]])
        b = tf.Variable(tf.zeros([1, layers[l+1]], dtype=tf.float32), dtype=tf.float32)
        a = tf.Variable(tf.constant(0.1, shape=[1, layers[l+1]]))
        weights.append(W)
        biases.append(b)
        acti_param.append(a)
    return weights, biases, acti_param
```

Figure 2: Initialization of NN with hyper-parameters like weights, biases and neuron-wise activation slopes. Activation slopes are initialized such that $na_k^i = 1$.

Figure 2 and 3 shows a self explanatory TensorFlow subroutines for the initialization of neural network and the actual neural network with neuron-wise locally adaptive tanh activation function, respectively.

The resulting optimization problem leads to finding the minimum of a loss function by optimizing $a_k^i$ along with weights and biases, i.e., we seek to find $(a_k^i)^* = \arg \min_{\{a_k^i\}^{\infty}} (J(a_k^i)), k = 1, 2, \cdots, D - 1, \ i = 1, 2, \cdots, N_k$. The process of training NN can be further accelerated by multiplying each activation slope with scaling factor $n > 1$. The final form of the activation function is given by $\sigma(na_k^i L_k(z^k - 1))$. It is important to note that the introduction of the scalable hyper-parameter does not change the structure of the loss function defined previously. Then, the final adaptive activation function based neural network representation of the solution is given by

$$u_{\Theta}(z) = (L_D \circ \sigma \circ na_D^{D-1} L_{D-1} \circ \sigma \circ na_{D-1}^{D-2} L_{D-2} \circ \cdots \circ \sigma \circ na_1 L_1)(z).$$

In this case, the set of trainable parameters $\Theta$ consists of $\{w_k, b_k\}_{k=1}^D$ and $\{a_k^i\}_{k=1}^{D-1}, \forall i = 1, 2, \cdots, N_k$. In all the proposed methods, the initialization of scalable hyper-parameters is done such that $na_k^i = 1, \forall n > 1$. Compared to single additional parameter of global adaptive activation function, the locally adaptive activation function based PINN has several additional scalable hyper-parameters to train. Thus, it is important to consider the additional computational cost required.
def neural_net(self, X, weights, biases, acti_param):
    num_layers = len(weights) + 1

    H = 2.0*(X - self.lb)/(self.ub - self.lb) - 1.0

    for l in range(0, num_layers-2):
        W = weights[l]
        b = biases[l]
        a = acti_param[l]
        H = tf.tanh(tf.multiply(tf.multiply(10.0, a), tf.add(tf.matmul(H, W), b)))

    W = weights[-1]
    b = biases[-1]
    u = tf.add(tf.matmul(H, W), b) # Network output
    return u

Figure 3: Neural network with neuron-wise locally adaptive activation function using scaling factor 10.

2.1. Expansion of parametric space and its effect on the computational cost

The increase of the parametric space leads to a high-dimensional optimization problem whose solution can be difficult to obtain. Between the previously discussed two approaches, i.e. L-LAAF and N-LAAF, N-LAAF introduces highest number of hyper-parameters for optimization. Let $\omega$ and $\beta$ be the total number of weights and biases in the NN. Then, the ratio $\mathcal{P}$ which is the size of parametric space of N-LAAF to that of fixed activation is

$$\mathcal{P} \approx \frac{1 + 2\varrho}{1 + \varrho},$$

where $\varrho = \beta/\omega$.

As an example, consider a fully connected NN with 3 hidden-layers involving 20 neurons in each layer, which gives the values of $\omega = 840$ and $\beta = 61$. Thus, $\mathcal{P} = 1.0677$, i.e., 6.77% increase in the number of hyper-parameters. This increment can further go down with an increase in the number of layers and neurons in each layer, which eventually results in negligible increase in the number of hyper-parameters. In such cases, the computational cost for fixed activation function and that of neuron-wise locally adaptive activations is comparable.

2.2. Loss function with slope recovery term

The main motivation of adaptive activation function is to increase the slope of activation function, resulting in non-vanishing gradients and fast training of the network. It is clear that one should quickly increase the slope of activation in order to improve the performance of NN. Thus, instead of only depending on the optimization methods, another way to achieve this is to include the slope recovery term based on the activation slope in the loss function as

$$\tilde{J}(\Theta) = MSE_F + MSE_u + S(a),$$

(3)

where the slope recovery term $S(a)$ is given by

$$S(a) = \begin{cases} \frac{1}{\sum_{i=1}^{N} |\mathcal{M}(a_i)|} & \text{for L-LAAF} \\ \frac{1}{\sum_{i=1}^{N} \sum_{j=1}^{n} \frac{|\frac{\partial}{\partial x_j} a_i|}{|\mathcal{M}(a_i)|}} & \text{for N-LAAF} \end{cases}$$

where $\mathcal{M}$ is a linear/nonlinear operator. Although, there can be several choices of this operator, including the linear identity operator, in this work we use the exponential operator. The main reason behind this is that such term contributes to the gradient of the loss function without vanishing. The overall effect of inclusion of this term is that it forces the network to increase the value of activation slope quickly thereby increasing the training speed. The following algorithm summarizes the LAAF-PINN algorithm with slope recovery term.
Algorithm 1: LAAF-PINN algorithm with slope recovery term.

**Step 1:** Specification of training set in space-time domain
Training data: \(u_{NN}\) network \(\{x_{n}, t_{n}\}^{N_{t}}_{n=1}\)
Residual training points: \(\mathcal{F}\) network \(\{x_{n}^{f}, t_{n}^{f}\}^{N_{t}}_{n=1}\)

**Step 2:** Construct neural network \(u_{NN}(\Theta)\) with random initialization of parameters \(\hat{\Theta}\).

**Step 3:** Construct the residual neural network \(\mathcal{F}\) by substituting surrogate \(u_{NN}\) into the governing equations using automatic differentiation [8] and other arithmetic operations.

**Step 4:** Specification of the loss function that includes the slope recovery term:

\[
\tilde{J}(\Theta) = \frac{1}{N_{t}} \sum_{i=1}^{N_{t}} |\mathcal{F}(x_{i}^{f}, t_{i}^{f})|^2 + \frac{1}{N_{u}} \sum_{i=1}^{N_{u}} |u_{i} - u(x_{i}^{f}, t_{i}^{f})|^2 + S(\alpha)
\]

**Step 5:** Find the best parameters using a suitable optimization method for minimizing the loss function

\[
\hat{\Theta} = \arg \min (\Theta)
\]

We now provide a theoretical result regarding the proposed methods. The following theorem states that a gradient descent algorithm minimizing our objective function \(\tilde{J}(\Theta)\) in [3] does not converge to a sub-optimal critical point or a sub-optimal local minimum, for neither L-LAAF nor N-LAAF, given appropriate initialization and learning rates. In the following theorem, we treat \(\Theta\) as a real-valued vector. Let \(\tilde{J}(0) = MSE_{\mathcal{F}} + MSE_{u}\) with the constant network \(u_{0}(z) = u_{0}(z') = c \in \mathbb{R}^{N_{0}}\) for all \(z, z'\) where \(c\) is a constant.

**Theorem 2.1.** Let \((\hat{\Theta}_{m})_{m \geq 1}\) be a sequence generated by a gradient descent algorithm as \(\hat{\Theta}_{m+1} = \hat{\Theta}_{m} - \eta_{m} \nabla \tilde{J}(\hat{\Theta})\). Assume that \(\tilde{J}(\Theta_{m}) < J(0) + S(0)\) for any \(c \in \mathbb{R}^{N_{0}}\). \(\tilde{J}\) is differentiable, and that for each \(i \in \{1, \ldots, N_{t}\}\), there exist differentiable function \(\varphi'\) and input \(\rho'\) such that \(|\mathcal{F}(x_{i}^{f}, t_{i}^{f})|^2 = \varphi'(u_{\Theta}(\rho'))\). Assume that at least one of the following three conditions holds.

(i) (constant learning rate) \(\nabla \tilde{J}\) is Lipschitz continuous with Lipschitz constant \(C\) (i.e., \(\|\nabla \tilde{J}(\hat{\Theta}) - \nabla \tilde{J}(\hat{\Theta}')\|_{2} \leq C\|\hat{\Theta} - \hat{\Theta}'\|_{2}\) for all \(\hat{\Theta}, \hat{\Theta}'\) in its domain), and \(\epsilon \leq \eta_{m} \leq (2 - \epsilon)/C\), where \(\epsilon\) is a fixed positive number.

(ii) (diminishing learning rate) \(\nabla \tilde{J}\) is Lipschitz continuous, \(\eta_{m} \to 0\) and \(\sum_{m=0}^{\infty} \eta_{m} = \infty\).

(iii) (adaptive learning rate) the learning rate \(\eta_{m}\) is chosen by the minimization rule, the limited minimization rule, the Armijo rule, or the Goldstein rule [3].

Then, for both L-LAAF and N-LAAF, no limit point of \((\hat{\Theta}_{m})_{m \geq 1}\) is a sub-optimal critical point or a sub-optimal local minimum.

The initial condition \(\tilde{J}(\hat{\Theta}_{0}) < J(0) + S(0)\) means that the initial value \(\tilde{J}(\hat{\Theta}_{0})\) needs to be less than that of a constant network plus the highest value of the slope recovery term. Here, note that \(S(1) < S(0)\). The proof of Theorem 2.1 is included in appendix.

3. Numerical experiments

In this section we shall solve a regression problem of a nonlinear function approximation using deep neural network, and the Burgers equation, which can admit high gradient solution using PINN. For the assessment of the proposed methods, various comparisons are made with the standard fixed as well as global adaptive activation functions.
3.1. Neural network approximation of nonlinear discontinuous function

In this test case a standard neural network (without physics-informed part) is used to approximate a discontinuous function. Here, the loss function consists of the data mismatch and the slope recovery term as

$$J(\hat{\Phi}) = \frac{1}{N_0} \sum_{j=1}^{N_0} |u^j - u(x_j^j, t_j^j)|^2 + S(a).$$

The following discontinuous function with discontinuity at $x = 0$ location is approximated by a deep neural network.

$$u(x) = \begin{cases} 
0.2 \sin(6x) & \text{if } x \leq 0 \\
1 + 0.1x \cos(18x) & \text{otherwise.}
\end{cases}$$

(4)

Here, the domain is $[-3, 3]$ and the number of training points used is 300. The activation function is $\tanh$, learning rate is 2.0e-4 and the number of hidden layers are four with 50 neurons in each layer. In this case, the ratio $P = 1.0257$, which shows just 2.57% increase in the number of hyper-parameters.

Figure 4 shows the solution (first column), solution in frequency domain (second column) and point-wise absolute error in log scale (third column). The solution by standard fixed activation function is given in the first row, GAAF solution is given in second row, whereas the third row shows the solution given by L-LAAF without and with (fourth row) slope recovery term. The solution given by N-LAAF without slope recovery term is shown in the fifth row and with slope recovery term in the sixth row. We see that the NN training speed increases for the locally adaptive activation functions compared to fixed and globally adaptive activations. Moreover, both L-LAAF and N-LAAF with slope recovery term accelerate training and yield the least error as compared to other methods. Figure 5 (top) shows the variation of $na$ for GAAF, whereas the second and third rows show the layer-wise variation of $na^L$ for L-LAAF without and with the slope recovery term. The fourth and fifth rows show the variation of scalable hyper-parameters for N-LAAF without and with the slope recovery term, where the mean value of $na^L$ along with its standard deviation (Std) are plotted for each hidden-layer. We see that the value of $na$ is quite large with the slope recovery term which shows the rapid increase in the activation slopes. Finally, the comparison of the loss function is shown in figure 5 for standard fixed activation, GAAF, L-LAAF and N-LAAF without the slope recovery (left) and for L-LAAF and N-LAAF with the slope recovery (right) using a scaling factor of 10. The Loss function for both L-LAAF and N-LAAF without the slope recovery term decreases faster, especially during the initial training period compared to the fixed and global activation function based algorithms.

3.2. Burgers equation

The Burgers equation is one of the fundamental partial differential equation arising in various fields such as gas dynamics, acoustics, fluid mechanics etc., see Whitham [9] for more details. The Burgers equation was first introduced by H. Bateman [3] and later studied by J.M. Burgers [5] in the context of theory of turbulence. We consider the Burgers equation given by

$$u_t + uu_x = \hat{\epsilon} u_{xx}, \quad x \in [-1, 1], \quad t > 0$$

(5)

with initial condition $u(x, 0) = -\sin(\pi x)$, boundary conditions $u(-1, t) = u(1, t) = 0$ and $\hat{\epsilon} = 0.01/\pi$. The non-linearity in the convection term develops a very steep gradient due to small value of diffusion coefficient. The analytical solution can be obtained using the Hopf-Cole transformation, see Basdevant et al. [2] for more details. The number of boundary and initial training points is 400, whereas the number of residual training points is 10000. The activation function is $\tanh$, learning rate is 0.0008 and the number of hidden layers are 6 with 20 neurons in each layer. In this case the ratio $P = 1.056$, which shows just a 5.6% increase in the number of hyper-parameters.

Figure 7 shows the evolution of frequency plots of the solution at three different times using the standard fixed activation function (first row), global adaptive activation function (second row), L-LAAF without (third row) and with (fourth row) slope recovery term, N-LAAF without (fifth row) and with (sixth row) slope recovery term using scaling factor 10. Columns from left to right represent the frequency plots of solution at $t = 0.25, 0.5$ and 0.75, respectively. As discussed in [6], $t = 0.25$ case needs large number of iterations for convergence, whereas both $t = 0.5$ and 0.75 cases converges faster. Again, for both L-LAAF and N-LAAF the frequencies are converging faster towards the exact
Figure 4: Discontinuous function: Neural network solution using standard fixed activation (first row), GAAF (second row), L-LAAF without (third row) and with (fourth row) slope recovery term, and N-LAAF without (fifth row) and with (sixth row) slope recovery term using the tanh activation. First column shows the solution which is also plotted in frequency domain (zoomed-view) as shown by the corresponding second column. Third column gives the point-wise absolute error in the log scale for all the cases.
Figure 5: Discontinuous function: comparison of variation of $n_{a}$ for GAAF (top row), L-LAAF without (second row) and with (third row) slope recovery term, and N-LAAF without (fourth row) and with (fifth row) slope recovery term using $tanh$ activation. In case of N-LAAF, the mean value of $n_{a}$ along with its standard deviation (Std) are plotted for each hidden-layer.

Figure 6: Comparison of loss function for standard fixed activation, GAAF, L-LAAF and N-LAAF without slope recovery term (left) and L-LAAF and N-LAAF with slope recovery term (right) using scaling factor 10.
Figure 8 shows contour plot of solution of the Burgers equation using L-LAAF after 2000 iterations (top row) and the comparison of solution of the Burgers equation using the standard fixed activation (second row), global adaptive activation function (third row), L-LAAF with slope regularization (fourth row), and N-LAAF with slope regularization (fifth row) using scaling factor 10. Both L-LAAF and N-LAAF gives more accurate solution compared to GAAF. Figure 9 shows the loss function for standard fixed, GAAF, L-LAAF and N-LAAF without slope recovery term (top left) and with slope recovery term (top right). Loss function decreases faster for all adaptive activations, in particular GAAF. Even though it is difficult to see from the actual solution plots given by figure 8, one can see from the table that both L-LAAF and N-LAAF gives smaller relative $L_2$ error using slope recovery term.

|                  | Standard | GAAF     | L-LAAF w/o SRT | N-LAAF w/o SRT | L-LAAF with SRT | N-LAAF with SRT |
|------------------|----------|----------|----------------|----------------|-----------------|-----------------|
| Relative $L_2$ error | 1.913973e-01 | 9.517134e-02 | 8.866356e-02 | 9.129446e-02 | 7.693435e-02 | 8.378424e-02 |

Table 1: Burgers equation: Relative $L_2$ error after 2000 iterations for fixed and all cases of adaptive activation functions. Slope recovery term is abbreviated as SRT.

Figure 10 shows the comparison of layer-wise variation of $n a_k$ for L-LAAF with and without slope recovery term. It can be seen that, the presence of slope recovery term further increases the slope of activation function thereby increasing the training speed. Among all the layers, the sixth hidden-layer shows large increment in the activation slope with slope recovery term since, most of the network learning takes place in the last few hidden-layers. Figure 11 shows the mean and standard deviation of $n a_k$ for N-LAAF with and without slope recovery term, which again validates that with slope recovery term, network training speed increases. This can be seen from the sixth hidden-layer, where activation slope with slope recovery term increases drastically.

4. Numerical results for deep learning problems

The previous sections demonstrated the advantages of adaptive activation functions with PINN for physics related problems. One of the remaining questions is whether or not the advantage of adaptive activations remains with standard deep neural networks for other types of deep learning applications. To explore the question, this section presents numerical results with various standard benchmark problems in deep learning.

MNIST [11], Fashion-MNIST [26] and KMNIST [24] are the data sets with handwritten digits, images of clothing and accessories, and Japanese letters, respectively. Apart from these, Semeion [23] is a handwritten digit data set that contains 1593 digits collected from 80 persons. SVHN [28] is another data set for street view house numbers obtained from house numbers in Google Street View images. CIFAR [15] is a popular data set containing color images. In particular, the CIFAR-10 data set contains 50000 training and 10000 testing images in 10 classes with image resolution of 32x32. CIFAR-100 is similar to the CIFAR-10, except it has 100 classes with 600 images in each class.

Figures 12 and 13 shows the mean values and the uncertainty intervals of the training losses for fixed activation function (standard), GAAF, L-LAAF, and N-LAAF, by using the standard deep learning benchmarks. The solid and dashed lines are the mean values over three random trials with random seeds. The shaded regions represent the intervals of 2×(the sample standard deviations) for each method. Figures 12 and 13 consistently show that adaptive activation accelerates the minimization process of the training loss values. Here, all of GAAF, L-LAAF and N-LAAF use the slope recovery term, which improved the methods without the recovery term. Accordingly, the results of GAAF are also new contributions of this paper. In general, L-LAAF improved against GAAF as expected.

The standard cross entropy loss was used for training and plots. We used pre-activation ResNet with 18 layers [10] for CIFAR-10, CIFAR-100, and SVHN data sets, whereas we used a standard variant of LeNet [11] with ReLU for other data sets; i.e., the architecture of the variant of LeNet consists of the following five layers (with the three hidden layers): (1) input layer, (2) convolutional layer with 64 5×5 filters, followed by max pooling of size of 2 by 2 and ReLU, (3) convolutional layer with 64 5×5 filters, followed by max pooling of size of 2 by 2 and ReLU, (4) fully connected layer with 1014 output units, followed by ReLU, and (5) Fully connected layer with the number of output...
Figure 7: Comparison of solution of the Burgers equation in frequency domain using standard fixed activation (first row), GAAS (second row), L-LAAF without (third row) and with (fourth row) slope recovery term, N-LAAF without (fifth row) and with (sixth row) slope recovery term using $n = 10$. Columns (left to right) represent the solution in frequency domain at $t = 0.25, 0.5$ and $0.75$, respectively.
Figure 8: Contour plot of solution of the Burgers equation using L-LAAF after 2000 iterations (top row) and the comparison of solution of the Burgers equation after 2000 iteration using standard fixed activation (second row), GAAF (third row), L-LAAF with slope recovery term (fourth row), and N-LAAF with slope recovery term (fifth row) using $n = 10$. Columns (left to right) represent the solution at $t = 0.25$, 0.5 and 0.75, respectively shown by the vertical white lines in the top contour plot.
Figure 9: Comparison of loss function for standard fixed, GAAF, L-LAAF and N-LAAF without slope recovery term (left) and L-LAAF, N-LAAF with slope recovery term (right).

Figure 10: Burgers equation: comparison of $a^k$ for L-LAAF for all six hidden-layers. First three columns represent results for L-LAAF without slope recovery term, whereas the last three columns are with slope recovery term. In all simulations, the scaling factor $n$ is 10.

Figure 11: Burgers equation: comparison of mean and standard deviation of $a^k$ for N-LAAF for all six hidden-layers. First three columns represent results for N-LAAF without the slope recovery term, whereas the last three columns are with slope recovery term. In all simulations, the scaling factor $n$ is 10.
Figure 12: Training loss in log scale versus epoch without data augmentation.
Figure 13: Training loss in log scale versus epoch with data augmentation.
units being equal to the number of target classes. All hyper-parameters were fixed a priori across all different data sets and models. We fixed the mini-batch size $s$ to be 64, the initial learning rate to be 0.01, the momentum coefficient to be 0.9 and we use scaling factor $n = 1$ and 2. The learning rate was divided by 10 at the beginning of 10th epoch for all experiments (with and without data augmentation), and of 100th epoch for those with data augmentation.

5. Conclusions

In this paper, we extended our previous work on global adaptive activation function for deep and physics-informed neural network by introducing the locally adaptive activations. In particular, we present two versions of locally adaptive activation functions namely, layer-wise and neuron-wise locally adaptive activation functions. Such local activation functions further improve the training speed of the neural network compared to its global predecessor. To further accelerate the training process, an activation slope based slope recovery term is added in the loss function for both layer-wise and neuron-wise activation functions, which is shown to enhance the performance of the neural network. To verify our claim, two test cases namely, nonlinear discontinuous function approximation and viscous Burgers equation are solved using deep and physics-informed neural networks, respectively. From these test cases, we conclude that the locally adaptive activations outperform fixed as well as global adaptive activations in terms of training speed. Moreover, while the proposed formulations increases the number of additional hyper-parameters compared to the fixed activation function, the overall computational cost is comparable. The proposed adaptive activation function with the slope recovery term is also shown to accelerate the training process in standard deep learning benchmark problems. Moreover, we theoretically prove that no sub-optimal critical point or local minimum attracts gradient descent algorithms in the proposed methods (L-LAAF and N-LAAF) with the slope recovery term under only mild assumptions.

Acknowledgement

This work was supported by the Department of Energy PhILMs grant DE-SC0019453, and by the DAPRA-AIRA grant HR00111990025.

Appendix A. Proof of Theorem 2.1

We first prove the statement by contradiction for L-LAAF. Suppose that the parameter vector $\hat{\Theta}$ consisting of $(w^k, b^k)_{k=1}^{D}$ and $\{a^j\}_{j=1}^{D-1}$ is a limit point of $(\hat{\Theta}_m)_{m \in \mathbb{N}}$ and a sub-optimal critical point or a sub-optimal local minimum.

Let $\ell'_j := \varphi'(u_b(\rho'))$ and $\ell''_j := |\rho' - u_b(x'_j, t'_j)|^2$. Let $z^k_i$ and $z^j_{u}$ be the outputs of the $k$-th layer for $\rho'$ and $(x'_j, t'_j)$, respectively. Define

$$h^{(j,k)} := na^k(w^{k,j}z^{j-1}_f + b^{k,j}) \in \mathbb{R},$$

and

$$h^{(j,k)}_u := na^k(w^{k,j}z^{j-1}_u + b^{k,j}) \in \mathbb{R},$$

for all $j \in \{1, \ldots, N_l\}$, where $w^{k,j} \in \mathbb{R}^{N \times N_{l-1}}$ and $b^{k,j} \in \mathbb{R}$.

Following the proofs in [4] Propositions 1.2.1-1.2.4], we have that $\nabla \tilde{J}(\hat{\Theta}) = 0$ and $\tilde{J}(\hat{\Theta}) < \tilde{J}(0) + S(0)$, for all three cases of the conditions corresponding the different rules of the learning rate. Therefore, we have that for all $k \in \{1, \ldots, D - 1\}$,

$$\frac{\partial \tilde{J}(\hat{\Theta})}{\partial a^k} = \frac{\partial S(a)}{\partial a^k} + n \sum_{j=1}^{N_l} \sum_{i=1}^{N_j} \frac{\partial \ell'_j}{\partial h^{(j,k)}_f}(w^{k,j}z^{j-1}_f + b^{k,j}) + n \sum_{j=1}^{N_l} \sum_{i=1}^{N_j} \frac{\partial \ell''_j}{\partial h^{(j,k)}_u}(w^{k,j}z^{j-1}_u + b^{k,j})$$

or

$$\frac{\partial \tilde{J}(\hat{\Theta})}{\partial a^k} = \frac{\partial S(a)}{\partial a^k} + n \sum_{j=1}^{N_l} \sum_{i=1}^{N_j} \frac{\partial \ell'_j}{\partial h^{(j,k)}_f}(w^{k,j}z^{j-1}_f + b^{k,j}) + n \sum_{j=1}^{N_l} \sum_{i=1}^{N_j} \frac{\partial \ell''_j}{\partial h^{(j,k)}_u}(w^{k,j}z^{j-1}_u + b^{k,j}) = 0.$$
Furthermore, we have that for all \( k \in [1, \ldots, D - 1] \) and all \( j \in [1, \ldots, N_k] \),

\[
\frac{\partial \tilde{J}(\hat{\Theta})}{\partial \tilde{w}^{k,j}} = \frac{n a^k}{N_f} \sum_{i=1}^{N_f} \frac{\partial \ell_f^j}{\partial h_f^{i,k,j}} (z_f^{i,k,j-1})^\top + \frac{n d^k}{N_u} \sum_{i=1}^{N_u} \frac{\partial \ell_u^j}{\partial h_u^{i,k,j}} (z_u^{i,k,j-1})^\top, 
\]

\[
= 0
\]

and

\[
\frac{\partial \tilde{J}(\hat{\Theta})}{\partial \hat{b}^{k,j}} = \frac{n a^k}{N_f} \sum_{i=1}^{N_f} \frac{\partial \ell_f^j}{\partial h_f^{i,k,j}} + \frac{n d^k}{N_u} \sum_{i=1}^{N_u} \frac{\partial \ell_u^j}{\partial h_u^{i,k,j}} = 0. 
\] (A.3)

By combining (A.1)–(A.3), for all \( k \in [1, \ldots, D - 1] \),

\[
0 = a^k \frac{\partial \tilde{J}(\hat{\Theta})}{\partial a^k} = a^k \frac{\partial S(a)}{\partial a^k} + \sum_{j=1}^{N} \left( \frac{n a^k}{N_f} \sum_{i=1}^{N_f} \frac{\partial \ell_f^j}{\partial h_f^{i,k,j}} (w_f^{k,j-1} + b^{k,j}) + \frac{n d^k}{N_u} \sum_{i=1}^{N_u} \frac{\partial \ell_u^j}{\partial h_u^{i,k,j}} (w_u^{k,j-1} + b^{k,j}) \right)
\]

\[
= a^k \frac{\partial S(a)}{\partial a^k} + \sum_{j=1}^{N} \left( w_f^{k,j} (\frac{\partial \tilde{J}(\hat{\Theta})}{\partial \tilde{w}^{k,j}})^\top + b^{k,j} (\frac{\partial \tilde{J}(\hat{\Theta})}{\partial \hat{b}^{k,j}}) \right)
\]

\[
= a^k \frac{\partial S(a)}{\partial a^k}.
\]

Therefore,

\[
0 = a^k \frac{\partial S(a)}{\partial a^k} = -a^k(D - 1) \left( \sum_{k=1}^{D-1} \exp(a^k) \right)^{-2} \exp(a^k),
\]

which implies that for all \( a^k = 0 \) since \((D - 1) \left( \sum_{k=1}^{D-1} \exp(a^k) \right)^{-2} \exp(a^k) \neq 0. \) This implies that \( \tilde{J}(\hat{\Theta}) = \tilde{J}(0) + S(0) \), which contradicts with \( \tilde{J}(\hat{\Theta}) < \tilde{J}(0) + S(0) \). This proves the desired statement for L-LAAF.

For N-LAAF, we prove the statement by contradiction. Suppose that the parameter vector \( \hat{\Theta} \) consisting of \( \{w^k, b^k\}_{k=1}^{D} \) and \( \{a^k\}_{k=1}^{D-1} \) \( \forall j = 1, 2, \cdots, N_k \) is a limit point of \( \{\hat{\Theta}_m\}_{m \in \Omega} \) and a sub-optimal critical point or a sub-optimal local minimum. Redefine

\[
h_r^{i,k,j} := n a^k (w_f^{k,j-1} + b^{k,j}) \in \mathbb{R},
\]

and

\[
h_r^{i,k,j} := n d^k (w_u^{k,j-1} + b^{k,j}) \in \mathbb{R},
\]

for all \( j \in [1, \ldots, N_k] \), where \( w_f^{k,j} \in \mathbb{R}^{1 \times N_k} \) and \( b^{k,j} \in \mathbb{R}^D \). Then, by the same proof steps, we have that \( \nabla \tilde{J}(\hat{\Theta}) = 0 \) and \( \tilde{J}(\hat{\Theta}) < \tilde{J}(0) + S(0) \), for all three cases of the conditions corresponding the different rules of the learning rate.
Therefore, we have that for all $k \in \{1, \ldots, D - 1\}$ and all $j \in \{1, \ldots, N_k\}$,

$$
\frac{\partial \tilde{J}(\Theta)}{\partial a_j} = \frac{n}{N_f} \sum_{i=1}^{N_f} \frac{\partial f_i}{\partial h_{ij}^k} (w^{k,j,i-1} + b^{k,j}) + \frac{n}{N_u} \sum_{u} \frac{\partial h_{ij}^k}{\partial h_{ij}^u} (w^{k,j,i-1} + b^{k,j}) + \frac{\partial S(a)}{\partial a_j}
$$

$$= 0.
$$

By combining (A.2)–(A.4), for all $k \in \{1, \ldots, D - 1\}$ and all $j \in \{1, \ldots, N_k\}$,

$$0 = a_j^k \frac{\partial \tilde{J}(\Theta)}{\partial a_j^k}$$

$$= \frac{n a_j^k}{N_f} \sum_{i=1}^{N_f} \frac{\partial f_i}{\partial h_{ij}^k} (w^{k,j,i-1} + b^{k,j}) + \frac{n a_j^k}{N_u} \sum_{u} \frac{\partial h_{ij}^k}{\partial h_{ij}^u} (w^{k,j,i-1} + b^{k,j}) + a_j^k \frac{\partial S(a)}{\partial a_j}
$$

$$= w^{k,j} (\frac{\partial \tilde{J}(\Theta)}{\partial w^{k,j}})^\top + b^{k,j} \left(\frac{\partial \tilde{J}(\Theta)}{\partial b^{k,j}}\right) + a_j^k \frac{\partial S(a)}{\partial a_j}
$$

$$= a_j^k \frac{\partial S(a)}{\partial a_j}$$

Therefore,

$$0 = a_j^k \frac{\partial S(a)}{\partial a_j} = -2a_j^k (D - 1) \left(\sum_{k=1}^{D-1} \exp \left(\frac{\sum_{j=1}^{N_k} a_j^k}{N_k}\right) \right)^{-2} \exp \left(\frac{\sum_{j=1}^{N_k} a_j^k}{N_k}\right) / N_k,
$$

which implies that for all $a_j^k = 0$ since $(D - 1) \left(\sum_{k=1}^{D-1} \exp \left(\frac{\sum_{j=1}^{N_k} a_j^k}{N_k}\right) \right)^{-2} \exp \left(\frac{\sum_{j=1}^{N_k} a_j^k}{N_k}\right) \neq 0$. This implies that $\tilde{J}(\Theta) = Jc(0) + S(0)$, which contradicts with $\tilde{J}(\Theta) < Jc(0) + S(0)$. This proves the desired statement for N-LAAF.

References

[1] D. P. Kingma, J. L. Ba, ADAM: A method for stochastic optimization, arXiv:1412.6980v9, 2017.
[2] C. Basdevant et al., Spectral and finite difference solution of the Burgers equation, Comput. Fluids, 14 (1986) 23-41.
[3] H. Bateman, Some recent researches on the motion of fluids, Monthly Weather Review, 43(4), 163-170, 1915.
[4] D.P. Bertsekas, Nonlinear programming, Athena scientific Belmont, 1999.
[5] J.M. Burgers, A mathematical model illustrating the theory of turbulence. In advances in applied mechanics, Vol. 1, pp. 171-199, 1948.
[6] AD Jagtap, GE Karniadakis, Adaptive activation functions accelerate convergence in deep and physics-informed neural networks, arXiv preprint arXiv:1906.01170, 2019.
[7] M. Dushkov, R. Ptucha, Adaptive Activation Functions for Deep Networks, Electronic Imaging, Computational Imaging XIV, pp. 1-5(5).
[8] A.G. Baydin, B.A. Pearlmutter, A.A. Radul, J.M. Siskind, Automatic differentiation in machine learning: a survey, Journal of Machine Learning Research, 18 (2018) 1-43.
[9] G.B. Whitham, Linear and nonlinear waves, Vol. 42, John-Wiley & Sons, 2011.
[10] K. He, X. Zhang, S. Ren, J. Sun, Identity mappings in deep residual networks, European conference on computer vision, pp. 630-645, 2016.
[11] Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner, Gradient-based learning applied to document recognition. Proceedings of the IEEE, 86(11): 2278-2324, 1998.
[12] B. Li, Y. Li and X. Rong, The extreme learning machine learning algorithm with tunable activation function, Neural Comput & Appl (2013) 22: 531-539.
[13] G. Hinton, L. Deng, D. Yu, G. Dahl, A. Mohamed, N. Jaitly, A. Senior, V. Vanhoucke, P. Nguyen, B. Kingsbury, et al. Deep neural networks for acoustic modeling in speech recognition. IEEE Signal processing magazine, 29, 2012.
[14] V. Kunc and J. Klema, On transformative adaptive activation functions in neural networks for gene expression inference, bioRxiv, doi:http://dx.doi.org/10.1101/587287, 2019.
[15] A. Krizhevsky and G. Hinton. Learning multiple layers of features from tiny images. Technical report, Citeseer, 2009.
[16] A. Krizhevsky, I. Sutskever, and G. Hinton. Imagenet classification with deep convolutional neural networks. In Advances in neural information processing systems, pages 1097–1105, 2012.

[17] M. Raissi, P. Perdikaris, G.E. Karniadakis. Physics-informed neural network: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. J. Comput. Phys., 378, 686–707, 2019.

[18] Dropout: A Simple Way to Prevent Neural Networks from Overfitting, N. Srivastava, G. Hinton, A. Krizhevsky, I. Sutskever, R. Salakhutdinov; Journal of Machine Learning Research, 15(Jun):1929–1958, 2014.

[19] J.-X Wang, et al., A comprehensive physics-informed machine learning framework for predictive turbulence modeling, arXiv:1701.07102.

[20] S. Ruder, An overview of gradient descent optimization algorithms, arXiv:1609.04747v2, 2017.

[21] S. Qian, et al. Adaptive activation functions in convolutional neural networks, Neurocomputing Volume 272, 10 January 2018, Pages 204-212.

[22] Y. Shen, B. Wang, F. Chen and L. Cheng. A new multi-output neural model with tunable activation function and its applications. Neural Processing Letters, 20: 85-104, 2004.

[23] Tactile Srl, Brescia, Italy (1994). Semeion Handwritten Digit Data Set. Semeion Research Center of Sciences of Communication, Rome, Italy.

[24] T. Clanuwat, M. Bober-Irizar, A. Kitamoto, A. Lamb, K. Yamamoto, D. Ha, "Deep Learning for Classical Japanese Literature", arXiv:1812.01718.

[25] Y. Wu, M. Schuster, Z. Chen, Q. V. Le, M. Norouzi, W. Macherey, M. Krikun, Y. Cao, Q. Gao, K. Macherey, et al. Googles neural machine translation system: Bridging the gap between human and machine translation. arXiv preprint arXiv:1609.08144, 2016.

[26] H. Xiao, K. Rasul, and R. Vollgraf. Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms. arXiv preprint arXiv:1708.07747, 2017.

[27] C. Yu, et al., An adaptive activation function for multilayer feedforward neural networks. 2002 IEEE Region 10 Conference on Computers, Communications, Control and Power Engineering. TENC0 '02. Proceedings.

[28] Yuval Netzer, Tao Wang, Adam Coates, Alessandro Bissacco, Bo Wu, Andrew Y. Ng Reading Digits in Natural Images with Unsupervised Feature Learning NIPS Workshop on Deep Learning and Unsupervised Feature Learning 2011.