Araştırma Makalesi

Research Article

A THEORETICAL INVESTIGATION ON TRAINING OF PIPE-LIKE NEURAL NETWORK BENCHMARK ARCHITECTURES AND PERFORMANCE COMPARISONS OF POPULAR TRAINING ALGORITHMS

Ozlem Imik SIMSEK* , Baris Baykant ALAGOZ

Inonu University, Engineering Faculty, Department of Computer Engineering, Malatya, Turkey

BORU-BENZERİ YAPAY SİNİR AĞI KARŞILAŞTIRMA MİMARİLERİNİN EĞİTİMİ HAKKINDA BİR TEORİK ARAŞTIRMA VE POPULAR EĞİTİM ALGORİTMALARIN PERFORMANS KARŞILAŞTIRILMALARI

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algoritmalarının genel performansının ölçüt tabanlı değerlendirmesi için Normalleştirilmiş Genel Performans Puanlaması (NGPP) uygulanmıştır.

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1. Introduction

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Neural networks have been gaining growing popularity in many fields of engineering and applied science for almost two decades. Their architectures and computation schemes have been progressively developed since the first appearance of the fundamental neural network models (Kim,2017). Today, the learning power of deep neural networks is harnessed for processing much bigger data stacks, and theoretical works and research competitions for deeper neural networks are continuing to boost learning capability of the deep neural networks (Coleman et al., 2017; Schmidhuber, 2015; Shrestha and Mahmood, 2019; Deng and Yu, 2013; Winkler and Le, 2017; Mhaskar et al., 2016).

Architectures of neural networks and the training algorithms have been occasionally progressed. The gradient vanishing problem was a major problem when adding more hidden layers to neural networks to reach much deeper networks (Kim, 2017). As the hidden layer count has increased, gradient vanishing problems have emerged, slowed down the training, reduced efficiency of backpropagation algorithms throughout deep layers, and the practical benefits in use of deeper layers began to disappear. Since around 2000, researches have came up with several solutions for the training problems of deep hidden layers; for instance use of more relevant activation functions (RELU and variants)(Kim, 2017; Oostwal et al., 2019), pre-training approaches (Hinton and Salakhutdinov, 2006), better random initial scaling (Glorot and Bengio, 2010), employment of better optimization methods (Martens, 2010), selection of more suitable neural network architectures (Shrestha and Mahmood, 2019; Bahrami et al., 2019; Arifovic and Gençay, 2001) and improved initialization techniques such as the orthogonal initialization and the random walk initialization (Sussillo and Abbott, 2014).

Besides the implementation of gradient based optimization methods in neural network training, there have been attempts to use metaheuristic optimization algorithms in the training process of neural networks. The metaheuristic optimization can provide a gradient-free search option and this becomes advantageous when searching the optimal points in low-gradient parametric search spaces (Martens, 2010). Metaheuristic methods employ a set and trial search strategy to seek optimal values of parameters in the complicated optimization problems (Arifovic and Gençay, 2001; Sussillo and Abbott, 2014). Due to these advantageous, there are several research works that have addressed the training of feedforward neural networks by using popular metaheuristics(Sexton and Gupta, 2000; Che et al., 2011; Gudise and Venayagamoorthy, 2003; Ince et al., 2010; Mosavi et al., 2016) and results were compared with the backpropagation method in the shallow feedforward neural network training problems: Sexton et al. showed that genetic algorithm could be effectively used for training of shallow neural networks for chaotic time series data and reported a superior training performance of genetic algorithm over the backpropagation methods (Sexton and Gupta, 2000). In a similar study, Che et al. concluded that the backpropagation algorithm can be preferred since it provides faster training of neural networks than the genetic algorithm; however it can suffer from the gradient vanishing problem where the genetic algorithm does not suffer (Che et al., 2011). Gudise et al. compared the neural network training performance of particle swarm optimization with performance of a backpropagation algorithm and reported that particle swarm optimization algorithm can faster converge to optimal weights than the backpropagation algorithm (Gudise and Venayagamoorthy, 2003). These contradicting reports on training performances of backpropagation and metaheuristic methods indicate the need for well-designed, standardized test and evaluation procedures.

^{*} İlgili yazar / Corresponding author: [oimiksimsek@gmail.com,](mailto:oimiksimsek@gmail.com) +90-530-416-8860

Later, performances of several contemporary metaheuristic algorithms were compared for the training of neural networks (Mosavi et al., 2016; Ghasemiyeh et al., 2017). Besides the training process of the neural network, metaheuristic optimization has also been performed for optimization of the network architectures to reach an improved training performance (Arifovic and Gençay, 2001). Although there are many efforts that compare performances of the learning methods (Sewak et al., 2018; Caruana and Niculescu-Mizil, 2006; Bala et al., 1992) and training algorithms (Bahrami et al., 2019; Zhao et al., 2010; Rusiecki, 2012; Karim et al., 2018; Can et al., 2019; Awolusi et al., 2019; Thakkar et al., 2020) in specific application domains, application-specific results obtained for arbitrary network architectures may not be relevant and consistent to have a common view on the training performances of the algorithms. For this reason, there is a demand for standard neural network training benchmark architectures, which are deliberately designed for hardto-train tests to uncover advantages and/or shortcoming of the training algorithms (Zhu et al., 2018; Fong et al., 2018). Such application-independent benchmarking is particularly useful to pinpoint major drawbacks of existing popular training algorithms and helpful to indicate new research directions for the ongoing research efforts.

This study investigates training performances of 9 widely used backpropagation training algorithms (e.g. LM, BFG, CGB etc.), which are implications of the gradient based optimization approaches, and 3 popular metaheuristic search methods (GA, PSO GWO) in the training problem of pipe-like deep neural network benchmark architectures. The pipe-like architecture of deep neural networks complicates the training process due to forming a long and narrowed learning bottleneck via an elongated feedforward path of neurons. In the experimental work, the body fat percentage estimation dataset, which may express biocomplexity of human metabolism, is used in training of this architecture with different pipe lengths (hidden layer counts). For the overall performance assessment of the training methods in pipe-like neural network architecture, a NOPS scheme is employed and the overall training performance and performance criterionbased selection of the training algorithms are shown. The addressed problems, novelties and main contributions of this study can be summarized as:

(i) A pipe-like neural network benchmark architecture, which is called pipe-like neural network benchmark architecture, is introduced. The pipe-like neural network benchmark architecture forms an extended bottleneck for the learning process. The training difficulties of this hard-to-train benchmark architecture are theoretically analyzed in the aspect of Baldi et al.'s learning channel theorem of neural networks. This effort contributes to using practical implications of the learning channel theorem for investigating training problems in deep neural networks.

(ii) A theorem to consider upper bounds of the training performance for gradient-based training algorithms is suggested. This theorem implements sensitivity derivative analysis on the pipe-like deep neural learning channel and it conjectures essential mechanisms that lead to gradient vanishing problems in deep neural networks. Suggestions of this theorem were observed in the experimental study and used to explain essential reasons for training performance degradations of gradient-based training in our experimental test.

(iii) To the best of our knowledge, this is the first experimental study that tests training performances of 9 popular NNBA algorithms and 3 fundamental MSA algorithms on the elongated pipe-like benchmark architectures from shallow one to deeper networks. The training performances of these algorithms are reported without any application-specific bias. The experimental results revealed performance drawbacks of these training algorithms and results indicated a requirement of designing new deep learning dedicated optimization algorithms, which are particularly specialized for training of deep neural network algorithms.

(iv) To enable performance criterion-based selection of the training algorithms, a NOPS scheme is illustrated. By allowing importance weighting of the performance criterion, NOPS can contribute to the solution of automated training algorithm evaluation and selection problems.

2. Preliminaries And Theoretical Background

This section provides preliminary knowledge on NNBA and MSA training algorithms that are tested in experimental study. Then, training difficulties of the pipe-like neural network benchmark architecture are theoretically analyzed by suggesting a theorem for upper bounds of training performance of this benchmark architecture. This theoretical background establishes a theoretical foundation to demonstrate suitability of the pipe-like neural network benchmark architecture for testing of training algorithm performances.

2.1. Backpropagation Training Algorithms

Training of an artificial neural network mathematically refers to finding optimal values of weight coefficients in order to minimize a predefined loss function. The loss functions are mathematical expressions that are used to evaluate the quality of the learning activity on the net. This optimization problem complicates as the number of layers in a neural network increases because of the increased function compositions to represent the network function (functional complexity of the network function) and growing weight and bias coefficient numbers to be optimized (high dimensionality of the optimization problem). To deal with complications associated with the training of multilayer feedforward neural network architectures, a "backpropagation" algorithm was proposed to cope with functional complexity of multilayer networks (Kim, 2017; Goodfellow et al., 2016). Then, the backpropagation has become the most fundamental training algorithm, and it has found a wide application area for the training of multilayer neural networks. It involves two essential stages (Kim, 2017): firstly, the input data propagates towards the output layer of neural networks; this stage is forward propagation of information, afterward, the error information, which is calculated at the output of the neural network, propagates back into the input layer of the neural network. This is the process of the backward propagation of the error information, where the term "backpropagation" comes from. Several training algorithms have been proposed to improve performance of the backpropagation training approach (Hagan et al., 1996; Cömert and Kocamaz, 2017; Hagan and Menhaj, 1994; Dennis and Schnabel, 1996; Mosavi et al., 2016; Pan et al., 2013). Table 1 shows a list of up-to-date backpropagation training algorithms that have been preferred in the training of multilayer feedforward neural networks in the current study. Training performance of backpropagation algorithms decrease when the hidden layer number of the feedforward neural networks increases because of the gradient vanishing problems: The decrease in gradient magnitudes can severely deteriorate the backward error propagation toward input layers, the weight updates slows down, and the training in deep layers begins to cease, practically. Therefore, consistent training performance analysis of algorithms should be carried out for deep and complicated neural network configurations.

Training Algorithms	Abbreviations	Related Works
Levenberg-Marquardt backpropagation	LM	(Hagan et al., 1996; Hagan and
		Menhaj, 1994; Powell, 1977)
Quasi-Newton backpropagation with Broyden,	BFG	
Fletcher, Goldfarb, and Shanno (BFGS) update		(Dennis and Schnabel, 1996)
Conjugate gradient backpropagation with Powell-	CGB	(Powell, 1977; Beale, 1972)
Beale restarts		
Conjugate gradient backpropagation with Polak-	CGP	(Hagan et al., 1996; Scales, 1985
Ribiére updates		; Fletcher, 1964)
Conjugate gradient backpropagation with Fletcher-	CGF	(Hagan et al., 1996; Scales,
Powell updates		1985; Fletcher, 1964
Variable learning rate gradient descent	GDX	(Vogl et al., 1988)
One-step secant backpropagation	_{OSS}	(Battiti, 1992)
Resilient backpropagation	RP	(Riedmiller and Braun, 1993)
Scaled conjugate gradient backpropagation	SCG	(Moller, 1993)

Table 1. The NNBA Types, Which Are Tested in This Study, and Their Abbreviations

2.2. Metaheuristic Training for Artificial Neural Networks

Metaheuristic optimization methods are easy-to-use, optimal solution seeking tools that have been widely implemented in engineering problems. They have been particularly used when the optimization problem is too complex to be solved numerically or analytically (Wong and Ming, 2019). These methods employ a set and trial search strategy that can provide a straightforward solution for empirical, complicated, even notwell structured optimization problems. This introduces an important advantage that makes them preferable in real-world engineering application works. However, they have some disadvantages such as concerns about the dependability of solutions, inefficiency of these methods while searching in high dimensional search spaces etc.

The candidate solution selection strategies of metaheuristic algorithms are very substantial for convergence performance of metaheuristic optimization, and they establish major discrimination points between metaheuristic optimization techniques. Some major problems, which were observed in use of the metaheuristic methods, can be summarized as (Gogna and Tayal, 2013; Chopard and Tomassini, 2018; Hinton, Salakhutdinov, 2006; Igel, 2014):

(i) Contemporary metaheuristic optimization methods cannot convey definite information whether or not the solution is globally optimal (Gogna and Tayal, 2013). However, the quality of solutions can be evaluated with the value of objective functions in applications (Parejo et al., 2012; Gunantara et al., 2019).

(ii) Metaheuristic optimization is commonly effective in the low dimensional search spaces. An increase in the dimension of search spaces, that is, more parameters to optimize, severely reduces the converge performance in the metaheuristic searching because of the exponential growth in the exploration fields for the set and trial searching of search agents. When the number of parameters, namely the dimension of the problem, increases, the computation time of the algorithms severely arises (Chopard and Tomassini, 2018; Parejo et al., 2012).

(iii) Many metaheuristic methods need the finite search spaces that are confined by the predefined search ranges of the optimized parameters. This may become an important shortcoming that can reduce practical efficiency of metaheuristic methods because it is not always an easy problem to determine predefined search ranges of parameters, which can include the global minimum or maximum. Therefore, improper configuration of parameter search regions can limit performance of metaheuristic search (Chopard and Tomassini, 2018; Birattari and Kacprzyk, 2009).

(iv) Metaheuristics methods commonly utilize random number generation in the search processes to differentiate search paths. However, this brings a problem of unrepeatability of the solutions even though the computers can generate pseudo-random numbers. The reliable results require a statistical evaluation of the repeated optimization tasks. However, the rerunning of the algorithms many times can considerably increase the computational burden (Gogna and Tayal, 2013; Parejo et al., 2012).

When the depth of a multi-layer feedforward neural network increases, training of the neural network introduces difficulties associated with gradient magnitudes for gradient-based optimization techniques. Therefore, there exist several efforts to implement gradient-free metaheuristic optimization as a substitute for backpropagation methods (Sexton and Gupta, 2000; Che et al., 2011; Gudise and Venayagamoorthy, 2003; Ince et al., 2010; Mosavi et al., 2016). Since a majority of metaheuristic methods perform gradientfree optimization algorithms, they are expected to present advantages over the gradient-based optimization algorithms when gradient calculations are problematic or ineffective. For the training of the multilayer feedforward networks, three widely preferred popular metaheuristic optimization methods in the literature are listed in Table 2 (Che et al., 2011; Ince et al., 2010; Mosavi et al., 2016). These methods are commonly used to minimize the sum of square error loss function of neural networks, which is written by

$$
\min E(w) = \frac{1}{2} \sum_{i=1}^{k} e_i^2 = \frac{1}{2} \sum_{i=1}^{k} (f_i(w, x_j) - y_i)^2
$$
\n(1)

where, $f_i(w, x_j)$ represents i th output function of the neural network for the input vector x_j . Training set is formed by the input-output data pairs $(x_j, y_1, y_2, \ldots, y_k)$. The weight vector w represents a collection of the weight coefficients of neural networks, which are optimized during the training of the network via a metaheuristic method. (Bias coefficients are computationally assumed as an input with a weight value of 1). Number of parameters to optimize, n layer neural network can be written by

$$
D = \sum_{h=1}^{n} (k_{(h-1)}k_h + k_h)
$$
, where k_h is the number of neurons in the hidden layer h and k_0 is the number

of inputs in a neural network. Parameter number *D* determines the dimension of the search space. The search space expands a D dimensional hypercube by the term $[w_l, w_u]^D$, where $[w_l, w_u]$ is the upper and lower boundaries of weight coefficient search ranges. Due to the exponential growth of the search space volume, the metaheuristic algorithms in Table 2 have been utilized in the training of shallow neural networks (Che et al., 2011; Ince et al., 2010; Mosavi et al., 2016). It will be useful to test these methods in training of the pipe-like architecture of deep neural networks to better observe the inherent shortcomings of the metaheuristic training approach.

2.3. A Theoretical Background on Pipe-like Architecture Deep Neural Network

Architecture types of neural networks affect the learning skills, and the proper selection of network architecture is a very important stage for the training performance (Ince et al., 2010; Hornik, 1991). Fundamentally, feedforward neural network architectures are divided into two main categories: These are the single layer neural networks in Figure 1 and the multi-layer neural networks in Figure 1. Later, multilayer feedforward neural networks were grouped into two major subcategories that are the shallow neural networks and the deep neural networks. Theoretical discussions on the architecture or the configuration of artificial neural networks are continuing on the bases of universal approximation theorems (Schmidhuber, 2015 ; Winkler and Le, 2017; Hornik, 1991; Csaji, 2001; Kratsios and Bilkoptov, 2020).

Conceptually, increasing the tunable parameter numbers (layers, weights, bias, generic activation function) can enhance fitting capability to data because it increases complexity in the compositional function representation of neural network and accordingly allows representation of more composite function models by using the deep neural network function $f_i(w, x_j)$. Thus, deep neural networks present

potential of better approximating to higher complexity compositional function models that cannot be well approximated by a shallow neural network (Mhaskar et al., 2016). On the other hand, in addition to enhancing approximation capability, increasing the depth of feedforward network was observed to enable more abstraction of the learned knowledge in the deeper layers similar to the biological neural network can do, for instance the convolution neural network can detect more complex features (irregular shape) in deep layers by using more primitive features (e.g. edges, curves) that are detected in the shallow layers (Deng and Yu, 2013). However, the overfitting problem, which causes a reduction in the generalization property in learning, emerges in deep neural networks because too many tunable parameters highly increase the approximation capability of neural network function to each data point in the training set. Overfitted models cause serious performance degradations in data applications in the cases of noisy data or insufficient data in training sets. Therefore, a proper generalization is preferable in data applications to obtain satisfactory practical performance.

In order to compare training performances of the training methods, hard-to-train neural network architectures are more suitable to reveal the performance shortcomings and superiorities. In this manner, authors used a pipe-like architecture deep neural network in the performance tests. The width of layers was set to 5 neurons and the length of the neural network was increased up to 20 layers by adding a hidden layer at each test. Figure 2 shows a depiction of the trained 5 neurons wide and 20 layers long pipe-like benchmark architecture. This generic pipe-like structure enables testing several pipe architecture versions from the shallow one to the deep networks by adjusting the hidden layer counts.

The communication and signaling phenomenon between neurons indicate the communication nature of the neural networks (Tagluk and Isik, 2019). A neural network resembles an information-adaptive narrowband communication channel with a learning property between the input layer and the output layer of the neural network. Previously, Baldi et al. have suggested the existence of a physical learning channel to convey information via the weights of the network (Isik and Sadowski, 2016) and they investigated the capacity of learning algorithms by considering the error gradients per weight. Thus, Baldi et al. conjectured a foundation for the learning channel theorem of neural networks. The current study contributes to the learning channel theorem of neural networks in a practical aspect by considering distribution of weight update magnitudes throughout a pipe-like deep neural network. Figure 2 depicts a one-neuron wide, pipelike network fraction (at middle schematic) that is composed of the hidden neuron model (at bottom schematic). Let's investigate the weight update magnitudes for this network to show hard-to-train nature of pipe-like benchmark networks:

Figure 2. A Block Diagram Of A 5 Neuron Wide And 20 Layer Long Pipe Architecture Neural Network (Top Schema), A Depiction Of One-Neuron Wide Pipe-Like Network Segment (Middle Schema), One Neuron In The Hidden Layer (Bottom Schema)

Essentially, the pipe-like architecture results in a long bottleneck for the training process because a pipelike architecture forms a narrowed and elongated network for forward and backward propagation of neural information and it exhibits two major training drawbacks for gradient based training algorithms that are the propagation delay problems related to narrowing of network and gradient vanishing problems related to elongation of network. To analyze these properties associated with the network architecture, let's denote the output function of the layer $\,h\,$ in the neural network by the function $f^{\,h}({w}^h,{x}^h_i)$ *j* $f^h(w^h, x_i^h)$, where the superscript

 $h\,$ is the layer index. When the layer number increases by adding more layers, the resulting output function of a deep neural network with n layers can be commonly expressed by using function compositions as (Mhaskar et al., 2016; Isik and Sadowski, 2016; Strang, 2018)

$$
y = f^{n}(w^{n}, f^{n-1}(w^{n-1}, f^{n-2}(w^{n-2}, \dots f^{2}(w^{2}, f^{1}(w^{1}, x^{1}_{j}))....)))
$$
 (2)

where the superscript n is the depth of this function composition.

By considering activation function and the weighted sum of neuron inputs in the form of $(f^h(w^h, x^h) = \varphi^h(\sum w_i^h \cdot \varphi_i^{h-1}) = \varphi^h(w^h \varphi^{h-1})$ *i h i* $y^h = f^h(w^h, x^h)$ = $\phi^h(\sum w^h_i \phi^{h-1}_i)$ = $\phi^h(w^h\phi^{h-1})$ (Isik and Sadowski, 2016; Mhaskar et al., 2016), the output of whole neural network is considered in the form of

$$
y = \varphi^{n} \left(\sum w^{n} \varphi^{n-1} \left(\sum w^{n-1} \varphi^{n-2} \left(\sum w^{n-2} \dots \varphi^{2} \left(\sum w^{2} \varphi^{1} \left(\sum w^{1} x_{j} \right) \right) \dots \right) \right) \right)
$$
(3)

 $(\sum w^2 \phi^{-1} (\sum w^2 - \omega^2)^{-2}) = (\sum w^2 - \omega^2)^{-2}$. ($w^2 \phi^{-1} (\sum w^2 \pi^2)$))) (3)

ggests a composite learning function formly of the weight coefficient vector w^4 . The ϕ^4 ()

critication in the tage of h . The weighted This equation suggests a composite learning function family of the weight coefficient vector $\ w^h$. The $\ \varphi^h(.)$ stands for the activation in the layer *h* . The weighted sum of neuron inputs in the layer *h* can be represented by the weighted sum of previous layer outputs $v^h = \sum w_i^h . \varphi_i^{h-1}$ *i h i* $v^h = \sum w_i^h \cdot \varphi_i^{h-1}$. For every optimal determination of the weight coefficient set of w^* = { w^1 , w^2 , w^3 ,.., w^h } at a minima of the loss function, the results yield a learned function $y_j = f(w^*, x_j)$ for an input vector x_j from the training set. The pipe-like architecture mainly narrows the width of the network, and this decreases the number of the weighted sum terms in the output function of the network. Consequently, this decreases the complexity of the composite learning function family that is represented by the Equation (3). Accordingly, a reduction in the complexity of the composite learning function tree decreases the representative nature of the output function. This is a factor that complicates the training tasks of a pipe-like architecture for all training algorithms.

The gradient-based algorithms use delta rule for the weight updates,

$$
w^h \leftarrow w^h + \Delta w^h \tag{4}
$$

where Δw^h is the weight update (Kim, 2017; Isik and Sadowski, 2016). The weight updates Δw^h are commonly performed in directions where the loss function decreases. Therefore, sensitivity function $\frac{d\mathbf{x}}{d\mathbf{w}^h}$ *E* õ õ

is widely used for the weight update $\Delta w^n = -\eta \frac{\Delta w}{\Delta h}$ *h w* $w^h = -\eta \, \frac{\partial E}{\partial w^h}$ $\Delta w^h = -\eta \frac{\partial E}{\partial x^h}$ in order to detect the descent directions of the loss

function, where $\,\eta > 0\,$ is the learning rate that is commonly used to regulate converge rate of gradient-

based optimization techniques. The magnitude of the weight updates $|\Delta w^n| = \eta \frac{\partial^2 w}{\partial x \partial y}$ *h w* w^h = $\eta \left| \frac{\partial E}{\partial w^{\prime}} \right|$ $\Delta w^h\Big| = \eta \Big| \frac{\partial E}{\partial h} \Big|$ is an indicator to

evaluate penetration of learning through the network. To consider training difficulties of pipe-like neural network architecture for gradient-based backpropagation training algorithms, it is useful to investigate an upper boundary of sensitivity function magnitude in the network.

Theorem 1 (An upper bound for sensitivity derivatives in pipe-like neural network models):

In cases of k numbers of the neuron in the each layer and gradient-based training algorithms, an upper bound for sensitivity derivatives at the first layer neurons can be expressed as

$$
\left|\frac{\partial E}{\partial w^1}\right| \leq \sum_{i}^{k} \left|\frac{\partial E}{\partial \varphi_i^n} \right| \left|\frac{\partial \varphi_i^n}{\partial v^n}\right| \left|w^n\right| \left|\frac{\partial \varphi_i^{n-1}}{\partial v^{n-1}}\right| w^{n-1} \dots \left|w^3\right| \left|\frac{\partial \varphi_i^2}{\partial v^2}\right| w^2 \left|\frac{\partial \varphi_i^1}{\partial v^1}\right| x_j \tag{5}
$$

Proof: To calculate sensitivity derivative $\frac{d^{2}y}{\partial w^{h}}$ *E* д $\frac{\partial E}{\partial \mathbf{r}}$ through the layers, a chain rule of derivative operators is

implemented to cope with the composite function form of the neural network output function. When the chain rule of derivative operator is used for the one-neuron wide and n layer pipe-like architecture, the sensitivity derivative can be written by

$$
\Delta w^{1} = -\eta \frac{\partial E}{\partial w^{1}} = -\eta \frac{\partial E}{\partial \varphi^{n}} \frac{\partial \varphi^{n}}{\partial v^{n}} \frac{\partial v^{n}}{\partial \varphi^{n-1}} \frac{\partial \varphi^{n-1}}{\partial v^{n}} \frac{\partial v^{n-1}}{\partial \varphi^{n-2}} \dots \frac{\partial v^{3}}{\partial \varphi^{2}} \frac{\partial \varphi^{2}}{\partial v^{2}} \frac{\partial v^{2}}{\partial \varphi^{1}} \frac{\partial \varphi^{1}}{\partial v^{1}} \frac{\partial v^{1}}{\partial w^{1}} \tag{6}
$$

for an update of weights in the first hidden layer (Roodschild et al., 2020). Here, by considering at the hidden layers $\frac{V}{h} = w^h$ *h h* $\frac{\partial v}{\partial \varphi^{h-1}} = w$ д $\frac{\partial^2 V}{\partial \varphi^{h-1}} = w^n$ and the first hidden layer $\frac{\partial^2 V}{\partial w^1} = x_j$ *w* $\frac{\partial v}{\partial w^1} =$ д 1 , the magnitude of sensitivity at the first hidden layer is expressed by the weight update magnitude as

$$
\left| \frac{\partial E}{\partial w^1} \right| = \left| \frac{\partial E}{\partial \varphi^n} \right| \left| \frac{\partial \varphi^n}{\partial v^n} \right| w^n \left| \frac{\partial \varphi^{n-1}}{\partial v^{n-1}} \right| w^{n-1} \dots w^3 \left| \frac{\partial \varphi^2}{\partial v^2} \right| w^2 \left| \frac{\partial \varphi^1}{\partial v^1} \right| x_j \tag{7}
$$

For k numbers of the neuron in the each layer (i.e., the learning channel width of k-neurons), one can aggregate contributions of all one-neuron path segments (See middle schema in Figure 2) in order to state an upper boundary for the sensitivity function magnitudes:

$$
\left|\frac{\partial E}{\partial w^1}\right| \leq \sum_{i}^{k} \left|\frac{\partial E}{\partial \varphi_i^n} \right| \left|\frac{\partial \varphi_i^n}{\partial v^n}\right| \left|w^n\right| \left|\frac{\partial \varphi_i^{n-1}}{\partial v^{n-1}}\right| w^{n-1} \dots \left|w^3\right| \left|\frac{\partial \varphi_i^2}{\partial v^2}\right| w^2 \left|\frac{\partial \varphi_i^1}{\partial v^1}\right| x_j
$$

Some Remarks and A Numerical Example:

By using Equation (5), an upper boundary for the weight updates at the first layer neurons can be obtained

$$
\left|\Delta w^{1}\right| = \eta \left|\frac{\partial E}{\partial w^{1}}\right| \leq \eta \sum_{i}^{k} \left|\frac{\partial E}{\partial \varphi_{i}^{n}}\right| \left|\frac{\partial \varphi_{i}^{n}}{\partial v^{n}}\right| \left|w^{n}\right| \left|\frac{\partial \varphi_{i}^{n-1}}{\partial v^{n-1}}\right| w^{n-1} \dots \left|w^{3}\right| \left|\frac{\partial \varphi_{i}^{2}}{\partial v^{2}}\right| w^{2} \left|\frac{\partial \varphi_{i}^{1}}{\partial v^{1}}\right| x_{j} \tag{8}
$$

This boundary reveals a restrictive factors for the learning activity of the pipe-like neural networks: The learning tendency of the network at each training epoch depends on the magnitude of activation function derivatives $\left| \frac{\partial \varphi}{\partial h} \right|$ *h ^v* $\frac{\partial \varphi^n}{\partial x^n}$, the magnitude of weight coefficients $|w^n|$, the learning rate η and the depth of the network (*n*). For the worst-case analysis, each partial derivative term of activation functions can be assumed $\left|\frac{\partial \varphi}{\partial h}\right| < 1$ д д *h h v* $\left|\frac{\partial v^*}{\partial v^h}\right|$ < 1 and the weight magnitudes are considered $\left|\frac{\partial v^*}{\partial \omega^{h-1}}\right| = \left|w^h\right|$ < 1 õ т, *h h h* $\left|\frac{v}{v}\right| = |w|$ φ , these conditions cause the whole chain rule approximating to zero, $\frac{d}{d\omega}$ \rightarrow 0 õ *w* $\left| \frac{E}{\cdot} \right| \rightarrow 0$, as the number of hidden layer (*n*) increases because of the subsequent multiplication of $\left|\frac{\partial \psi}{\partial x}\right| < 1$ д д *h h v* $\left|\frac{\varphi}{\varphi}\right|$ < 1 and $|w^h|$ < 1 terms. This effect results in the weight updates also converging to zero, $|\Delta w^1|\!\rightarrow\!0$, and it can severely slow down the training process.

According to Theorem 1, the deep pipe-like network encounters two major training complications for NNBA methods: (i) gradient vanishing problem $\left(\frac{\partial \mathbf{L}}{\partial w_1} \rightarrow 0\right)$ д *w* $\frac{E}{\hbar}$ \rightarrow 0) because of the multiplication of terms with

 $<\!1$ д д *h h v* $\left|\frac{\varphi^{\alpha}}{h}\right|$ < 1 and $|w^h|$ < 1 as the hidden layer number increases, and (ii) slowing down the training process

though the pipe-like networks as neuron counts *k* (the channel width) decreases in the narrowed layers. For a numerical illustration of the gradient vanishing problem in the pipe-like neural networks, it is useful to consider upper bounds of sensitivity derivatives at the first hidden layer for a fundamental activation function. For illustration purpose, a pipe-like neural network with the sigmoid activation function (*v e* $v = \frac{1}{1+e^{-t}}$ $\varphi(v) = \frac{1}{(1 - v^2)}$ is investigated based on the inequality (5). The unit weight coefficients $|w^i| = 1$ and the

unit input $|x_j|=1$ are assumed in order to compensate for effects of weight and input parameters. Thus, one can consider only effects of the activation function selection on the training process. Let us consider sigmoid activation functions, it is obvious that $\left|\frac{p}{\sigma} \right| \leq 0.25$ д õ *h h v* $\left|\frac{\varphi}{\varphi}\right|$ \leq 0.25. For an upper boundary analysis, the

maximum value $\left|\frac{\partial \varphi}{\partial x}\right| = 0.25$ $\left|\frac{\partial \psi}{\partial v^h}\right|$ = 0.25 can be used in inequality (5). Figure 3 shows change of logarithmic scaled $\partial\pmb{\varphi}^h$

sensitivity function amplitude ($\left|\frac{\partial \mathbf{L}}{\partial w^1}\right|$ *E* д $\frac{\partial E}{\partial \mathbf{r}}\big|_0$ at the first layer neurons while increasing hidden layer numbers up to 20 layers. The upper bound of the sensitivity derivative up to 20 hidden layer network is about д *E*

≤ 9.09 · 10^{-13} , which also implies that the weight updating $\left|\Delta w^1\right|$ ≤ η 9.09 · 10^{-13} is at a negligible ∂w^1 *w*

level at the first layer. This problem suppresses backward propagation of error signals through deep neural networks. This result indicates a severe gradient vanishing problem with almost cessation of the training process under the presumed conditions. However, according to this conjecture, one can suggest that the learning rate $\eta,$ can be adaptively used to amplify the sensitivity function amplitudes to deal with this issue.

3. An Experimental Study

This section reports experimental results for training performance of 9 popular NNBA algorithms and 3 fundamental MSA algorithms on the elongated pipe-like benchmark architectures. The advantages and disadvantages of the tested training algorithms are revealed in training of this benchmark architecture.

3.1. A Comparison of Training Algorithms from Shallow to Deep Training

Artificial neural networks have been widely used for the black-box modeling of the physical and biological systems and they have been implemented in the model-based prediction problems (Chen et al., 2020; Zhao et al., 2020). Due to higher level of complexity and chaotic dynamics, biological system modeling benefits from highly nonlinear function approximation skills of the artificial neural networks. To conduct the training experiments, the body fat rate estimation problem is solved by using body fat data from Matlab. This dataset is composed of 13 anatomical measurements of the human body as input data, and the neural network is trained to predict body fat percentages based on these anatomical features (Zamri et al., 2018). This dataset involves highly nonlinear relations and noisy data, which make it preferable for training algorithm tests.

Figure 4 shows the average MSE performance of NNBA training tests. Figure 5 and Figure 6 illustrate the maximum MSE and the minimum MSE performances of NNBA training processes for 10 repeated tests. A large increase in layer counts cannot consistently improve MSE performance because of emergence of the gradient vanishing and saturation problems as suggested in remarks of theorem 1. In overall, one can observe that the BFG, LM, CGB and RP backpropagation algorithms provide an improved average MSE performance when training the neural network architectures from 1 layer to 10 layers. However, for 10 repeated tests, the minimum MSE performances are produced by the LM algorithm for all configurations in Figure 6. These results indicate the potential of the LM algorithm to reach the lowest MSE when training of the neural networks is repeated adequately.

Figure 5. Maximum MSE Performances of The NNBA Trainings

Number of Layers

5

6

8

10

 10

SCG

10

9

Figure 6. Minimum of MSE performances of the NNBA trainings

Figure 7 shows the average MSE performance of the training tests by using MSAs. Figure 8 and 9 illustrate the maximum MSE and the minimum MSE performances for 10 repeated training tests of each neural network configuration. Increasing the hidden layer number to 2 layers or more severely deteriorated the tested MSE performances because MSAs need much more computation time in searching optimal points as

the dimension of search spaces increases. The dimension of search space ($D=\sum (k_{_{(h-1)}}k_{_h}+1)$ $D = \sum_{h=1}^{n} (k_{(h-1)}k_h + k_h)$) grows *h* 1

fast with the layer number *n* in neural networks. Another factor that affects the performance of MSAs is the geometry of search spaces. Loss functions of shallow networks introduce rather multimodal search spaces and a higher exploration skill becomes an advantage to find better solutions, and this effect can increase average performance of search agents in multimodal search spaces. As the number of hidden layers increases in neural networks, the convexity of their search space increases because more hidden layers increase depth and optimization parameters, and accordingly approximation performance of the composite neural network function.

Figure 7 and 8 reveal that the GA can provide better average MSE and maximum MSE performances up to 8 hidden layer networks. A main reason for this result is that the GA is more explorative than swarm-based search algorithms (GWO, PSO) because of randomly applied genetic processes such as random mutation and crossover. These processes occasionally lead to random spreading of population into the search space at each generation, and such dispersion of individuals makes it more probable to find better solutions in multi-modal search space of shallow networks. On the other hand, GWO and PSO algorithms perform more exploitative search because search agents (individuals) of the swarm tend to move towards the best individual. Therefore, minimum MSE performance of GWO and PSO begins to improve after 8 hidden layers in Figure 9 as a result of the increase in convexity of the search space. Due to enhanced exploitation capability of GWO, the GWO algorithm can provide the lowest minimum MSE values when the training is repeated adequately. These results reveal that the GWO algorithm can be advantageous to obtain a minimum MSE in the case that the training of the deep neural networks is repeated.

Figure 9. Minimum MSE Performances of The MSAs

The computation time per weight parameter is useful to consider the computation load of an optimization method in the training process. It expresses the average of training time that a training algorithm is used to perform a weight update. It eliminates effects of network depth on training time measurements of algorithms. It is computed by dividing the total computation time ($T_{_C}$) by the number of weight parameters

(N_w) as T_c / N_w . Figure 10 shows the average computation times per weight in the training processes of

NNBAs. The figure reveals that the BFG training method consumes considerably more time during the training process. Figure 11 shows the average computation times per weight in MSAs during the training process. The figure reveals a lower computation time of the GA algorithm compared to GWO and PSO algorithms in this regression problem because automatic stopping criteria of Matlab ga() can decrease the computation time. GWO and PSO algorithms do not stop before performing the maximum iteration number (Maximum iteration number is 1000 iterations for GWO and PSO). Figure 12 compares NNBAs and MSAs in terms of computation time per the weight coefficient. For these network configurations (up to 10 hidden layers), it is apparent that the computation times of MSAs is much higher than those of the NNBAs and such a high computation time is another important disadvantage of MSAs for the deep neural network training tasks. A reason for high computation time of MSAs is that MSAs are multi-agent (population-based) search algorithms, and they perform a loss function calculation for each agent of the population. This is an important factor that increases the training time of MSAs depending on the population size. Since population size and iteration numbers of MSAs are the same while the number of layers increases, the computation time per weight is relatively steady in Figure 11.

Figure 10. Computation Time (In Sec) During Training of The Neural Network Configurations By using NNBAs

Figure 11. Computation Times (In Sec) During Training of The Neural Network Configurations By Using MSAs

Table 3 lists the training test results of algorithms on a pipe-like deep neural network architecture with 20 hidden layers. In the case of 20 hidden layers, the lowest average MSE is provided by the GWO algorithm and the lowest maximum MSE is provided by the PSO algorithm as a result of the increased convexity in the search space. On the other hand, due to the gradient vanishing problem of the pipe-like deep neural network, which was analyzed by using Theorem 1, training performances of NNBAs can reduce to levels that are comparable with training performances of MSAs. The performance of MSAs deteriorated because of the high-dimensional search space with 646 optimization parameters. However, the lowest minimum MSE is still provided by the LM algorithm (The lower minimum MSE implies accessibility to the best MSE performance in the case of multiple training.) and the lowest standard deviation of the MSE is provided by the CGF algorithm. (The lower standard deviation implies consistency of the MSE performance in multiple tests.) The lowest average computation time per weight is provided by the RP algorithm because The RP uses the sign of the partial derivative of the activation functions and this improves convergence speed however reduces convergence accuracy (Riedmiller an Braun, 1993). Although the lowest average MSE is possible by using the GWO, it's computation time is much higher than all NNBAs. Table 3 showed that NNBA methods consume quite less computation time. Deep neural network training applications require faster algorithms in order to process large amounts of data. The speed of training algorithms is an important asset for deep neural network training in big data applications (Zhu et al.,2018).

Figure 12. The Computation Time (In Sec) Comparison Between NNBAs And MSAs

When an optimization algorithm is developed to be successful in hard-to-training benchmark networks, it will be more specialized and more dedicated for deep neural network training tasks. This unveils a research motivation that the optimization algorithms should be designed dedicated to the neural networks "deep learning dedicated optimization algorithms" in order to surpass the training performance standards of general purpose optimization algorithms.

Table 3. Test Results of The Pipe Architecture Deep Neural Network With 20 Hidden Layers For Analyses Of MSE Performances And Computation Times For 10 Repeated Training (The Number Of Weights To Be Updated At Each Iteration Is 646)

3.2. Overall Performance Analysis and Criterion-based Selection of Training Algorithms

For criterion-based assessment on the practical effectiveness of training algorithms, a normalized overall performance scoring (NOPS) is adopted to statistical properties in Table 3 as follows:

$$
NOPS = \sum_{i=1}^{p} W_i \frac{P_i}{\sum_{j=1}^{m} P_i}
$$
\n
$$
(9)
$$

where the parameter P_i , $i = 1,2,.., p$ stands for the value of the properties (performance indices) in the analyses of *m* different algorithm options. Authors used 5 properties to evaluate training algorithm performance ($p = 5$). Accordingly, the property P_1 is the average MSE value, the property P_2 is the maximum MSE value, the property $\,P_{\rm 3}\,$ is the minimum MSE value, the property $\,P_{\rm 4}\,$ is the standard deviation and the property P_5 is the average computation time per weight. Previously, the weighted sum formula has been considered for decision-making problems (Stanujkic and Zavadskas, 2015 ; Goh et al., 1996). We modified it for the criterion-based selection of the training algorithms by using importance weighting. It should be noticed that all properties should be minimized for a desirable performance in this training algorithm selection problem. Therefore, an algorithm with a lower NOPS is better in criterion-based overall performance. The parameter W_i stands for the importance weight of the property i and the importance

weight should satisfy the normalization condition $\sum W_i = 1$ $\sum_{i=1}^p W_i =$ *i* $W_{i} = 1$ to perform a weighted average. For the equal

importance of the properties, the importance weight is set to a constant value of *p* $W_i = \frac{1}{n}$. Table 4 and Table

5 show NOPS lists of NNBAs and MSAs for three type importance weighting: the equal importance weights with $W_{\!\scriptscriptstyle i} = [0.2 \ 0.2 \ 0.2 \ 0.2 \ 0.2]$, the NOPS_1 importance weights with $W_{\!\scriptscriptstyle i} = [0.4 \ 0.1 \ 0.2 \ 0.0 \ 0.3]$ (it attributes more importance for average and minimum MSE performances to express accuracy and for computation time to express speed of the training algorithms) and NOPS_2 importance weights with $W_{\scriptscriptstyle \hat{i}} = [0.4 \,\, 0.0 \,\, 0.0 \,\, 0.3 \,\, 0.3]$ (it attributes more importance for average MSE and standard deviation to express accuracy and consistency and for computation time to express speed of the training algorithms).

Due to their higher speed and accuracy requirements, NOPS_1 can be preferable for training algorithm selection tasks of deep learning applications for big data analytics. Since MSAs have very high computation time, NOPS calculations were separately performed for NNBAs and MSAs categories. According to the NOPS analyses, the LM, CGB and CGP training algorithms can be advantageous for speed and accuracy requirements due to their low scores in Table 4. Improvements on nonlinear optimization (Marquardt, 1963) can contribute to NNBAs. Among the tested MSAs in Table 5, GA algorithms can be useful in terms of speed and accuracy weighting. However, one should consider that these MSAs have extremely high computation time as shown in Table 3, and they are not effective for deep neural network training.

Training Algorithm Types	Algorithm	NOPS for Equal Importance	NOPS_1 for Speed and Accuracy Importance	NOPS 2 for Speed and Consistency Importance
NNBA	LM	0.0608	0.0795	0.1155
NNBA	CGB	0.0552	0.0823	0.0869
NNBA	CGP	0.0591	0.0838	0.0894
NNBA	SCG	0.0583	0.0897	0.0827
NNBA	OSS	0.0572	0.0965	0.0805
NNBA	RP	0.0612	0.1047	0.0640
NNBA	CGF	0.0581	0.1049	0.0629
NNBA	GDX	0.1629	0.1402	0.1927
NNBA	BFG	0.0563	0.2184	0.2254

Table 4. NOPS Analyses of NNBAs For The Pipe Architecture Deep Neural Network With 20 Hidden Layers

Table 5. NOPS Analyses of MSAs For The Pipe Architecture Deep Neural Network With 20 Hidden Layers

3.3. A Discussion on Experimental Results:

Some significant observations from experimental results can be summarized as

(i) For training of the shallow networks with a hidden layer of 5 neurons, MSE performances of the tested NNBAs and MSAs are comparable. However, when two or more hidden layers were added to the network, MSE values of the MSAs sharply increased and the training performances severely deteriorated. While increasing the hidden layer numbers, MSE performances of NNBAs rather slowly deteriorate because the gradient vanishing problem gradually becomes effective as the layer number increases as suggested by Theorem 1. Therefore, authors concluded that the tested MSAs are suitable for the training of shallow neural networks. This shortcoming is mainly caused by the fact that the tested MSA methods are practicable for low dimensional optimization problems (Fong et al., 2018). An increase in hidden layers largely increases the number of weight and bias coefficients, namely the dimension of the search space of the loss function. For this reason, in order to train deep neural networks via MSAs, it is necessary to design algorithms that can be particularly effective for high dimensional optimization problems. Consequently, research efforts on high dimensional optimization problems will be very strategic for the deep learning research community. Authors anticipated that development of deep learning dedicated optimization methods can be more effective than the adaptation of general purpose optimization methods for neural network training. In a recent work, Manoharan et al. discussed performance improvement of neural network dedicated metaheuristics for several datasets (Manoharan and Sathesh, 2020).MSAs were preferably utilized in network architecture optimization problems because architecture optimization introduces lowerdimensional optimization problems compared to training tasks. MSAs can more effectively optimize hyperparameters of neural networks such as layer numbers, neuron numbers and configuration of neural elements. Several works have discussed benefits of such neuroevolutionary approaches in deep learning (Stanley et al., 2019; Floreano et al., 2008; Suganuma, 2017; Ding et al., 2013; Galván and Mooney, 2021).

(ii) The computation load of the MSAs is much larger than those of the tested NNBAs. This is another substantial shortcoming of MSAs in the training of deep neural networks. The main reason is that metaheuristic optimization commonly uses multi-agents (population) global search techniques. NNBAs use the single search agent and perform the local search according to the gradient direction. This property of NNBAs becomes an advantage for reduction of algorithmic computation complexity and it can significantly reduce the computation load of the training process. Nonetheless, low average MSE results of GWO in Table 3 can support the idea, suggesting that the gradient free metaheuristic search can be a solution to deal with the complications associated with the gradient-based deep neural network training, such as the gradient vanishing and gradient exploding problems. However, the computation time of GWO is severely high, which becomes an important disadvantage for deep learning applications.

For consistent evaluation of training algorithms, hyperparameters of each training algorithm type have been configured to similar values. Some significant hyperparameters of the training algorithms are summarized in Table 6. Upper and lower bounds of weight coefficients are important parameters because they can affect the training performance for MSA methods. When these bounds are set symmetrical in positive and negative ranges, MSAs can obtain both negative and positive weight coefficients in the optimization stage. Besides, we configured the upper and lower bounds of weight coefficients in the narrow range of [-10, 10] as in Table 6. This can lead to a regularization effect (data generalization) in the neural learning process by preventing large differences between weight coefficients. Since the number of optimized weight coefficients in the training process exponentially grows the search space of MSAs, population size of MSAs can be increased to maintain the search performance for large search spaces.

Table 6. Hyperparameter Setting of Training Algorithms

4. Conclusions

This study introduced the pipe-like neural network benchmark architecture and performance analysis results of popular training algorithms were reported for different depths of the generic pipe-like neural network architecture. Training difficulties of this network were theoretically demonstrated by extending the learning channel theory to an aggregated one-neuron learning channel conjecture in Theorem 1. The weight update bounds of aggregated one-neuron learning channels and gradient vanishing problem of pipelike deep networks were analyzed for a fundamental neuron model. In the experimental studies, training processes of a pipe-like deep neural network took several weeks run-time for a high performance computer (Intel I7 processors and 16 GB RAM) without interruptions.

Some remarks and suggestions can be summarized as follows:

* Upper bounds theorem of training performance demonstrated training complications of the pipe-like neural network benchmark architecture on the basis of learning channel theorem, and the experimental study validates these performance complications for 9 popular NNBA algorithms and 3 fundamental MSA algorithms.

* A major weaknesses of the tested popular NNBA algorithms originates from decrease of sensitivity

function magnitudes ($\left| \frac{\partial E}{\partial w^h} \right|$ *E* д $\frac{\partial E}{\partial \mathbf{r}}$) through hidden layers according to remarks of Theorem 1. This effect causes

severe attenuation of backward error signal propagation in the deep neural networks for backpropagation algorithms. Possible solutions to this problem may be reducing of gradient dependence of optimization methods (e.g., use of gradient-free optimization methods (Sexton and Gupta, 2000; Che et al., 2011; Gudise and Venayagamoorthy, 2003; Ince et al., 2010; Mosavi et al., 2016)), implementation of gradient magnitude balancing mechanisms to regulate backward error propagation (e.g., adjustment of additional gain coefficients (Roodschild et al., 2020) to balance gradient magnitudes through hidden layers), improving activation function (Kim, 2017; Oostwal et al., 2019) to enhance gradient magnitude of the activation

function
$$
\left(\frac{\partial \varphi^h}{\partial v^h}\right)
$$
.

*An essential shortcoming of the tested popular MSA algorithms is related to a high increase of computation burden as the dimension of optimization problems (the number of parameters to optimize) increases. Dimension of optimization problem for the training of neural networks grows very fast as the layer number increases. Population sizes and iteration numbers of MSAs should be increased to deal with the high dimension issue, however this can severely increase the computation time and cause the tested MSAs to be impractical for the deep neural network training task. Possible solutions of this problem may be enhancement of search strategies by specializing them to perform more effective searching on neural network function types. Such metaheuristics are referred to as deep learning dedicated MSAs.

The current study introduced a hard-to-train benchmark network that can be utilized as a test bench for development of training algorithms. Future works can address designing and testing of the deep learning dedicated optimization algorithms by using a pipe-like neural network test benches.

Conflict of Interest

No conflict of interest was declared by the authors.

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