Article

Bound the parameters of neural networks using Particle Swarm Optimization

Ioannis G. Tsoulos[1,*], Alexandros Tzallas[1], Evangelos Karvounis[1], Dimitrios Tsalikakis[2]

[1] Department of Informatics and Telecommunications, University of Ioannina, Greece
[2] University of Western Macedonia, Department of Engineering Informatics and Telecommunications, Greece
* Correspondence: itsoulos@uoi.gr;

Abstract: Artificial Neural Networks are machine learning models widely used in many sciences as well as in practical applications. The basic element of these models is a vector of parameters, the values of which should be estimated using some computational method, and this process is called training. For effective training of the network, computational methods from the field of global minimization are often used. However, for global minimization techniques to be effective, the bounds of the objective function should also be clearly defined. In this paper, a two-stage global optimization technique is presented for efficient training of artificial neural networks. In the first stage, the bounds for the neural network parameters are estimated using Particle Swarm Optimization and, in the second phase, the network parameters are trained within the bounds of the first phase using global optimization techniques. The proposed technique was applied to a number of well-known problems in the literature and the experimental results were more than encouraging.

Keywords: Global optimization; local optimization; stochastic methods; evolutionary techniques; termination rules.

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1. Introduction

Artificial neural networks (ANNs) are parametric machine learning models [1,2], which have been widely used during the last decades in a variety of practical problems from many different fields such as physics problems [3–5], chemistry problems [6–8], problems related to medicine [9,10], economic problems [11–13] etc. Also, recently ANNs have been applied to models solving Differential Equations [14,15], agricultural problems [16,17], facial expression recognition [18], wind speed prediction [19], the gas consumption problem [20], intrusion detection [21] etc. Usually, neural networks are defined as a function $N(\overrightarrow{x},\overrightarrow{w})$, where the vector $\overrightarrow{x}$ is the input pattern to the network and the vector $\overrightarrow{w}$ is called the weight vector. To estimate the weight vector, the so-called training error is minimized, which is defined as the sum:

$$E(N(\overrightarrow{x},\overrightarrow{w})) = \sum_{i=1}^{M}\left(N(\overrightarrow{x}_i,\overrightarrow{w}) - y_i\right)^2 \tag{1}$$

In equation 1 the values t $\left(\overrightarrow{x_i}, y_i\right),\ i = 1,\ldots,M$ defined the training set for the neural network. The values y_i denote the expected output for the pattern $\overrightarrow{x_i}$.

To minimize the quantity in equation 1, several techniques have been proposed in the relevant literature such as: Back Propagation method [22,23], the RPROP method [24–26], Quasi Newton methods [28,29], Simulated Annealing [30,31], Genetic Algorithms [32,33], Particle Swarm Optimization [34,35],Differential Optimization methods [36], Evolutionary Computation [37], the Whale optimization algorithm [38], the Butterfly optimization algorithm [39], etc. In addition, many researchers have focused their attention on techniques for initializing the parameters of artificial neural networks, such as the usage of decision trees to initialize neural networks [40], a method based on Cachy's inequality [41], usage of genetic algorithms [42], initialization based on discriminant learning [43] etc. In addition, many researchers were also concerned with the construction of artificial neural network architectures, such as the usage of Cross Validation to construct the architecture of neural networks [44], incorporation of the Grammatical Evolution technique [46] to construct the architecture of neural networks as well as to estimate the values of the weights [45], evolution of neural networks using a method based on cellular automata [47] etc. Also, since in recent years there has been a leap forward in the development of parallel architectures, a number of works have been presented that take advantage of such computational techniques [48,49].

However, in many cases, the training methods of artificial neural networks suffer from the problem of overfitting, i.e. although they succeed in significantly reducing the training error of equation 1, they do not perform similarly on unknown data that was not present during training. These unknown data sets are commonly called test sets. The overfitting problem is usually tackled through a variety of methods, such as weight sharing [50,51], pruning of parameters, i.e reducing the size of the network [52–54], the dropout technique [55,56], weight decaying [57,58], the Sarporp method [59], positive correlation methods [60] etc. The overfitting problem is thoroughly discussed in Geman et all [61] and in the article by Hawkins [62].

A key reason why the problem of overtraining in artificial neural networks is present, is that there is no well-defined interval of values in which the network parameters are initialized and trained by the optimization methods. This, in practice, means that the values of the parameters are changed indiscriminately in order to reduce the value of the equation 1. In this work it is proposed to use the Particle Swarm Optimization (PSO) technique [63] for the reliable calculation of the value interval of the parameters of an artificial neural network. The PSO method was chosen since it is a fairly fast global optimization method, easily adaptable to any optimization problem, and does not require many execution parameters to be defined by the user. The PSO method was applied with success to many difficult problems, such as problems that arise in physics [64,65], chemistry [66,67], medicine [68,69], economics [70] etc. In the proposed method, the PSO technique is used to minimize the equation 1 to which a penalty factor has been added, so as not to allow the parameters of artificial neural networks to vary uncontrollably. After the minimization of the modified function is done, the parameters of the neural network are initialized in an interval of values around the optimal value located by the PSO method, and then the original form of equation 1 is minimized without a penalty factor this time.

The rest of this article is organized as follows: in section 2 the proposed method is fully analyzed and discussed, in section 3 the experimental datasets as well as the experimental results are listed and discussed and finally in section 4 some conclusions are presented.

2. The proposed method

2.1. Preliminaries

Consider a neural network with one processing level that uses the so - called sigmoid function as activation function. The sigmoid function is defined as:

$$\sigma(x) = \frac{1}{1+\exp(-x)} \tag{2}$$

This function is graphically illustrated in Figure 1.

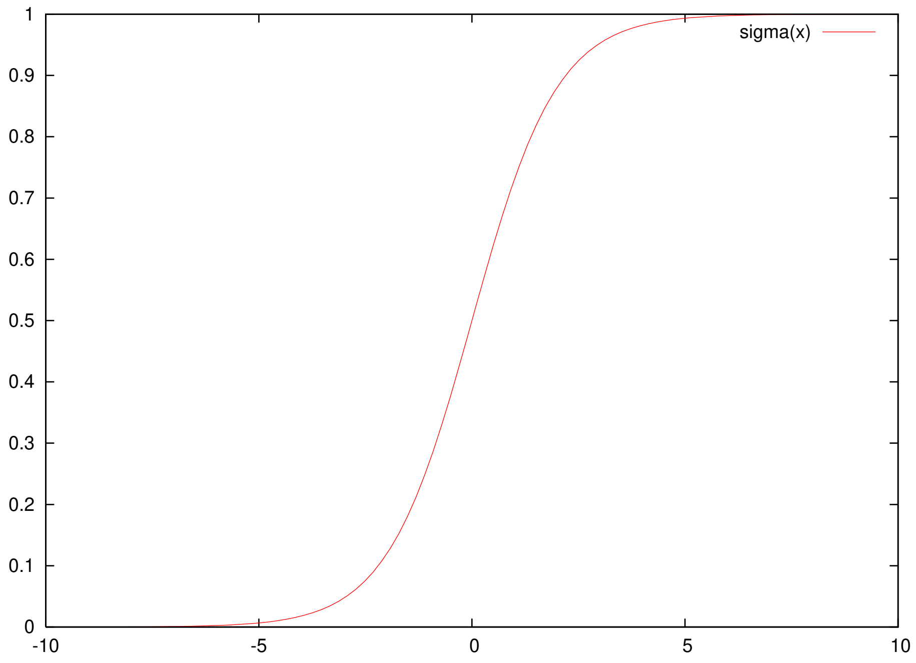

Figure 1. Plot of the sigmoid function.

The equation for every hidden node of the neural network has as:

$$o_i(x) = \sigma\left(w_i^T x + \theta_i\right), \tag{3}$$

where the vector w_i stands for the the weight vector and the value θ_i denotes the bias the node i. The equation for a neural network with H hidden is defined as:

$$N(x) = \sum_{i=1}^{H} v_i o_i(x), \tag{4}$$

The value v_i denotes the output weight for node i. Therefore writing the overall equation of the artificial neural network using equations 3 and 4 has as:

$$N(\overrightarrow{x}, \overrightarrow{w}) = \sum_{i=1}^{H} w_{(d+2)i-(d+1)} \sigma\left(\sum_{j=1}^{d} x_j w_{(d+2)i-(d+1)+j} + w_{(d+2)i}\right) \tag{5}$$

The value d stands for the dimension of the input vector $\overrightarrow{x}$. Observing the equation 5 but also the shape of the sigmoid function in figure 1, it is obvious that in many cases, the sigmoid function is driven to 1 or 0 and as a consequence the training error of the neural network can get trapped in local minima and finally, the neural network it will lose its generalization abilities. Therefore, a technique should be devised by which the values of the sigmoid will be restricted to some interval of values. In the present work, the limitation of the neural network parameters to a range of values is carried out using the Particle Swarm Optimization method.

2.2. The bounding algorithm

In the case of the sigmoid function of equation 2 , if the parameter x is large, then the function will very quickly tend to 1 and if it is very small, it will very quickly tend to 0. This means that the function will very quickly lose any generalizing abilities it has. Therefore, the parameter x should somehow be in some interval of values, so that there are no generalization problems. For this reason, the quantity $B(L)$ is estimated, where L is a limit for the absolute value of the parameter x of the sigmoid function. The steps for this calculation are shown in Algorithm 1. This function will eventually return the average of the overruns made for the x parameter of the sigmoid function. The higher this average is, the more likely it is that the artificial neural network will not be able to generalize satisfactorily.

Algorithm 1 Calculation of the quantity $B(L)$ for a given parameter L. The parameter M stands for the number of patterns for the neural network $N(x,w)$.

```
1. Function $B(L)$
2. Define $v = 0$
3. For $i = 1..H$ Do
   (a) For $j = 1..M$ Do
       i. If $\left|\sum_{k=1}^{d}\left(w_{(d+2)i-(d+i)+k}x_{jk}\right)+w_{(d+2)i}\right| > L$ then $v = v + 1$
   (b) EndFor
4. EndFor
5. Return $\frac{v}{H\star M}$
6. End Function
```

2.3. The PSO algorithm

The Particle Swarm Optimization method is based on a population of vectors that are also called particles. These particles are also possible global minima of the objective function. Each particle is associated with two vectors: the current position denoted as $\overrightarrow{p}$ and the corresponding speed $\overrightarrow{u}$ at which they are moving towards the global minimum. In addition, each particle maintains in the vector $p_{i,b}$ the best position in which it has been so far and the total population, maintains in the vector p_{best} the best position that any of the particles have found in the past. The purpose of the method is to move the total population toward the global minimum through a series of iterations. In each iteration, the velocity of each particle is calculated based on its current position, its best position in the past and the optimal position of the population.

In the present work, the PSO technique is used to train artificial neural networks by minimizing the error function as defined in the equation 3 along with a penalty factor depending on the function $B(L)$ defined in subsection 2.2. Hence, the PSO technique will minimize the equation:

$$E_T(N(x,w),L) = \sum_{i=1}^{M}\left(N\left(\overrightarrow{x}_i,\overrightarrow{w}\right)-y_i\right)^2 \times (1+\alpha B(L)) \tag{6}$$

where α is a penalty factor with $\alpha > 1$. Hence, the main steps of a PSO algorithm are shown in Algorithm 2.

Algorithm 2 The base PSO algorithm executed in one processing unit.

```
1. Initialization Step .
    (a) Set $k = 0$, as the iteration number.
    (b) Set $H$ the number of hidden nodes for the neural network.
    (c) Set $m$ as the total number of particles. Each particle corresponds to a randomly
        selected set of parameters for the neural network
    (d) Set $\mathrm{k_{max}}$ as the maximum number of iterations allowed.
    (e) Initialize randomly the velocities $u_1, u_2, ..., u_m$.
    (f) For $i = 1..m$ do $p_{i,b} = p_i$. The vector $p_{i,b}$ corresponds to the best located
        position of particle $i$.
    (g) Set $p_{\mathrm{best}} = \arg\min_{i \in 1..m} f(p_i)$
2. If $k \geq k_{\mathrm{max}}$, then terminate.
3. For $i = 1..m$ Do
    (a) Compute the velocity $u_i$ using the vectors $u_i,\ p_{i.b}$ and $p_{\mathrm{best}}$
    (b) Set the new position $p_i = p_i + u_i$
    (c) Calculate the $f(p_i)$ for particle $p_i$ using the equation 6 as $f(p_i) =
        E_T(N(x, p_i), L)$
    (d) If $f(p_i) \leq f(p_{i,b})$ then $p_{i,b} = x_i$
4. End For
5. Set $p_{\mathrm{best}} = \arg\min_{i \in 1..m} f(p_i)$
6. Set $k = k + 1$.
7. Goto Step 2
```

The velocity of each particle p_i usually is calculated as: 119

$$u_i = \omega u_i + r_1 c_1 (p_i - x_i) + r_2 c_2 (p_{\mathrm{best}} - x_i) \tag{7}$$

where 120

1. The variables $r_1,\ r_2$ are random numbers defined in $[0, 1]$. 121
2. The constants $c_1,\ c_2$ are defined in $[1, 2]$. 122
3. The variable ω is called inertia, proposed in [71]. 123

For the proposed algorithm, the inertia calculation used in [72–74] was used and it is 124
defined as: 125

$$\omega_k = \frac{k_{\mathrm{max}} - \mathrm{k}}{\mathrm{k_{max}}} (\omega_{\mathrm{max}} - \omega_{\mathrm{min}}) + \omega_{\mathrm{min}} \tag{8}$$

where ω_{min} and ω_{max} are the minimum and the maximum value for inertia respectively. 126

2.4. *Application of local optimization* 127

After the Particle Swarm Optimization is completed in the vector p_{best} is the optimal 128
set of parameters for the artificial neural network. From this set, a local optimization 129
method can be started in order to achieve an even lower value for the neural network 130
error. In addition, the optimal set of weights can be used to calculate an interval for the 131
parameters of the neural network. The error function of the equation 3 will be minimized 132
inside this interval. The interval $[LW, RW]$ for the parameter vector w of the neural network 133
is calculated through the following procedure: 134

1. **For** $i = 1..n$ **do** 135
    (a) **Set** $LW_i = -F \times \left|p_{\mathrm{best},i}\right|$ 136
    (b) **Set** $RW_i = F \times \left|p_{\mathrm{best},i}\right|$ 137
2. **EndFor** 138

The value F will be called margin factor with $F > 1$. In the proposed algorithm, the BFGS variant of Powell [75] was used as the local search procedure, which is a version of the BFGS local optimization procedure [76], that utilizes bounds for the objective function.

3. Experiments

The proposed method was applied to a number of well-known problems in the literature and compared with other well-known artificial neural network training techniques. In addition, experiments were carried out to show the dependence of the method on its basic parameters. The classification datasets incorporated in the relevant experiments can be found at:

1. UCI dataset repository, https://archive.ics.uci.edu/ml/index.php
2. Keel repository, https://sci2s.ugr.es/keel/datasets.php[77].

The majority of regression datasets was found in the Statlib URL ftp://lib.stat.cmu.edu/datasets/index.html.

3.1. Experimental datasets

The classification datasets used in the conducted experiments are:

1. **Appendictis** a medical dataset, found in [78].
2. **Australian** dataset [79]. It is a dataset related to credit card applications.
3. **Balance** dataset [80], a cognitive dataset.
4. **Cleveland** dataset, a medical datasets found in a variety of papers[81,82].
5. **Bands** dataset, a dataset related to printing problems.
6. **Dermatology** dataset [83], a medical dataset.
7. **Hayes roth** dataset [85].
8. **Heart** dataset [84], a medical dataset about heart diseases.
9. **HouseVotes** dataset [86].
10. **Ionosphere** dataset, found in the Johns Hopkins Ionosphere database and it has been thoroughly studied in many papers [87,88].
11. **Liverdisorder** dataset [89], a medical dataset.
12. **Mammographic** dataset [90], a medical dataset.
13. **Page Blocks** dataset [91], related to documents.
14. **Parkinsons** dataset [92], a medical dataset related to Parkinson's decease.
15. **Pima** dataset [93], a medical dataset..
16. **Popfailures** dataset [94], that is related to climate model simulation crashes of simulation crashes.
17. **Regions2** dataset. It is created from liver biopsy images of patients with hepatitis C [95].
18. **Saheart** dataset [96], a medical dataset about heart disease.
19. **Segment** dataset [97].
20. **Wdbc** dataset [98], a medical dataset about breast tumors.
21. **Wine** dataset, a dataset about chemical analysis for wines wines [99,100].
22. **Eeg** datasets [17], it is medical datasets about EEG signals and three distinct cases used here named Z_F_S, ZO_NF_S and ZONF_S respectively.
23. **Zoo** dataset [101].

The regression datasets used in the conducted experiments have as follows:

1. **Abalone** dataset [103], used to predict the age of abalone from various measurements.
2. **Airfoil** dataset, a dataset used by NASA [104].
3. **Baseball** dataset, used to estimate the salary of baseball players.
4. **BK** dataset [105], a dataset used to predict the points in a basketball game.
5. **BL** dataset, related to a experiment on the affects of machine adjustments on the time to count bolts.
6. **Concrete** dataset [106], a civil engineering dataset.
7. **Dee** dataset, used to predict the price of the electricity energy in Spain.

8. **Diabetes** dataset, a medical dataset.
9. **Housing** dataset [107].
10. **FA** dataset, used to fit body fat to other measurements.
11. **MB** dataset [108].
12. **MORTGAGE** dataset, related to economic data information of USA.
13. **PY** dataset, (Pyrimidines problem)[109].
14. **Quake** dataset, used to approximate the strength of a earthquake.
15. **Treasure** dataset, which contains Economic data information of USA from 01/04/1980 to 02/04/2000 on a weekly basis.
16. **Wankara** dataset, which contains weather information.

3.2. Experimental results

In order to validate the efficiency of the proposed method, the ten - fold validation method was used and and 30 experiments were conducted using different seeds for the random generator each time. The average classification or regression error on the test set is reported in the experimental tables. The parameters used in the experiments are shown in Table 1. The proposed method is compared against some other methods from the relevant literature:

1. A simple genetic algorithm using m chromosomes, denotes by GENETIC in the experimental tables. Also, in order to achieve a better solution, the local optimization method BFGS is applied to the best chromosome of the population when the genetic algorithm terminates.
2. The optimization method Adam [110] as provided by the OptimLib, freely available from https://github.com/kthohr/optim.
3. The Rprop method [24] as provided by the FCNN programming package [111].
4. The NEAT method (NeuroEvolution of Augmenting Topologies) [112]. The method is implemented in the EvolutionNet programming package downloaded from https://github.com/BiagioFesta/EvolutionNet.

The results for the classification datasets are listed in Table 2 and the results for the regression datasets in Table 3. For every table, an additional row was added with the title AVERAGE indicating at the end showing the average classification or regression error for all datasets. All the experiments were conducted on AMD Epyc 7552 equipped with 32GB of RAM. The operating system was the Ubuntu 20.04 operating system.

Table 1. The values for the parameters of the proposed method.

PARAMETER	MEANING	VALUE
m	Number of particles or chromosomes	200
$k_{\max}$	Maximum number of iterations	200
$\omega_{\min}$	Minimum value for inertia	0.4
$\omega_{\max}$	Maximum value for inertia	0.9
H	Number of weights	10
α	Penalty factor	100.0
L	The limit for the function $B(L)$	10.0
F	The margin factor	5.0

Table 2. Experimental results for the classification datasets.

DATASET	GENETIC	ADAM	RPROP	NEAT	PROPOSED
Appendicitis	18.10%	16.50%	16.30%	17.20%	16.97%
Australian	32.21%	35.65%	36.12%	31.98%	26.96%
Balance	8.97%	7.87%	8.81%	23.14%	7.52%
Bands	35.75%	36.25%	36.32%	34.30%	35.77%
Cleveland	51.60%	67.55%	61.41%	53.44%	48.40%
Dermatology	30.58%	26.14%	15.12%	32.43%	14.30%
Hayes Roth	56.18%	59.70%	37.46%	50.15%	36.33%
Heart	28.34%	38.53%	30.51%	39.27%	18.99%
HouseVotes	6.62%	7.48%	6.04%	10.89%	7.10%
Ionosphere	15.14%	16.64%	13.65%	19.67%	13.15%
Liverdisorder	31.11%	41.53%	40.26%	30.67%	32.07%
Lymography	23.26%	29.26%	24.67%	33.70%	27.05%
Mammographic	19.88%	46.25%	18.46%	22.85%	17.37%
PageBlocks	8.06%	7.93%	7.82%	10.22%	6.47%
Parkinsons	18.05%	24.06%	22.28%	18.56%	14.60%
Pima	32.19%	34.85%	34.27%	34.51%	26.34%
Popfailures	5.94%	5.18%	4.81%	7.05%	5.27%
Regions2	29.39%	29.85%	27.53%	33.23%	26.29%
Saheart	34.86%	34.04%	34.90%	34.51%	32.49%
Segment	57.72%	49.75%	52.14%	66.72%	18.99%
Wdbc	8.56%	35.35%	21.57%	12.88%	6.01%
Wine	19.20%	29.40%	30.73%	25.43%	10.92%
Z_F_S	10.73%	47.81%	29.28%	38.41%	8.55%
ZO_NF_S	8.41%	47.43%	6.43%	43.75%	7.11%
ZONF_S	2.60%	11.99%	27.27%	5.44%	2.61%
ZOO	16.67%	14.13%	15.47%	20.27%	5.80%
AVERAGE	**23.47%**	**30.81%**	**25.37%**	**28.87%**	**18.21%**

Table 3. Experiments for regression datasets.

DATASET	GENETIC	ADAM	RPROP	NEAT	PROPOSED
ABALONE	7.17	4.30	4.55	9.88	4.34
AIRFOIL	0.003	0.005	0.002	0.067	0.002
BASEBALL	103.60	77.90	92.05	100.39	58.78
BK	0.027	0.03	1.599	0.15	0.03
BL	5.74	0.28	4.38	0.05	0.02
CONCRETE	0.0099	0.078	0.0086	0.081	0.003
DEE	1.013	0.63	0.608	1.512	0.23
DIABETES	19.86	3.03	1.11	4.25	0.65
HOUSING	43.26	80.20	74.38	56.49	21.85
FA	1.95	0.11	0.14	0.19	0.02
MB	3.39	0.06	0.055	0.061	0.051
MORTGAGE	2.41	9.24	9.19	14.11	0.31
PY	105.41	0.09	0.039	0.075	0.08
QUAKE	0.04	0.06	0.041	0.298	0.044
TREASURY	2.929	11.16	10.88	15.52	0.34
WANKARA	0.012	0.02	0.0003	0.005	0.0002
AVERAGE	**18.55**	**11.70**	**12.44**	**12.70**	**5.42**

In both cases, the superiority of the proposed technique over other artificial neural network training methods is evident, especially in the case of regression. The average gain from the next best method is 22% for the classification case and 54% for the regression case. In fact, in many cases the profit exceeds 50% compared to the immediate best technique.

In addition, in order to see if there is a dependence of the results on the critical parameters L and F of the proposed method, a series of additional experiments were carried out in which these parameters were varied. In the first phase, the proposed technique was applied to the regression datasets for different values of the coefficient L varying from 2.5 to 20.0 and the average regression error is graphically shown in Figure 2.

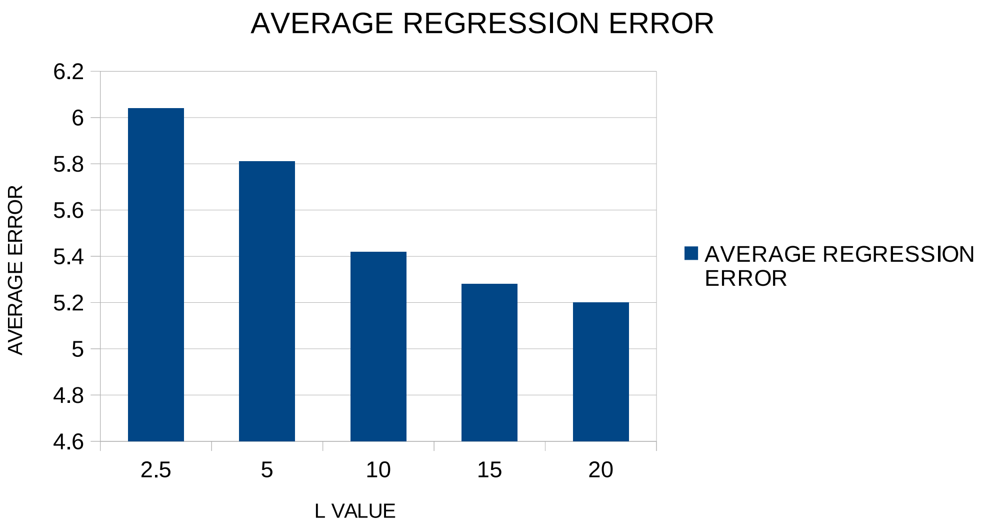

Figure 2. Experiments with the L parameter for the regression datasets.

From the results, it is obvious that increasing the value of this parameter also reduces the average error, but this reduction is not extremely large to radically change the behavior of this technique.

In addition, corresponding experiments were performed with the value of the coefficient F increasing from 2 to 15 and these are graphically illustrated in figure 3.

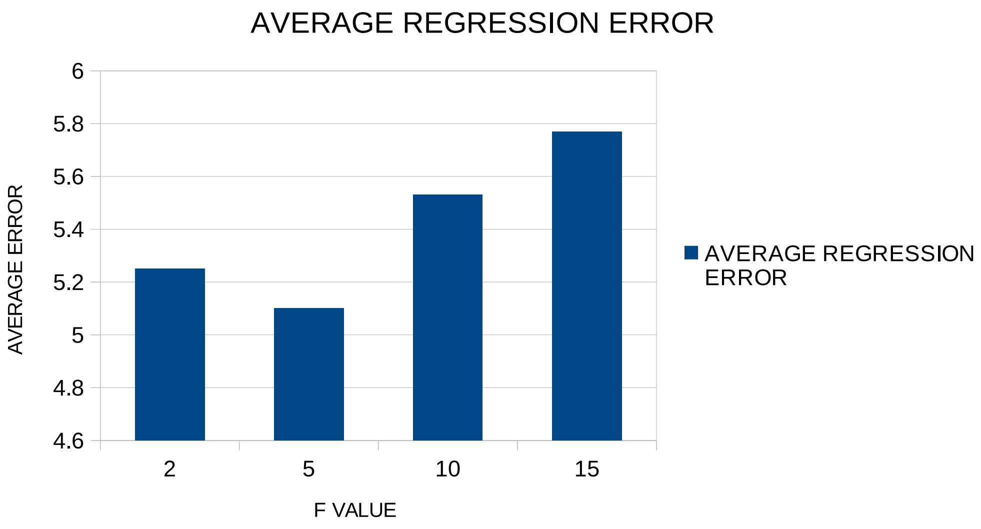

Figure 3. Experiments with the value of parameter F for the regression datasets.

From these results it follows that the proposed method achieves the best results for the value of the parameter to be equal to 5, although again there is no significant difference in the effectiveness of the method for large changes in the value of this parameter.

4. Conclusions

In this paper, a two-stage technique for efficient training of artificial neural networks for classification and regression problems was presented. In the first phase, a widely used global optimization technique such as the Particle Swarm Optimization was used to minimize the training error of the artificial neural network to which a penalty factor had been added. This penalty factor is used in order to maintain the effectiveness of the artificial neural network to generalize to unknown data as well. The calculation of the penalty factor is based on the observation that the artificial neural network can lose its generalization abilities when the input values in the sigmoid activation function exceed some predetermined threshold. After the particle optimization technique is performed in the second phase, the best particle is used both as an initializer of a local optimization method and as a basis for calculating bounds on the parameters of the artificial neural network.

The proposed method was applied to a wide range of classification and regression problems from the relevant literature and the experimental results were more than encouraging. In addition, when comparing the proposed technique with other widely used methods from the relevant literature, it appears that the proposed technique significantly outperforms, especially in the case of regression problems. In relevant experiments carried out regarding the sensitivity of the proposed technique on its critical parameters, it was found to be quite robust without large error fluctuations.

Future extensions of the technique may include its application to other network cases such as Radial Basis Function artificial neural networks (RBFs), as well as the use of global optimization methods in the second stage of the proposed technique or even the creation of appropriate termination techniques.

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