

Bound the parameters of neural networks using Particle Swarm Optimization

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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.

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], agriculture 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 $N(\vec{x}, \vec{w})$, where the vector \vec{x} is the input pattern to the networks and the vector \vec{w} is called the weight vector. To estimate the weight vector, the so-called training error is minimized, which is defined as the sum:

$$E(N(\vec{x}, \vec{w})) = \sum_{i=1}^M (N(\vec{x}_i, \vec{w}) - y_i)^2 \quad (1)$$

In equation 1 the values $t(\vec{x}_i, y_i)$, $i = 1, \dots, M$ defined the training set for the neural network. The values y_i denote the expected output for the pattern \vec{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 Cauchy's inequality [41], usage of genetic

Citation: Tsoulos, I.G.; Tzallas, A.I.; Karvounis E; Tsalikakis D Bound the parameters of neural networks using Particle Swarm Optimization. *Journal Not Specified* **2022**, *1*, 0.
<https://doi.org/>

Received:

Accepted:

Published:

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.

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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 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 are commonly called test set. The overfitting problem usually is 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 the Geman et al [61] and in the article of 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 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 appear in physics [64,65], chemistry [66,67], medicine [68,69], economics [70] etc. In the proposed method, the PSO technique is used to minimize 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:

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

This function is graphically illustrated in Figure 1.

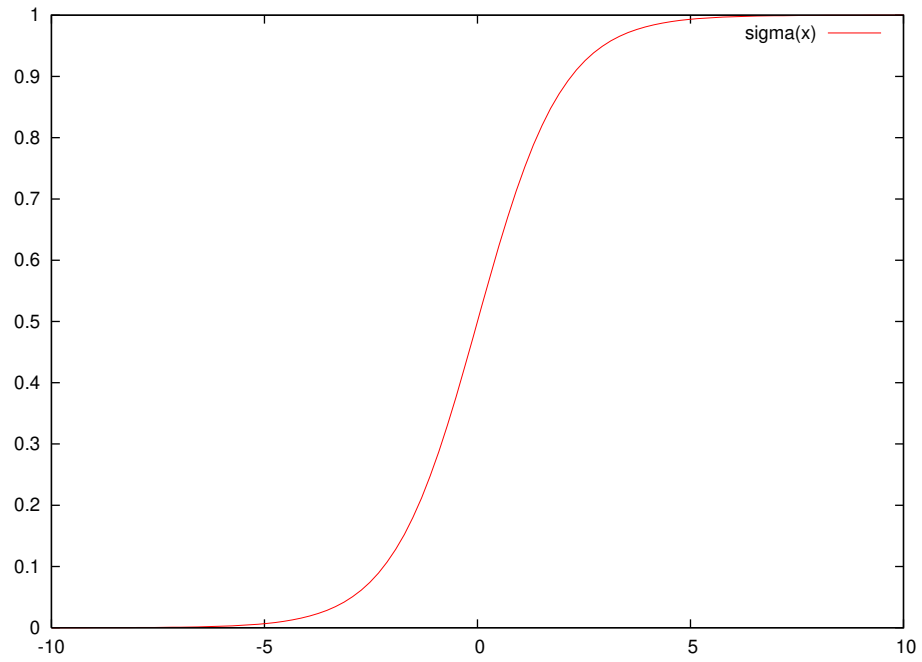


Figure 1. Plot of the sigmoid function.

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

$$o_i(x) = \sigma(w_i^T x + \theta_i), \quad (3)$$

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:

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

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:

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

The value d stands for the dimension of input vector \vec{x} . Observing 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 therefore the training error of the neural network can get trapped in local minima and consequently 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 PSO algorithm

The Particle Swarm Optimization method is based on a population of vectors that 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 \vec{p} and the corresponding speed \vec{u} at which they are moving towards to 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. The main steps of a PSO algorithm are shown in Algorithm 1.

Algorithm 1 The base PSO algorithm executed in one processing unit.

1. **Initialization Step** .
 - (a) **Set** $k = 0$.
 - (b) **Set** m as the total number of particles.
 - (c) **Set** k_{\max} as the maximum number of iterations allowed for the serial algorithm.
 - (d) **Initialize** randomly, the positions p_1, p_2, \dots, p_m for the particles. The initial positions must be within the domain of the objective function.
 - (e) **Initialize** randomly the velocities u_1, u_2, \dots, u_m .
 - (f) **For** $i = 1..m$ **do** $p_{i,b} = p_i$. The vector $p_{i,b}$ represents the best located position of particle i .
 - (g) **Set** $p_{\text{best}} = \arg \min_{i \in 1..m} f(p_i)$
 2. **Termination Check Step** . The termination criterion for the serial algorithm is checked. If the termination criterion is true, then the method terminates.
 3. **For** $i = 1..m$ **Do**
 - (a) **Compute** the velocity u_i as a combination of the vectors u_i , $p_{i,b}$ and p_{best}
 - (b) **Set** the new position for the particle as: $p_i = p_i + u_i$
 - (c) **Calculate** the $f(p_i)$ for particle p_i using the objective function $f(x)$.
 - (d) **If** $f(p_i) \leq f(p_{i,b})$ **then** $p_{i,b} = p_i$
 4. **End For**
 5. **Set** $p_{\text{best}} = \arg \min_{i \in 1..m} f(p_i)$
 6. **Set** $k = k + 1$.
 7. **Goto** Step 2
-

3. Experiments

The proposed method is evaluated on a series of classification and regression problems from the relevant literature. The classification problems used for the experiments were found in most cases in two internet databases:

1. UCI dataset repository, <https://archive.ics.uci.edu/ml/index.php>
2. Keel repository, <https://sci2s.ugr.es/keel/datasets.php>[71].

The regression datasets are in most cases available from the Statlib URL <ftp://lib.stat.cmu.edu/datasets/index.html>. The proposed method is compared against a neural network trained by a genetic algorithm and the results are reported.

3.1. Experimental datasets

The following classification datasets were used:

1. **Appendictis** a medical dataset, proposed in [72].
2. **Australian** dataset [73], the dataset is related to credit card applications.
3. **Balance** dataset [74], which is used to predict psychological states.
4. **Cleveland** dataset, a dataset used to detect heart disease used in various papers[75,76].
5. **Bands** dataset, a printing problem used to identify cylinder bands.
6. **Dermatology** dataset [77], which is used for differential diagnosis of erythematous-squamous diseases.
7. **Hayes roth** dataset. This dataset[79] contains 5 numeric-valued attributes and 132 patterns.

8. **Heart** dataset [78], used to detect heart disease. 121
9. **HouseVotes** dataset [80], which is about votes in the U.S. House of Representatives 122
Congressmen. 123
10. **Ionosphere** dataset. The ionosphere dataset contains data from the Johns Hopkins 124
Ionosphere database and it has been studied in a bunch of papers [81,82]. 125
11. **Liverdisorder** dataset [83], used for detect liver disorders in peoples using blood 126
analysis. 127
12. **Mammographic** dataset [84]. This dataset be used to identify the severity (benign or 128
malignant) of a mammographic mass lesion from BI-RADS attributes and the patient's 129
age. It contains 830 patterns of 5 features each. 130
13. **Page Blocks** dataset [85], used to detect the page layout of a document. 131
14. **Parkinsons** dataset. This dataset is composed of a range of biomedical voice measure- 132
ments from 31 people, 23 with Parkinson's disease (PD)[86]. 133
15. **Pima** dataset [87], used to detect the presence of diabetes. 134
16. **Popfailures** dataset [88], that is related to climate model simulation crashes of simula- 135
tion crashes. 136
17. **Regions2** dataset. It is created from liver biopsy images of patients with hepatitis 137
C [89]. From each region in the acquired images, 18 shape-based and color-based 138
features were extracted, while it was also annotated form medical experts. The 139
resulting dataset includes 600 samples belonging into 6 classes. 140
18. **Saheart** dataset [90], used to detect heart disease. 141
19. **Segment** dataset [91]. This database contains patterns from a database of 7 outdoor 142
images (classes). 143
20. **Wdbc** dataset [92], which contains data for breast tumors. 144
21. **Wine** dataset, used to detect through chemical analysis determine the origin of wines 145
and is been used in various research papers [93,94]. 146
22. **Eeg** datasets. As an real word example, consider an EEG dataset described in [17] 147
is used here. The dataset consists of five sets (denoted as Z, O, N, F and S) each 148
containing 100 single-channel EEG segments each having 23.6 sec duration. With 149
different combinations of these sets the produced datasets are Z_F_S, ZO_NF_S, 150
ZONF_S. 151
23. **Zoo** dataset [95], where the task is classify animals in seven predefined classes. 152

Also, the following regression datasets were used: 153

1. **Abalone** dataset [97]. This data set can be used to obtain a model to predict the age of 154
abalone from physical measurements. 155
2. **Airfoil** dataset, which is used by the NASA for a series of aerodynamic and acoustic 156
tests [98]. 157
3. **Baseball** dataset, a dataset to predict the salary of baseball players. 158
4. **BK** dataset. This dataset comes from Smoothing Methods in Statistics [99] and is used 159
to estimate the points scored per minute in a basketball game. 160
5. **BL** dataset: This dataset can be downloaded from StatLib. It contains data from an 161
experiment on the affects of machine adjustments on the time to count bolts. 162
6. **Concrete** dataset. This dataset is taken from civil engineering[100]. 163
7. **Dee** dataset, used to predict the daily average price of the electricity energy in Spain. 164
8. **Diabetes** dataset, a medical dataset. 165
9. **Housing** dataset. This dataset was taken from the StatLib library which is maintained 166
at Carnegie Mellon University and it is described in [101]. 167
10. **FA** dataset, which contains percentage of body fat and ten body circumference mea- 168
surements. The goal is to fit body fat to the other measurements. 169
11. **MB** dataset. This dataset is available from Smoothing Methods in Statistics [102] and 170
it includes 61 patterns. 171
12. **MORTGAGE** dataset, which contains the Economic data information of USA. 172
13. **PY** dataset, (Pyrimidines problem). The source of this dataset is the URL: <https://www.dcc.fc.up.pt/~ltorgo/Regression/DataSets.html> and it is a problem of 27 173
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attributes and 74 number of patterns. The task consists of Learning Quantitative Structure Activity Relationships (QSARs) and provided by [103].

14. **Quake** dataset. The objective here is to approximate the strength of an 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

Table 1. Experimental results for the classification datasets.

DATASET	GENETIC	ADAM	RPROP	NEAT	PSO1	PSO2
Appendicitis	18.10%	16.50%	16.30%	17.20%	17.07%	17.90%
Australian	32.21%	35.65%	36.12%	31.98%	18.26%	17.37%
Balance	8.97%	7.87%	8.81%	23.14%	7.12%	7.43%
Bands	35.75%	36.25%	36.32%	34.30%	34.89%	34.31%
Cleveland	51.60%	67.55%	61.41%	53.44%	49.85%	49.52%
Dermatology	30.58%	26.14%	15.12%	32.43%	11.20%	10.81%
Hayes Roth	56.18%	59.70%	37.46%	50.15%	35.90%	37.03%
Heart	28.34%	38.53%	30.51%	39.27%	19.43%	20.26%
HouseVotes	6.62%	7.48%	6.04%	10.89%	6.91%	7.03%
Ionosphere	15.14%	16.64%	13.65%	19.67%	13.61%	13.98%
Liverdisorder	31.11%	41.53%	40.26%	30.67%	32.39%	31.95%
Lymography	23.26%	29.26%	24.67%	33.70%	26.91%	26.40%
Mammographic	19.88%	46.25%	18.46%	22.85%	17.47%	17.40%
PageBlocks	8.06%	7.93%	7.82%	10.22%	7.05%	6.88%
Parkinsons	18.05%	24.06%	22.28%	18.56%	15.49%	14.69%
Pima	32.19%	34.85%	34.27%	34.51%	26.26%	25.62%
Popfailures	5.94%	5.18%	4.81%	7.05%	5.26%	5.32%
Regions2	29.39%	29.85%	27.53%	33.23%	28.30%	28.86%
Saheart	34.86%	34.04%	34.90%	34.51%	32.59%	32.25%
Segment	57.72%	49.75%	52.14%	66.72%	15.95%	15.61%
Wdbc	8.56%	35.35%	21.57%	12.88%	4.79%	4.67%
Wine	19.20%	29.40%	30.73%	25.43%	8.12%	8.53%
Z_F_S	10.73%	47.81%	29.28%	38.41%	8.08%	7.97%
ZO_NF_S	8.41%	47.43%	6.43%	43.75%	5.43%	5.47%
ZONF_S	2.60%	11.99%	27.27%	5.44%	2.44%	2.51%
ZOO	16.67%	14.13%	15.47%	20.27%	5.20%	5.27%
AVERAGE	23.47%	30.81%	25.37%	28.87%	17.54%	17.50%

Table 2. Experiments for regression datasets.

DATASET	GENETIC	ADAM	RPROP	NEAT	PSO1	PSO2
ABALONE	7.17	4.30	4.55	9.88	4.39	4.33
AIRFOIL	0.003	0.005	0.002	0.067	0.003	0.003
BASEBALL	103.60	77.90	92.05	100.39	62.61	56.59
BK	0.027	0.03	1.599	0.15	0.027	0.027
BL	5.74	0.28	4.38	0.05	0.006	0.005
CONCRETE	0.0099	0.078	0.0086	0.081	0.003	0.003
DEE	1.013	0.63	0.608	1.512	0.23	0.23
DIABETES	19.86	3.03	1.11	4.25	0.59	0.62
HOUSING	43.26	80.20	74.38	56.49	22.69	15.51
FA	1.95	0.11	0.14	0.19	0.02	0.02
MB	3.39	0.06	0.055	0.061	0.05	0.05
MORTGAGE	2.41	9.24	9.19	14.11	0.21	0.16
PY	105.41	0.09	0.039	0.075	0.10	0.11
QUAKE	0.04	0.06	0.041	0.298	0.04	0.04
TREASURY	2.929	11.16	10.88	15.52	0.28	0.21
WANKARA	0.012	0.02	0.0003	0.005	0.0002	0.0002
AVERAGE	18.55	11.70	12.44	12.70	5.70	4.87

4. Conclusions

Author Contributions: All authors have conceived of the idea and methodology. A.T. and I.G.T. conducted the experiments, employing several datasets and provided the comparative experiments. D.T. and E.K. performed the statistical analysis and prepared the manuscript. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Institutional Review Board Statement: Not applicable.

Acknowledgments: The experiments of this research work were performed at the high performance computing system established at Knowledge and Intelligent Computing Laboratory, Department of Informatics and Telecommunications, University of Ioannina, acquired with the project “Educational Laboratory equipment of TEI of Epirus” with MIS 5007094 funded by the Operational Programme “Epirus” 2014–2020, by ERDF and national funds.

Conflicts of Interest: The authors declare no conflict of interest.

Sample Availability: Not applicable.

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