A two phase evolutionary method to train RBF networks

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Abstract

This article proposes a two phase hybrid method to train RBF neural networks for classification and regression problems. During the first phase a range for the critical parameters of the RBF network is estimated and in the second phase a genetic algorithm is incorporated to locate the best RBF neural network for the underlying problem. The method is compared against other training methods of RBF neural networks on a wide series of classification and regression problems from the relevant literature and the results are reported.

Keywords: RBF networks, classification, regression, genetic algorithms.

1 Introduction

In machine learning appear many practical problems such as classification and regression problems. A good programming tool that can be used to tackle this problem is Radial Basis Function (RBF) networks[1]. These networks typically are expressed as a function:

$$y(x) = \sum_{i=1}^{k} w_i \phi \left(\|x - c_i\| \right) \tag{1}$$

where $\overrightarrow{x}$ is the input pattern, the vector $\overrightarrow{w}$ is called the weight vector and $y(x)$ is the predicted value of the network. RBF networks are feedforward neural networks[2] with three computational layers:

1. The input layer, where the problem is presented in the form of patterns to the neural network

2. The processing layer, where a computation is performed using the Gaussian processing units $\phi(x)$. These units can have many forms in the relevant literature but the most used form is the Gaussian function expressed

as:

$$\phi(x) = \exp\left(-\frac{(x-c)^2}{\sigma^2}\right) \tag{2}$$

The value $\phi(x)$ depends only on the distance of vector $\overrightarrow{x}$ from some other vector $\overrightarrow{c}$, which typically is called centroid.

3. The output layer where the output of every function $\phi(x)$ is multiplied by a corresponding weight value w_i.

RBF networks have been used in many classification and regression problems from the areas of physics [3, 4, 5, 6], medicine [7, 8, 9], solution of differential equations [10, 11], chemistry [12, 13, 14], economics [15, 16, 17], digital communications [18, 19] etc. Also, recently the RBF networks have been used in more difficult problems such as authentication assurance of meat products [20], trajectory tracking for electro-hydraulic servo systems, identification of geographical origin for foods [22], prediction of solution gas-oil ratio of crude oil systems [23], prediction of occurrences of haloketones in tap water [24] , health monitoring [25] etc. Because of the extensive use of RBF networks, many methods have been proposed in the recent literature to enhance them. There are methods that parallelize the RBF networks [26, 27], methods that improve the initialization of the RBF parameters [28, 29, 30], methods that alter the architecture of the network [31, 32, 33], methods aimed to locate the best set of the RBF parameters with global optimization techniques[34, 35, 36] etc. This article transforms the problem of RBF training into an optimization problem and applies a modified genetic algorithm technique to solve it. The global optimization problem is defined as :

$$\min\left(E\left(y\right)\right) = \sum_{i=1}^{m}\left(y\left(x_i\right) - t_i\right)^2 \tag{3}$$

where m is the total number of input patterns and t_i is the output for pattern x_i. The suggested approach has two phases: firstly reasonable bounds for the RBF parameters are estimated using the k-means [38] algorithm and in the second phase the modified algorithm is used to solve the problem of equation 3 inside the bounds located in the first phase.

The rest of this paper is organized as follows: in section 2 the proposed method is described, in section 3 the conducted experiments are listed and the proposed method is compared against the traditional training of RBF networks and finally in section 4 some conclusions are derived.

2 Method description

The proposed method can be divided into two main phases: during the first phase an approximation for the bound of RBF parameters is made using the K-Means algorithm in the second phase the optimization problem is solved using a modified genetic algorithm. These phases are outlined in detail in the following subsections.

Figure 1: The layout of the chromosomes in the proposed genetic algorithm.

c_{11}	c_{12}	...	c_{1d}	σ_1	c_{21}	c_{22}	...	c_{2d}	σ_2	...	c_{k1}	c_{k2}	...	c_{kd}	σ_k

2.1 Bound location phase

The proposed genetic algorithm has chromosomes with dimension $(d+1)\times k$, where d is the dimension of the input problem, i.e. the dimension of the vector $\overrightarrow{x_i}$ in equation 3 and k is the total number of processing units of the RBF network. The layout of each chromosome is presented in Figure 1. Every center $\overrightarrow{c_i}$ in the equation 1 is a vector of dimension d and also an additional parameter is reserved for the parameter σ of every $\phi(x)$ function. The centroids and the corresponding variances are estimated using the k-means algorithm that described in algorithm 1. The value σ_i for every $\phi_i(x)$ is calculated as:

$$\sigma_i = \sum_{j=1}^{d} s_{ij}^2 \tag{4}$$

After the estimation of c_i and σ_i the vectors $\overrightarrow{L}$, $\overrightarrow{R}$ with dimension $(d{+}1){\times}k$ are constructed. These vectors will serve as the bounds for the chromosomes of the genetic population. These vector are constructed using the following procedure:

```
1. Set m=0
2. Set $F > 1$
3. For $i = 1..k$ do
    (a) For $j = 1..d$ do
        i. Set $L_m{=}{-F} \times c_{ij}$, $R_m{=}F \times c_{ij}$
        ii. Set $m = m + 1$
    (b) EndFor
    (c) Set $L_m = -F \times \sigma_i$, $R_m = F \times \sigma_i$
    (d) Set $m = m + 1$
4. EndFor
```

2.2 Main algorithm

The genetic algorithm used here is based on the algorithm denoted as GA (c_{r1}, l) in the paper of Kaelo and Ali[39] with a modified stopping rule as proposed in [37]. The basic steps of the main algorithm are given below:

1. **Initialization Step**
    - (a) **Read** the train set with m patterns of d dimension.

Algorithm 1 The k-means algorithm.

```
1. Repeat
    (a) $S_j = \{\}\,,\ j = 1..k$
    (b) For every sample $x_i$ Do
        i. Set $j^* = \min_{i=1}^{k} \{D(x_i, c_j)\}$, where $j^*$ is the nearest center for sample $x_i$.
        ii. Set $S_{j^*} = S_{j^*} \cup \{x_i\}$.
    (c) EndFor
    (d) For every center $c_j$ Do
        i. Set $M_j$=number of elements in $S_j$
        ii. Update $c_j$
                $c_j = \frac{1}{M_j} \sum_{i=1}^{M_j} x_i$
    (e) EndFor
2. Calculate the corresponding variances
        $s_j^2 = \frac{\sum_{i=1}^{M_j} (x_i - c_j)^2}{M_j}$
3. Terminate when $c_j$ no longer change.
```

(b) **Set** k the number of nodes for the RBF network.

(c) **Estimate** the vectors $\overrightarrow{L}$, $\overrightarrow{R}$ using the procedure of subsection 2.1.

(d) **Initialize** a genetic population of N_C random chromosomes inside $[L, R]$.

(e) **Set** the selection rate $p_s \in [0,1]$, the mutation rate $p_M \in [0,1]$, $iter = 0$, and i_{max} the maximum number of generations.

2. **Evaluation Step**

   For every chromosome g **calculate** using the procedure defined in subsection 2.3 the fitness f_g.

3. **Genetic operations step**
   During this step three genetic operations are performed: selection, crossover and mutation.

   (a) **Selection procedure.** Firstly the chromosomes are sorted with relevance to their corresponding fitness value. The best $(1 - p_s) \times N_c$ are transferred without change to the next generation and the remain ones are substituted by offsprings created through the crossover procedure. In the crossover procedure the mating parent are selected using tournament selection for every parent. The tournament selection has as follows:

   i. Select as set of $T > 2$ chromosomes from the population

   ii. Return the chromosome with the best fitness value in this subset.

   (b) **Crossover procedure** : For every pair (z, w) of selected parents create two new offsprings $\tilde{z}$ and $\tilde{w}$:

$$\begin{aligned} \tilde{z_i} &= a_i z_i + (1 - a_i) w_i \\ \tilde{w_i} &= a_i w_i + (1 - a_i) z_i \end{aligned} \tag{5}$$

   with a_i a random number and $a_i \in [-0.5, 1.5]$ [39]. This crossover scheme will be able to better explore the search space of the train error.

   (c) **Mutation procedure** : For every element of each chromosome create a random number $r \in [0,1]$. If $r \leq p_m$ then change randomly this element. The mutation is performed in a way similar to other approaches of genetic algorithms[37] and it is described in subsection 2.5.

   (d) **Replace** the $p_s \times N_c$ worst chromosomes in the population with the generated offsprings.

4. **Termination Check Step**

   (a) **Set** $iter = iter + 1$

   (b) **Terminate** if the termination criteria of subsection 2.4 are satisfied, **else Goto** Evaluation Step.

2.3 Fitness evaluation

In this step a valid RBF network $y(x) = \sum_{i=1}^{k} w_i \phi\left(\|x - c_i\|\right)$, is created using the chromosome g and subsequently is trained using the typical training procedure for RBF networks. The main steps to calculate the fitness f_g of a chromosome g are the following:

1. **Decode** the chromosome g to the parts (centers and variances) of the RBF network as defined by the layout of Figure 1.
2. **Calculate** the output vectors $w_1, w_w, \ldots, w_k$ by solving the an induced system of equations:
   (a) **Set** $W = w_{kj}$ the matrix of k weights, $\Phi = \phi_j\left(x_i\right)$ and $T = \{t_i\}$.
   (b) **Solve:**
   $$\Phi^T \left(T - \Phi W^T\right) = 0 \tag{6}$$
   $$W^T = \left(\Phi^T \Phi\right)^{-1} \Phi^T T = \Phi^{\dagger} T \tag{7}$$
   The matrix $\Phi^{\dagger} = \left(\Phi^T \Phi\right)^{-1} \Phi^T$ is the pseudo-inverse of Φ, with
   $$\Phi^{\dagger} \Phi = I \tag{8}$$
3. **Set** $f_g = \sum_{i=}^{m} \left(y\left(x_i\right) - t_i\right)^2$

2.4 Stopping rule

Define as g_{best} the best chromosome in the population and define as $\sigma^{(\text{iter})}$ the variance of best fitness $f\left(g_{\text{best}}\right)$ at generation iter. If fitness $f\left(g_{\text{best}}\right)$ has not improved for a number of generations, then probably the algorithm should terminate. Hence, the termination rule is defined as:

$$\text{iter} \geq i_{\max} \text{ OR } \sigma^{(\text{iter})} \leq \frac{\sigma^{(\text{klast})}}{2} \tag{9}$$

where klast is the last generation where a new minimum was found.

2.5 Mutation procedure

Let $w = (w_1, w_2, ..., w_n)$ be the chromosome to be mutated. The proposed mutation procedure modifies w_i with probability p_m and the resulting element w_i' is given by

$$w_i' = \begin{cases} w_i + \Delta\left(\text{iter}, R_i - w_i\right), \text{ if} & t > \frac{1}{2}0 \\ w_i - \Delta\left(\text{iter}, w_i - L_i\right), \text{ otherwise} & \end{cases} \tag{10}$$

where t is a random number with $t \in [0, 1]$. The function $\Delta(\text{iter}, y)$ is given by:

$$\Delta(\text{iter}, y) = y\left(1 - r^{\left(1 - \frac{\text{iter}}{\text{ITERMAX}}\right)^b}\right) \tag{11}$$

Table 1: Experimental parameters.

PARAMETER	VALUE
k	10
N_c	200
p_s	0.90
p_m	0.05
F	3.0
i_{max}	200

where r is a random number in $[0,1]$ and b controls the change of element w_i. In the proposed algorithm the value $b=5$ was used.

3 Experiments

In order to evaluate the performance of the proposed method, comparative experiments were performed on a series of well - known classification and regression datasets from the relevant literature.

3.1 Experimental setup

The RBF network was coded in ANSI C++, using the Armadillo library [40] and the optimization was performed using the Genetic optimization method of the optimization package OPTIMUS, that is freely available from `https://github.com/itsoulos/OPTIMUS/`. Also, to have more reliability in the results the common used method of 10 - fold cross validation was used, which means that the the original data was randomly partitioned into 10 equal sized subsamples. Subsequently, 10 independent experiments were conducted: in each experiments one subsample is used as the testing data and all the others as the training data. The average error on the test data is the total test error. All the experiments were executed 30 times with different initialization for the random generator each time. The random generator used was the function drand48() of C programming language. The execution environment was an Intel Xeon E5-2630 multi core machine using the OpenMP library [42] for parallelization and the Ubuntu Linux operating system. The parameters for the genetic algorithm are displayed in Table 1. The parameters of the method were chosen so that there is a balance between speed and efficiency of the method.

3.2 Experimental datasets

The classification problems used for the experiments were found in most cased 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`[41].

The following classification datasets were used:

1. **Alcohol** dataset which is related to alcohol consumption [43].
2. **Appendictis** dataset, proposed in [44].
3. **Australian** dataset [45], which refers to credit card applications.
4. **Balance** dataset [46], which is used to predict psychological states.
5. **Cleveland** dataset, a dataset used to detect heart disease used in various papers[47, 48].
6. **Dermatology** dataset [49], which is used for differential diagnosis of erythemato-squamous diseases.
7. **Glass** dataset. The dataset contains glass component analysis and it has been used in a variety of papers [50, 51].
8. **Hayes roth** dataset [52].
9. **Heart** dataset [53], used to detect heart disease.
10. **HouseVotes** dataset [54], which is about votes in the U.S. House of Representatives Congressmen.
11. **Ionosphere** dataset. The ionosphere dataset contains data from the Johns Hopkins Ionosphere database and it has been studied in a bunch of papers [55, 56].
12. **Liverdisorder** dataset [57], used for detect liver disorders in peoples using blood analysis.
13. **Mammographic** dataset [58], used to identify the severity of a mammographic mass lesion.
14. **Parkinsons** dataset. This dataset is composed of a range of biomedical voice measurements from 31 people, 23 with Parkinson's disease (PD)[59].
15. **Pima** dataset [60], used to detect the presence of diabetes.
16. **Popfailures** dataset [61], that is related to climate model simulation crashes of simulation crashes.
17. **Regions2** dataset, is created from liver biopsy images of patients with hepatitis C [62].
18. **Ring** dataset [63]. It is an 20 dimensional problem with two classes. Each class is drawn from a multivariate normal distribution.
19. **Saheart** dataset [64], used to detect heart disease.

20. **Segment** dataset [65]. This database contains patterns from a database of 7 outdoor images (classes).

21. **Sonar** dataset [66]. The task is discriminate between sonar signals bounced off a metal cylinder.

22. **Spiral** dataset: The spiral artificial dataset contains 1000 two-dimensional examples that belong to two classes.

23. **Tae** dataset [67], which concerns evaluations of teaching performance.

24. **Thyroid** dataset, which concerns Thyroid disease records[79].

25. **Wdbc** dataset [68], which contains data for breast tumors.

26. **Wine** dataset, used to detect through chemical analysis determine the origin of wines and is been used in various research papers [69, 70].

27. **Eeg** datasets, the eeg dataset in [72] is utilized. The dataset consists of five sets (denoted as Z, O, N, F and S) each containing 100 single-channel EEG segments each having 23.6 sec duration. With different combinations of these sets the produced datasets are Z_F_S, ZO_NF_S, ZONF_S.

28. **Zoo** dataset [71], where the task is classify animals in seven predefined classes.

The regression datasets are in most cases available from the Statlib URL `ftp://lib.stat.cmu.edu/datasets/index.html`:

1. **Abalone** dataset [73]. This data set can be used to obtain a model to predict the age of abalone from physical measurements.

2. **Airfoil** dataset, which is used by the NASA for a series of aerodynamic and acoustic tests [74].

3. **Anacalt** dataset [75]. This contains information about the decisions taken by a supreme court.

4. **BK** dataset [81], used to estimates the points in a basketball game.

5. **BL** dataset: This dataset can be downloaded from StatLib. It contains data from an experiment on the affects of machine adjustments on the time to count bolts.

6. **Concrete** dataset, used to measure the concrete compressive strength [76].

7. **Housing** dataset. This dataset was taken from the StatLib library which is maintained at Carnegie Mellon University and it is described in [77].

8. **Laser** dataset. Dataset used in laser experiments. It has been obtained from the The Santa Fe Time Series Competition Data repository.

9. **MB** dataset. This dataset is available from Smoothing Methods in Statistics [78].
10. **NT** dataset. This dataset contains data from [80] that examined whether the true mean body temperature is 98.6 F.
11. **Quake** dataset. The objective here is to approximate the strength of a earthquake. It has been obtained from the Bilkent University Function Approximation Repository.

3.3 Experimental results

The results for the classification datasets are listed in Table 2 and for the regression datasets the results are reported in Table 3. For the first case the average classification error is reported and for the case of regression datasets the total test error is reported. The column KRBF denotes the classic RBF training method, GRBF denotes the method proposed in [82] and the column PROPOSED denotes the proposed method. The KBF simply consists of two phases: in the first phase centers and variances are estimated through the k-means algorithm and in the second phase a system of equations is solved to obtain the weights w_i of the RBF network.

From the experimental results it is clear that the proposed method is significantly superior to other methods in almost all datasets. In the proposed method the appropriate initialization interval is found for the parameters of RBF using k-means. A parallel genetic algorithm was then applied to this previous value range creating a variety of neural networks. This combination of techniques obviously has very good results as it combines a very efficient clustering method and an excellent optimization method that is ideally parallelized. Of course, the new method requires much more execution time, due to the presence of the genetic algorithm but the parallel execution of the software drastically reduces this time. Also, in order to study the effectiveness of the selection of parameter F an additional experiment were conducted, where the best fitness of the genetic algorithm is plotted for the WINE problem. The outcome of this experiment is graphically outlined in Figure 2. The graph shows that the behavior of the proposed method does not change significantly for different values of the parameter F. Also the plot for the WINE dataset of best, worst and average fitness for $F = 3$ is shown in Figure 3. An additional experiment was performed to evaluate the effect of the parameter change k on the results. In Figure 4 the plot for different values of k for the Housing dataset is outlined and in Figure 5 the same experiment is shown for the Z_F_S classification dataset. Of course from the value $k = 4$ onwards the error falls but not at the same rate. The proposed value $k = 10$ was used in all data sets in order to have a balance between the speed and the efficiency of the method. Finally, classification performance was evaluated based on two evaluation metrics: precision and recall for some datasets as show in Table 4.In these results, the precision of the proposed method showed the best classification performance under different datasets. We found the same trends in recall metric in the two of three datasets (spiral and EEG datasets).

Table 2: Classification error for different datasets.

DATASET	KRBF	GRBF	PROPOSED
Alcohol	46.63%	52.30%	21.86%
Appendicitis	12.23%	16.83%	16.03%
Australian	34.89%	41.79%	22.97%
Balance	33.42%	38.02%	12.88%
Cleveland	67.10%	67.47%	51.75%
Dermatology	62.34%	61.46%	37.37%
Glass	50.16%	61.30%	49.16%
Hayes Roth	64.36%	63.46%	35.26%
Heart	31.20%	28.44%	17.80%
HouseVotes	6.13%	11.99%	3.67%
Ionosphere	16.22%	19.83%	10.33%
Liverdisorder	30.84%	36.97%	28.73%
Mammographic	21.38%	30.41%	17.25%
Parkinsons	17.42%	33.81%	17.37%
Pima	25.78%	27.83%	24.00%
Popfailures	7.04%	7.08%	5.44%
Regions2	38.29%	39.98%	25.81%
Ring	21.65%	50.36%	2.09%
Saheart	32.19%	33.90%	29.38%
Segment	59.68%	54.25%	39.44%
Sonar	27.85%	34.20%	19.62%
Spiral	44.87%	50.02%	18.98%
Tae	60.07%	61.78%	52.44%
Thyroid	10.52%	8.53%	7.12%
Wdbc	7.27%	8.82%	5.29%
Wine	31.41%	31.47%	8.67%
Z_F_S	13.16%	23.37%	4.21%
ZO_NF_S	9.02%	22.18%	4.17%
ZONF_S	4.03%	17.41%	2.18%
ZOO	21.93%	33.50%	9.00%

Table 3: Regression error for different datasets.

DATASET	KRBF	GRBF	PROPOSED
ABALONE	2559.48	4161.66	1960.22
AIRFOIL	5.49	18.15	0.58
ANACALT	11.628	5.58	0.003
BK	0.17	0.21	0.23
BL	0.05	0.019	0.0009
CONCRETE	1.15	1.50	0.52
HOUSING	2884.09	4784.50	693.22
LASER	2.35	6.94	1.04
MB	11.33	2.44	0.63
NT	72.14	0.22	0.09
QUAKE	15.36	171.43	7.86

Figure 2: Plot of best fitness for the WINE problem for different values of parameter F.

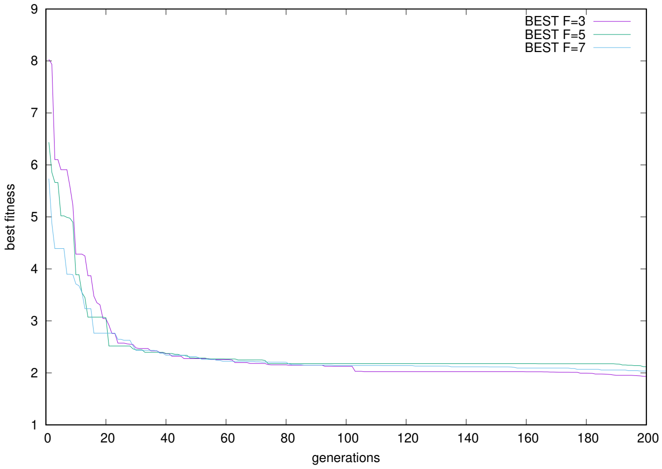


Table 4: Comparison of precision and recall between the traditional RBF and the proposed method for some datasets.

DATASET	PRECISION KRBF	RECALL KRBF	PRECISION PROPOSED	RECALL PROPO
HOUSEVOTES	90.61%	95.60%	96.44%	94.25%
SPIRAL	55.53%	55.93%	82.93%	84.66%
ZONF_S	92.76%	87.23%	97.27%	94.55%

Figure 3: Plot of best, worst and average fitness for the Wine dataset and $F = 3$.

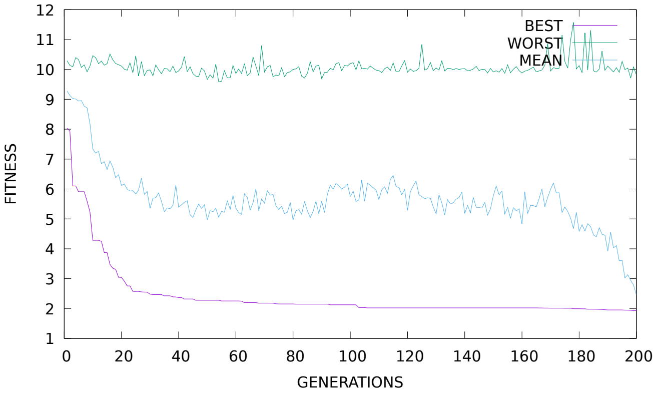


Figure 4: Experiments with different values of k for the Housing dataset.

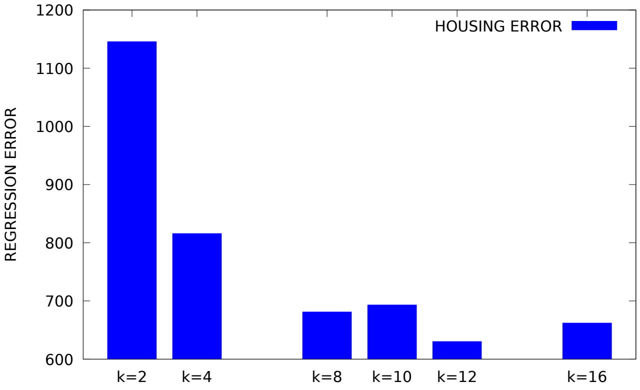
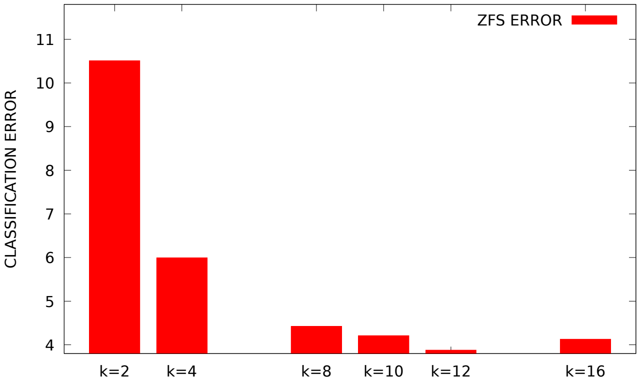


Figure 5: Classification error of Z_F_S dataset for different values of k.



4 Conclusions

A two phase method was proposed in this article to train RBF neural networks for classification and regression problems. Firstly, a common used clustering method was used to estimate an interval for the critical parameters of the neural network. Subsequently, a parallel genetic algorithm was incorporated to locate the best RBF network with good generalization capabilities. The used software was coded using ANSI C++ and open source libraries such as the Armadillo library and the OpenMP library for parallelization. Future research may include

1. Use parallel methods for the k-means clustering phase of the method.

2. Dynamic selection of K in k-means algorithm.

3. More advanced stopping rules for the genetic algorithm.

4. Replace the Genetic algorithm with other optimization methods such as Particle Swarm Optimization, Ant Colony Optimization etc.

Acknowledgments

The experiments of this research work was performed at the high performance computing system established at Knowledge and Intelligent Computing Laboratory, Dept 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 finds.

Compliance with Ethical Standards

All authors declare that they have no conflict of interest.

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