Comparative performance of some popular ANN algorithms on benchmark and function approximation problems

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Abstract. We report an inter-comparison of some popular algorithms within the artificial neural network domain (viz., Local search algorithms, global search algorithms, higher order algorithms and the hybrid algorithms) by applying them to the standard benchmarking problems like the IRIS data, XOR/N-Bit parity and Two Spiral. Apart from giving a brief description of these algorithms, the results obtained for the above benchmark problems are presented in the paper. The results suggest that while Levenberg-Marquardt algorithm yields the lowest RMS error for the N-bit Parity and the Two Spiral problems, Higher Order Neurons algorithm gives the best results for the IRIS data problem. The best results for the XOR problem are obtained with the Neuro Fuzzy algorithm. The above algorithms were also applied for solving several regression problems such as cos(x) and a few special functions like the Gamma function, the complimentary Error function and the upper tail cumulative $\chi^2$-distribution function. The results of these regression problems indicate that, among all the ANN algorithms used in the present study, Levenberg-Marquardt algorithm yields the best results. Keeping in view the highly non-linear behaviour and the wide dynamic range of these functions, it is suggested that these functions can be also considered as standard benchmark problems for function approximation using artificial neural networks.

Keywords. Artificial Neural Network, Benchmark problems, Function approximation, Special functions

PACS Nos 07.05.Mh, 7.05Kf, 2.60GF, 29.85

1. Introduction

An artificial neural network (ANN) is an interconnected group of artificial neurons that use a mathematical model for information processing to accomplish variety of tasks [1]. They can be configured in various arrangements to perform a range of tasks including pattern recognition and classification [2]. While the theory and the implementation of ANN has been around for more than 50 years, it is only...
recently that they have found widespread practical applications. This is primarily due to the advent of high speed, low cost computers that can support the rather computationally intensive requirement of an ANN of any real complexity.

Artificial neural networks have been used successfully in various fields, like, pattern recognition, financial analysis, biology, engineering and so on, because of their merits such as self-learning, self-adapting, good robustness and capability of dealing with non-linear problems. They have also been employed extensively in several branches of astronomy for automated data analysis and other applications like star/galaxy classification, time series analysis (e.g. prediction of solar activity), determination of photometric redshifts, characterization of peculiar objects such as QSO’s, ultraluminous IR galaxies[3][4]. With the increase of quantity and the distributing complexity of astronomical data, its scientific exploitation requires a variety of automated tools, which are capable of performing variety of tasks, such as data preprocessing, feature selection, data reduction, data mining and data analysis[5]. In some recent applications the IUCAA group (and their collaborators) have used ANNs with remarkable success for problems like star/galaxy classification, stellar spectra classification etc. Employing principal component analysis (PCA) for reducing the dimensionality of the data and a multilayer backpropagation network based ANN scheme, a fast and robust method has been developed in [6] for classifying a library of optical stellar spectra for O to M type stars. It has been demonstrated in their work that the PCA when combined with ANN reduces the network configuration (and hence computational time) drastically without compromising on the classification accuracy. An automated classification scheme based on the above idea has been also used for classifying 1273 stars in the CFLIB data base [7] with an added advantage that by employing a generalized PCA technique, the authors were able to restore missing data for 300 stars. A supervised back-propagation algorithm was used to classify 2000 bright sources from the Calgary database of IRAS (Infrared Astronomical Satellite) spectra into 17 predefined classes and a success rate of 80% has been reported by the authors [8]. Stellar spectra classification using the probabilistic Neural Network (PNN) for automated classification of about 5000 Solan Digital Sky Survey (SDSS) spectra into 158 spectral classes has also been performed in [9] with some encouraging results. The use of ANN-based technique to develop a pipeline for automated segregation of star/galaxies to be observed by the Tel-Aviv University Ultra-Violet Experiment (TAUVEX) is also validated by using synthetic spectra in the UV region as the training set and International Ultraviolet Explorer (IUE) low resolution spectra as the test set [10][11].

An important research activity in the field of neural networks is to compare the performance of different ANN algorithms on benchmark problems and to develop more efficient algorithms for solving real world problems with noisy and scarce data. It has been also noticed by several workers, that neural network algorithms are often benchmarked rather poorly [12]. More importantly, it is also found in the literature that performance of any algorithm is only compared to the standard backpropagation algorithm [13] even though there are several powerful and widely used algorithms readily available now. Keeping this in mind, we present a detailed study in this paper where the performance of three generations of neural network algorithms i.e 1st order algorithms (Standard Backpropagation and Resilient Backpropagation), 2nd order algorithms (Conjugate Gradient, Levenberg-Marquardt,
Comparative performance ... Radial Basis Function, Simulated Annealing), the Hybrid models like the Higher Order Neuron model and Neuro-Fuzzy system, is examined by applying them to standard benchmarking problems like IRIS data, XOR/N-Bit parity and Two Spiral data. In addition to benchmark problems discussed above, we have also applied the above mentioned neural network algorithms for solving several regression problems such as \( \cos(x) \) and a few special functions like the Gamma function, the complimentary Error function and the upper tail cumulative \( \chi^2 \)-distribution function. A short introduction to ANN methodology and a brief description of the ANN algorithms used in the present work has also been presented in the paper so that the manuscript can be easily followed by researchers who are not experts in the field of neural networks.

2. ANN Methodology and brief description of algorithms used

In a feed-forward ANN model, the network is constructed using layers where all nodes in a given layer are connected to all nodes in a subsequent layer. The network requires at least two layers, an input layer and an output layer. In addition, the network can include any number of hidden layers with any number of hidden nodes in each layer. The signal from the input vector propagates through the network layer by layer till the output layer is reached. The output vector represents the predicted output of the ANN and has a node for each variable that is being predicted. The task of training the ANN is to find the most appropriate set of weights for each connection which minimizes the output error. All weighted-inputs are summed at the neuron node and this summed value is then passed to a transfer (or scaling) function. The selection of the transfer function is part of the neural network design and some examples of the transfer functions are the sigmoid, hyperbolic tangent, Sine, decaying exponential, gaussian, cauchy functions etc. Apart from being smooth and differentiable, the transfer function is chosen in such a manner so that it can accept input in any range, and produce an output in a strictly limited range. To train an ANN, initially all the neurons of the ANN are assigned random weights and the inputs and desired output vectors are presented to the ANN. The ANN uses the input vector to produce an output vector. The ANN generated output vector is compared with the desired output vector to calculate the error [14]. The ANN learns by adjusting its weights such that in the next iteration the net error produced by the ANN is generally smaller than that in the current iteration. However, there are several issues involved in designing and training a multilayer neural network. These are: (a) Selecting appropriate number of hidden layers in the network; (b) Selecting the number of neurons to be used in each hidden layer; (c) Finding a globally optimal solution that avoids local minima; (d) Converging to an optimal solution in a reasonable period of time; (e) Validating the neural network to test for overfitting.

Depending upon the architecture in which the individual neurons are connected and the choice of the error minimization procedure, there can be several possible ANN configurations. As discussed above, the ANN algorithms, which have been used in the present work, can be broadly categorized into three main categories viz., Local search algorithms, Global search algorithms and Hybrid algorithms. While
algorithms like Standard backpropagation and Resilient backpropagation come under
the category of Local search algorithms, Conjugate Gradient methods, Lavenberg-
Marquardt algorithm, Radial basis function and Simulated Annealing Technique
belong to the category of Global search algorithm. Hybrid algorithm category
constitutes models like Higher order neurons and Neuro-fuzzy systems. A brief
description of the most promising ANN algorithms is presented below.

The standard backpropagation network [15] is the most thoroughly investigated
ANN algorithm. Backpropagation using gradient descent often converges very
slowly. The success of this algorithm in solving large-scale problems critically de-
dpends on user-specified learning rate and momentum parameters and, there are
no standard guidelines for choosing these parameters. Unfortunately, if incorrect
values are specified, the convergence may be exceedingly slow, or it may not con-
erge at all. The Resilient backpropagation (RProp) algorithm was proposed by
Reidmiller [16], to expedite the learning of a backpropagation algorithm. Unlike
the standard Backpropagation algorithm, RProp uses only partial derivative signs
to adjust weight coefficients. The algorithm uses the so-called ‘learning by epoch’,
which means that the weight adjustment takes place after all the patterns from the
learning sample are presented to the network.

As already discussed, the learning schemes followed by Backpropagation or the
Resilient Backpropagation, based on the gradient descent methods, have several
limitations. In these gradient-based algorithms it is difficult to obtain a unique set
of optimal parameters due to the existence of multiple local optima [17]. The pres-
ence of these local minima hampers the search for global minimum because these
algorithms frequently get trapped in local minima regions and hence incorrectly
identify local minimum as the global minimum. The traditional conjugate gradient
algorithm uses the gradient to compute a search direction and then a line search
algorithm is used to find the optimal step size along a line in the search direction.
The Scaled conjugate gradient algorithm developed by Moller [18] is an improve-
ment over conjugate gradient which besides giving higher accuracy also reduces the
number of iterations and computation time. The Levenberg algorithm [19] involves
the use of "blending" between the steepest descent method employed by the back-
propagation algorithm and the quadratic rule employed in conjugate algorithms.

The original Levenberg algorithm was improved further by Marquardt, resulting in
the Lavenberg-Marquardt algorithm, by incorporating the local curvature information.
In essence, the model suggests that we should move further in the direction in
which the gradient is smaller in order to get around the classic ”error valley”. Ra-
dial Basis Functions are powerful techniques for interpolation in multidimensional
space and in artificial neural networks they are utilized as activation functions [20].
Simulated annealing is a generic probabilistic algorithm for the global optimization
problem, namely locating a good approximation to the global optimum of a given
function in a large search space [21]. Starting from some random point, the error at
this point ($E_A$) is evaluated from the model or data. Then a nearby point is chosen
at random and the error at this point ($E_B$) is again evaluated. If this new point has
a lower error, the process is repeated to find a still lower error point. However if it
has a higher error, there is still a chance for finding a lower error valley within the
error surface. The probability of this is given by $p=\exp(E_A-E_B)/kT$ [22]. In other
words ”'uphill’” moves are permitted, albeit with decreasing probability for large
Comparative performance ... differences. This has the effect of managing to ‘escape’ from the local minima.

The limitations of standard backpropagation can be overcome either by global techniques or by higher order models. Global search methods like the conjugate algorithms may reduce the architectural complexity but not the learning complexity. Higher order neuron model is the one which includes the quadratic and higher order basis functions in addition to the linear basis functions to reduce the learning complexity. A higher order neuron model [23] has many aggregation and activation functions. The aggregation functions can be linear weighted sum (linear basis function), quadratic or higher order basis functions. Here the cross product of the input terms is added into the model where each component in the input pattern multiplies the entire input vector. Neuro-fuzzy systems [24,25] refer to hybrids of artificial neural networks and fuzzy logic which result in a hybrid intelligent system that synergizes these two techniques by combining the human-like reasoning style of fuzzy systems with the learning and connectionist structure of neural networks.

3. Benchmarking of ANN algorithms

The comparative performance of the ANN algorithms described above have been studied by applying them to standard benchmarking problems like IRIS data, XOR/N-Bit parity, Two Spiral data and Cosine(x). While we used standard ANN package contained in the MATLAB software for implementing the Lavenberg-Marquardt algorithm, the implementation of other algorithms like Backpropagation, Resilient Backpropagation, Conjugate Gradient Method, Radial Basis Functions, Simulated Annealing, Neuro-Fuzzy etc., were done by using the dedicated ANN simulator package BIKAS (BARC - IIT Kanpur ANN Simulator). Written in Java environment, this dedicated ANN package contains a variety of neural network algorithms like the standard backpropagation, resilient, scale and self conjugate, higher order network functions, simulated annealing and radial basis methods, adaptive resonance theory algorithms, self growing networks and fuzzy algorithms. An exhaustive library of about 15 error minimization functions (like the conventional RMS error function, Hyperbolic square error, Minkowski error, Hubers error function, Cauchy error function etc.) and about 25 activation functions (like the sigmoid function, hyperbolic tan, sine, cosine, decaying exponential, Gaussian, bipolar logarithmic etc.) are also provided in this package.

The training and testing of all the ANN algorithms used in the present work has been done on a Pentium P-III 700 MHz machine. Rigorous checks were also performed at various stages to ensure that the ANN configuration used for a particular problem was properly optimized with respect number of nodes in the hidden layer. This was done by monitoring the RMS error while training the ANN. The RMS error employed here is defined as:

\[
RMS = \frac{1}{PI} \sqrt{\sum_{p=1}^{P} \sum_{i=1}^{I} (D_{pi} - O_{pi})^2}
\]  

(1)

where \(D_{pi}\) and \(O_{pi}\) are the desired and the observed values, \(P\) is number of training patterns and \(I\) is the number of output nodes.
The optimized configuration yielded a RMS error which reduced only marginally when the number of nodes in the hidden layer was increased further, but at the cost of a much larger computation time. It is worth mentioning here that while the number of nodes in the hidden layer used varied from 2 for XOR to 15 for IRIS data, the number of nodes in the hidden layer was kept same for a particular problem in different ANN algorithms to avoid any biasing towards a particular algorithm. The training of the above networks was 'early-stopped' to avoid any overfitting effects and this was done as soon as the RMS error reached a plateau. A maximum of \( \sim 2000 \) iterations were found to be optimum for all the problems which are considered in this work. However, it is important to note that the number of iterations needed for the ANN to learn the input/output mapping depends on the complexity of the problem. In real world problems, e.g. star/galaxy classification [6], spectra classification, primary energy estimation of cherenkov telescopes [26] etc. \( \sim 10,000 \) iterations have been used.

3.1 IRIS problem

Fisher [27] introduced a benchmark dataset that contains the sepal and petal measurements of different types of iris flowers. There are 150 training samples available, each of which consists of four inputs and one output. The inputs are the measured lengths and widths of the petals and the sepals, and the output is the type of iris flower, such as Setosa, Versicolor, and Virginica. The distributions of the samples with respect to the dimensions of the sepals and petals are shown in Fig.1 for an easy visualization. It is quite evident from Fig.1 that the classes of Versicolor and Virginica overlap, whereas the class of Setosa is clearly separated from the other two classes. In order to convert the training data in the \([0,1]\) interval, all measurement values were first divided by 10. The three iris species setosa, versicolor, and virginica were categorized with the numbers 1, 2 and 3, respectively. The configuration employed for training the ANN consists of 4:15:1 i.e, 4 neurons in the input layer, 15 neurons in the hidden layer and 1 neuron in the output layer corresponding to the category of the species. The choice of 15 neurons was found to be optimum for this task. Since the final RMS error also depends upon the choice of initial parameters (like \( \alpha, \beta \) and the initial weights), these parameters were changed randomly 5 times and final RMS error presented here is the mean of these five RMS error values. The RMS error obtained at the end of the training process for all the algorithms along with time taken for completing the training is presented in Table.1. The test set for the IRIS data is similar to the training set except that this data has not been presented during the training of the nets. It consists of 45 data points (15 from each class). Instead of testing the performance of all the algorithms with test data, we have only chosen one (or sometimes two) ANN algorithm for testing purpose and these are the ones which yield the lowest RMS error during their training stage. Since for the IRIS data case both Higher Order and Lavenberg Marquardt algorithm yield the lowest (and reasonably comparable also) RMS error, we have used only these algorithms for checking their performance on the test data. The test results obtained for these algorithms suggest that while 100% classification is achievable for class Setosa, the classification for Versicolor and Virginica is only
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Figure 1. IRIS data distribution with respect to the sepal and petal lengths.

80%. The reason for not being able to obtain 100% classification between versicolor and virginica seems to be the overlapping between these two species (Fig.1).

3.2 XOR and N-Bit parity problems

XOR is a standard and thoroughly investigated problem in the field of neural network research. Its popularity originates from the fact that, being able to solve it was a breakthrough achieved by back-propagation algorithm, compared to the situation faced when no learning algorithm was known to solve a non linearly separable classification task such as XOR [28]. Apart from the XOR problem we also applied the other ANN algorithms to the generalized XOR problem i.e the N-bit parity, where the task requires to classify the sequence consisting of 1’s and 0’s according to whether number of 1’s is odd or even [28]. The target for the net here is 1 or 0 depending on whether the sequence is odd or even. In the XOR problem the algorithm used has the form 2:2:1 i.e 2 neurons in the input layer, 2 neurons in the hidden layer and 1 neuron in the output layer. Also, for training the networks, more data points were also generated by incorporating random noise of 10% at the XOR inputs. The RMS error obtained for the XOR problem at the end of the training process, for all the algorithms, alongwith time taken for completing the training is presented in Table 2. As seen from Table 2, the lowest RMS error for the XOR problem is yielded by the Neuro-Fuzzy and the Marquardt-Lavenberg al-
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**Algorithm**
P RO

**RMS**

| ANN Algorithm | BAC | RES | LAV | CON | RAD | SIM | NEU | HIG | ORD |
|----------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| RMS Error      | 1.20×10⁻³ | 1.14×10⁻³ | 1.21×10⁻⁵ | 1.20×10⁻³ | 1.14×10⁻³ | 1.21×10⁻⁵ | 1.20×10⁻³ | 1.14×10⁻³ | 1.21×10⁻⁵ |

**Time (s)**

| ANN Algorithm | BAC | RES | LAV | CON | RAD | SIM | NEU | HIG | ORD |
|----------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Time           | 16  | 14  | 15  | 16  | 18  | 12  | 15  | 28  | 16  |

Table 1. Mean RMS error and training time of various ANN algorithms with a configuration of 4:15:1 for the IRIS problem. The abbreviations used for different ANN algorithms are the following: BAC PRO – Backpropagation; RES BAC – Resilient Backpropagation; LAV MAR – Lavenberg-Marquardt; CON GRA – Conjugate Gradient; RAD BAS – Radial Basis; SIM ANN – Simulated Annealing; NEU FUZ – Neuro Fuzzy; HIG ORD – Higher Order

Table 2. Mean RMS error and training time of various ANN algorithms with a configuration of 2:2:1 for the XOR problem. Full form of the abbreviations used for different ANN algorithms can be seen in the Caption of Table 1.

algorithms and hence performance testing on test data sample is done only for these two algorithms. Both these networks show ~100% success rate in reproducing the XOR truth table.

The parity problem too is a demanding classification task for neural networks to solve, because the target-output changes whenever a single bit in the input vector changes. The N-bit parity consists of 2ᴺ (here N = 4) training pairs. A 4:2:1 architecture was used by us for studying this problem. The RMS error obtained for the N-Bit problem, at the end of the training process, for all the algorithms, alongwith time taken for completing the training is presented in Table.3. The test set for N-Bit parity problem consists of 10 randomly generated noisy events (noise 10%). Testing of the net was done only with the Marquardt-Lavenberg algorithm network since compared to other algorithms considered in this works, it gives the lowest RMS error. The results obtained on the test data suggest that the 4-Bit parity is reproduced with an accuracy of ~ 90%.

3.3 Two-spiral problem

The original two intertwined spirals benchmark problem was designed by Lang and Wittbrock [29] to test the performance of classification on binary data. This particular task is difficult for most current algorithms since it requires the ANN model
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| ANN Algorithm | BAC | RES | LAV | CON | RAD | SIM | NEU | HIG |
|---------------|-----|-----|-----|-----|-----|-----|-----|-----|
| RMS Error     | 9.81×10⁻⁷ | 7.12×10⁻⁷ | 3.43×10⁻⁸ | 4.03×10⁻⁷ | 1.27×10⁻⁴ | 9.01×10⁻⁷ | 3.42×10⁻³ | 5.16×10⁻⁴ |
| Time (s)      | 26  | 40  | 50  | 16  | 28  | 28  | 44  | 55  |

Table 3. Mean RMS error and training time of various ANN algorithms with a configuration of 4:2:1 for the 4-Bit parity problem. Full form of the abbreviations used for different ANN algorithms can be seen in the Caption of Table 1.

to learn the highly non-linear separation of the input space. In this benchmarking problem, two spirals, each of which has three complete turns, are created inside a unit square Fig.2. The two-interwined spirals problem has also been used quite extensively by other researchers as standard benchmark problem and requires the neural network to learn a mapping that distinguishes between points on two intertwined spirals. The data used by us for the 2-Spiral problem contains 194 data points (97 samples per spiral). The network configuration chosen to represent this problem has the 2:15:1 architecture, where the two inputs correspond to \(a_1\), \(a_2\) values of the two spirals and the 1 output corresponds to whether the value belongs
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to the spiral 1 or spiral 2 (1 if the point falls on one spiral and 0 if it falls on other spiral). Out of these 194 data points 164 were used for training and 30 points (15 from each spiral) were used for testing. The training results obtained for all the ANN algorithms used in the present study are presented in Table 4 and it is quite evident from this table that the Levenberg-Marquardt gives the best convergence results. However, from training time considerations, the standard backpropagation and the resilient backpropagation algorithms are seen to consume minimum training time. Performance check of the Levenberg-Marquardt algorithm, on test data for 30 points (15 from each spiral), indicates that ∼70% of the events are classified in the proper spiral category. This is much better as compared to resilient backpropagation which can classify only ∼50% of the events properly.

A consolidate report of the mean RMS error yielded by various ANN algorithms used in the present work for all the 4 benchmark problems is presented in Table 5. A plot of the RMS error as a function of number of iterations, for all the 4 benchmark problems is also shown in Fig. 3 so that the performance of the backpropagation algorithm can be compared with other algorithms. For the sake of clarity, the RMS error is shown only for the Backpropagation algorithm and one more specific algorithm which yields the minimum RMS error (i.e Higher Order for IRIS, Neuro-fuzzy for XOR and Levenberg-Marquardt method for N bit parity

| ANN Algorithms | IRIS problem | XOR problem | N-bit parity problem | 2-spiral problem |
|----------------|--------------|-------------|----------------------|-----------------|
| Backprop       | $2.00 \times 10^{-3}$ | $1.23 \times 10^{-4}$ | $9.81 \times 10^{-4}$ | $1.51 \times 10^{-4}$ |
| Resilient      | $1.75 \times 10^{-3}$ | $7.72 \times 10^{-4}$ | $7.12 \times 10^{-4}$ | $7.13 \times 10^{-4}$ |
| Lavenberg      | $1.92 \times 10^{-3}$ | $1.59 \times 10^{-4}$ | $3.43 \times 10^{-4}$ | $1.99 \times 10^{-4}$ |
| Conjugate      | $9.64 \times 10^{-4}$ | $6.66 \times 10^{-4}$ | $4.03 \times 10^{-4}$ | $1.23 \times 10^{-4}$ |
| Rad. Basis     | $3.99 \times 10^{-4}$ | $2.70 \times 10^{-4}$ | $1.27 \times 10^{-4}$ | $1.37 \times 10^{-4}$ |
| Sim. Annealing | $1.20 \times 10^{-3}$ | $1.18 \times 10^{-4}$ | $9.01 \times 10^{-4}$ | $1.70 \times 10^{-4}$ |
| N. Fuzzy       | $1.14 \times 10^{-3}$ | $2.88 \times 10^{-4}$ | $3.42 \times 10^{-4}$ | $1.38 \times 10^{-4}$ |
| Hig. Order     | $1.21 \times 10^{-3}$ | $3.67 \times 10^{-4}$ | $5.16 \times 10^{-4}$ | $1.13 \times 10^{-4}$ |

Table 5. Comparison of mean RMS error for the different ANN algorithms considered for the study of benchmark problems.
Comparative performance ... and 2 spiral problem). It is evident from Fig. 3 and Table 5 that the Lavenberg-

Marquardt method yields a lower RMS error as compared to the standard backpropagation method. Even for the IRIS and XOR problems, where Higher Order and Neuro Fuzzy algorithms, respectively are found to yield the lowest RMS error, the performance of the Levenberg-Marquardt is always better than the remaining ANN algorithms. The reason for the superior performance of Levenberg-Marquardt is due to the fact that it is a combination of gradient decent and Gauss-Newton method which combines the advantages of the local convergence properties of the Gauss-Newton method and the global properties of gradient descent. However, the computational complexity of backpropagation is only \(O(n)\) as against \(O(n^3)\) for the Levenberg-Marquardt algorithm (where \(n\) is the total number of weights in the network).

4. Application of ANN algorithms to regression problems

Artificial neural networks have become a popular tool for approximating non-linear functions in higher dimensions. Although they are not the panacea for these type of problems, they are nevertheless recognized as a useful tool for approximating non-linear functions. Other well known methods which are conventionally used for these
problems include splines [30], additive models [31], MARS [32], hinging hyperplanes [33] and CART [34]. While none of these methods are likely to perform consistently better than the others across a wide range of problems, it is indeed a non-trivial task to develop a method that is truly effective for all types of non-linear functions. Keeping in view the superior ability of ANNs to capture non-linear behaviour of a function and its reasonably fast computation speed, we were tempted to apply the ANN as a regression tool for approximating functions like \( \cos(x) \) and a few special functions like the Gamma function, the complimentary Error function and the upper tail cumulative \( \chi^2 \)-distribution function [35].

4.1 Approximation to \( \cos(x) \)

To test the performance of the ANN algorithms as a regression analysis tool, we have first applied the ANN algorithms to a simple trigonometric function like \( y = \cos(x) \). In order to keep the output range of the network between 0 and 1, we follow the approach given in [28] where the function is changed to \( y = (\cos(2x) + 1)/3 \). The ANN configuration chosen for this problem (i.e., 1:2:1) and the number of data points used for training (=200) is again similar to that used by [28]. The training data set for this problem is synthesized by evaluating the function \( y = (\cos(2x) + 1)/3 \) at 200 randomly chosen points which are picked uniformly in the interval \([0, \pi]\) range (Fig. 4a). Additional 100 data points, following the same prescription, were also generated for testing the best ANN algorithm which produces the lowest RMS error during training. The training results obtained for all the ANN algorithms used in the present study are presented in Table 6. The results of the generalization performance of the Levenberg-Marquardt algorithm, which yields the lowest RMS error during training, is shown in Fig. 4. In this figure, we have plotted the relative error in \( y \) (defined as \( (y_{ANN} - y_{EXP}) / y_{EXP} \)) as a function of \( x \) for 100 random data points generated uniformly in the interval \([0, \pi]\). Here, for a given value of \( x \), \( y_{ANN} \) is the value predicted by the ANN and \( y_{EXP} \) is expected value of the function \( (\cos(2x) + 1)/3 \). It is evident from Fig. 4b that except for \( x \) values in the vicinity of

| Algorithm | BAC PRO | RES BAC | LAV MAR | CON GRA | RAD BAS | SIM ANN | NEU FUZ | HIG ORD |
|-----------|---------|---------|---------|---------|---------|---------|---------|---------|
| RMS Error | 9.83\times10^{-6} | 7.61\times10^{-5} | 3.29\times10^{-7} | 7.30\times10^{-6} | 4.15\times10^{-5} | 4.61\times10^{-6} | 6.71\times10^{-6} | 8.12\times10^{-7} |
| Time (s)  | 7       | 7       | 12      | 8       | 12      | 15      | 25      | 20      |

Table 6. Mean RMS error and training time of various ANN algorithms with a configuration of 1:2:1 for the \((\cos(2x) + 1)/3\) problem. The abbreviations used for different ANN algorithms are the following: BAC PRO – Backpropagation; RES BAC – Resilient Backpropagation; LAV MAR – Lavenberg-Marquardt; CON GRA – Conjugate Gradient; RAD BAS – Radial Basis; SIM ANN – Simulated Annealing; NEU FUZ – Neuro Fuzzy; HIG ORD – Higher Order.
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\[ y = \frac{\cos(2x) + 1}{3} \]

\[ \frac{\pi}{2} \text{ radians, where the function } y = \frac{\cos(2x) + 1}{3} \text{ itself becomes close to zero, the relative error in } y \text{ is in general } < 1\% \text{ for all other values of } x. \]

### 4.2 Approximation to a few special functions

In this section, we apply the ANN algorithms as a function approximation tool to few special functions like the Gamma function, the complementary Error function and the upper tail cumulative \( \chi^2 \)-distribution function. The training and test data sets for the above special functions have been generated by using the MATHEMATICA software package.

The Gamma-function (\( \Gamma(z) \)) has one argument and is defined by the following integral:

\[
\Gamma(z) = \int_0^\infty t^{z-1}e^{-t} \, dt
\]  \hspace{1cm} (2)

The approximation of the Gamma function was implemented with an ANN configuration of 1:20:1, where the one node in the input corresponds to the \( z \) value in the range 0\(<\)\( z <\)20 and the output node corresponds to \( \ln \Gamma(z) \). The purpose of using \( \ln \Gamma(z) \) instead of \( \Gamma(z) \) directly was to avoid overflow problems even at a quite modest value of \( z \). The training of the ANN algorithms has been done with \( \sim 1000 \) values and only those values of \( z \) and \( \ln \Gamma(z) \) are used for which \( \Gamma(z) < 1.2 \times 10^{17} \).
The second special function chosen by us to test the function approximation
capability of the ANN is the complimentary function, \( \text{erfc}(x) \). The complimentary
error function has one argument and is defined by the following integral:

\[
\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} \, dt
\]  

(3)

Since there is direct relationship between between the complimentary error function
and the cumulative distribution for the Gaussian distribution, we have tried
to apply the ANN algorithms for approximating the normal tail integral. The upper
tail integral, or the cumulative upper distribution function, \( Q(x) \) for Gaussian
probability distribution with argument \( x \) is defined by

\[
Q(x) = \frac{1}{\sqrt{2\pi}} \int_x^\infty e^{-t^2/2} \, dt = \frac{1}{2} \text{erfc}\left(\frac{x}{\sqrt{2}}\right)
\]  

(4)

The function approximation for the normal tail probability integral was imple-
mented with a ANN configuration of 1:20:1, where the one input node corresponds
to the \( x \) value ranging between 0 to 20 and the output node corresponds to \( \ln Q(x) \).
The values of \( Q(x) \) are in the range \( \sim 2.767 \times 10^{-89} \) to 0.5. About 1000 values of \( x \)
and (ln \( Q(x) \)) were used for training the ANN algorithms.

The third special function chosen for testing the function approximation capa-
bility of the ANN is the cumulative distribution function of the \( \chi^2 \)-probability
distribution. The chi-square distribution is one of the most widely used theoretical
probability distribution in inferential statistics, i.e. in statistical significance tests.
The best known situation in which the \( \chi^2 \)-distribution is used are the common
\( \chi^2 \)-tests for goodness of fit of an observed distribution to a theoretical one. The
\( \chi^2 \)-upper tail cumulative distribution function \( (Q(\chi^2|\nu)) \) is defined by the following
integral:

\[
Q(\chi^2|\nu) = \frac{1}{2^{\nu/2} \Gamma(\nu/2)} \int_{\chi^2}^\infty e^{-t^2/2} \nu^{\nu/2-1} \, dt ; \quad \text{for } \nu > 0, \chi^2 \geq 0
\]  

(5)

Where \( \nu \) is the degrees of freedom. The approximation of the \( \chi^2 \) upper tail cumu-
lative distribution function \( (Q(\chi^2|\nu)) \) was implemented with a ANN configuration
of 2:20:1 where the two input nodes correspond to the \( \chi^2 \) and \( \nu \) values. The output
node of the ANN represents the (ln \( Q(\chi^2|\nu) \)) value. About 1000 values with \( 1 \leq \chi^2 \)
\leq 100 and \( 1 \leq \nu \leq 100 \) were used for training the ANN algorithms. The training of
the ANN was performed with only those values of \( \chi^2 \) and \( \nu \) which yield a \( (Q(\chi^2|\nu)) \)
between \( \sim 1.757 \times 10^{-23} \) to 0.999. The results of the training regarding the mean
error for all the three special functions discussed above are presented in Table 7.

Performance of the Levenberg-Marquardt algorithm in terms of relative error in
approximating the three special functions is shown in Fig.5. A data sample of 100
values each is used for testing the approximation for the Gamma function (Fig. 5a)
and Gaussian upper tail probability integral (Fig. 5b). The corresponding data
samples used for testing the \( \chi^2 \) upper tail probability integral is 400 for 4 differ-
ent values of \( \nu \). Referring first to the approximation of the Gamma function, it is
| Algorithm                  | RMS error (Gamma Function) | RMS error (Upper tail Normal dist.) | RMS error (Upper tail $\chi^2$ dist.) |
|----------------------------|----------------------------|-------------------------------------|--------------------------------------|
| Backpropagation            | $2.25 \times 10^{-2}$      | $9.16 \times 10^{-1}$               | $2.91 \times 10^{-9}$                |
| Resilient Backprop         | $8.97 \times 10^{-2}$      | $1.51 \times 10^{-1}$               | $2.01 \times 10^{-8}$                |
| Lavenberg-Marquardt        | $1.25 \times 10^{-3}$      | $2.08 \times 10^{-3}$               | $1.72 \times 10^{-7}$                |
| Conjugate Gradient         | $5.01 \times 10^{-4}$      | $2.14 \times 10^{-2}$               | $4.87 \times 10^{-2}$                |
| Radial Basis               | $5.68 \times 10^{-4}$      | $7.33 \times 10^{-3}$               | $5.71 \times 10^{-2}$                |
| Simulated Annealing        | $5.23 \times 10^{-3}$      | $1.52 \times 10^{-2}$               | $4.20 \times 10^{-3}$                |
| Neuro-Fuzzy                | $4.12 \times 10^{-2}$      | $8.96 \times 10^{-2}$               | $1.16 \times 10^{-3}$                |
| Higher-Order               | $7.16 \times 10^{-3}$      | $9.86 \times 10^{-3}$               | $6.42 \times 10^{-4}$                |

Table 7. Mean RMS Error of various ANN algorithms with a configuration of 1:20:1 for function approximation of 3 special functions.

evident from Fig. 5a that the relative error in $\Gamma(z)$ is $<0.25\%$ for $2<z<20$. However, for $0<z<2$, the relative error increases significantly to $>\pm0.5\%$. Regarding the approximation of the Gaussian upper tail probability integral, the relative error in $Q(x)$ is within $\pm0.3\%$ for all values of $x$ in the range 0 to 20. The results for the approximation of $\chi^2$ upper tail probability integral (Fig.5c and Fig.5d) indicate that the relative error in $Q(\chi^2|\nu)$ is in general significantly more than that of the other 2 special functions possibly because of the presence of 2 input parameters ($\chi^2$ and $\nu$) instead of 1 as in the case of other two special functions. Keeping in view the fact that these special functions are being approximated over a very wide dynamic range ($\sim 0.88 \times 10^{17}$ for Gamma function, $\sim 2.7 \times 10^{-89}$ to 0.5 for Gaussian upper tail integral and $\sim 1.8 \times 10^{-23}$ to 0.999 for $\chi^2$ upper tail integral), we believe that the results obtained are rather encouraging. However, there is a strong need to further improve these results if one demands that approximation using ANN algorithms should yield a performance which is comparable to that of the conventional methods using numerical algorithms or other ad hoc approximations. Furthermore, keeping in view the widespread use of these functions and also their highly non-linear behaviour with a very wide dynamic range, we feel that these functions can be considered as standard benchmark problems for function approximation studies using ANNs.

5. Discussion and conclusion

Artificial neural network algorithms have been applied to a variety of problems in various diverse areas of physics, biology, medicine, computer research etc. The main aim of most of these studies has been to use ANN-based algorithms (generally standard backpropagation) as an alternative method to conventional analysis for achieving better results. While comparative performance of some ANN algorithms like standard backpropagation, fuzzy logic, genetic algorithms, fractals etc., has been studied for various applications, a rigorous intercomparison of some of powerful algorithms (e.g. the ones studied in this work) is still missing from the
literature. The primary aim of this work has been to provide a rigorous comparative study of various powerful algorithms, by first applying them to standard benchmark problems and then applying them as a regression tool for approximating functions like \( \cos(x) \) and a few special functions. Our results suggest that while Levenberg-Marquardt algorithm yields the lowest RMS error for the N-bit Parity and the Two Spiral problems, Higher Order Neurons algorithm gives the best results for the IRIS data problem. The best results for the XOR problem are obtained with the Neuro Fuzzy algorithm. It is worth mentioning here that benchmark problems (IRIS, XOR/N-Bit Parity and 2-Spiral) have been also studied by numerous other workers. For example, using a 2:2:1 configuration for the XOR problem, Wang [28] has reported that one can achieve an accuracy of \( \sim 80\% \) with \( \sim 5000 \) epochs of training. Other benchmark problems like Parity and \( \cos(x) \) has been also studied by the same author, but comparison is done only for the backpropagation and simulated annealing techniques. Likewise, the 2-Spiral problem has been studied by several workers using different algorithms like vanilla backpropagation [36] with configuration of 2:5:5:1, generalised regression model [37], vector quantization method [38], input coding scheme [39]. Complicated ANN configurations like 2:20:20:1 for the 2-Spiral problem with 50000 training epochs and 4:4:2:1 for the IRIS problem with 30000 training epochs has also been attempted by Lee [40] for achieving reasonably accurate results for these benchmark problems.

Regarding application of neural network algorithms for solving regression problems, such as evaluation of special functions like the Gamma function, the complementary Error function and the upper tail cumulative \( \chi^2 \)-distribution function, we
believe that such an attempt has been made in this work for the first time. The results obtained in this work indicate that, among all the ANN algorithms used in the present study, Levenberg-Marquardt algorithm yields the best results. Conventionally, two groups of approximations are found in the literature which are used for calculating these special functions. One group consists of standard numerical algorithms which, at least in theory, allow computation of the above integral to arbitrarily high precision. However, computation using these numerical algorithms requires massive computation. The second group consists of so called “ad hoc approximations” which require only a few carefully chosen numeric constants. Importantly, a serious limitation of most of the approximations in both the groups is that they are designed to work in a predefined range of input parameter values and the accuracy of the approximation rapidly deteriorates when the input parameters takes a value outside the predefined range.

In order to appreciate the complexity of evaluating the special functions studied in this paper, it is worth discussing here some of important approximations used for these functions. A well known method for calculating the gamma function is the so called Lanczos approximation [41] which computes the value of $\Gamma(z)$ any positive real argument with a high level of accuracy. Likewise, a compilation of useful approximations used for evaluating the upper tail integrals for the Gaussian and $\chi^2$ distributions can be found in [42] and [43], respectively.

Although the comparative performance of different ANN algorithms is in general problem dependent, we feel that the study undertaken in this paper does give an insight into the power of various powerful ANN algorithms. Since for real world problems it is not an easy task to identify the most suitable ANN algorithm by just having a look at the problem, our results suggest that while investigating the comparative performance of other ANN algorithm, the Levenberg-Marquardt algorithm deserves a serious consideration and cannot be rejected outright because of its training time overheads.

6. Acknowledgements

We would like to thank all the members of the BIKAS (BARC - IIT Kanpur ANN Simulator; BRNS- 2000/36/5-B) collaboration for useful discussions and suggestions. We would also like to thank the anonymous referee his valuable comments and suggestions for improving the paper.

References

[1] J. Hertz et al., Neural Computation, Addison-Wesley Publishing, Santa Fe (1991).
[2] M.Caudill et al., Neural Networks-Computer explorations 1 2 (1992).
[3] A.S. Miller., Vistas in astronomy 36 141 (1993).
[4] R.Tagliaferri et al., Neural Networks 16 297 (2003).
[5] R.Gupta et al., Automated Data Analysis in Astronomy, Narosa Publishing (2002).
[6] H.P.Singh et al., MNRAS 295 312 (1998).
[7] H.P.Singh et al., Publ.Astron. Soc. Japan 58 177 (2006).
[8] R.Gupta et al., Astron. Phys. Jour. Sci 152n2 201 (2004).
[9] M. Bazarghan et al., *Astro. Phys. Sp. Sci* **315** 201 (2008).
[10] A.Bora et al., *MNRAS* **384** 827 (2008).
[11] A.Bora et al., *New Astronomy* **14** 649 (2009).
[12] M.D. Christopher et al., *World Congress on Computational Intelligence IEEE* 1213 (1994).
[13] R.K.Bock et al., *Nucl. Instr and Meth. A* **516** 511 (2004).
[14] R. Sinkus, *Nucl. Instr and Meth. A* **361** 290 (1995).
[15] D.E. Rumelhart et al., *Nature* **323** 533 (1986).
[16] M. Reidmiller et al., *Proc. Int. Conf. Neural Networks ICNN* 586 (1993).
[17] McInerney et al., *Technical Report No. CS89-157* (1989).
[18] R.K. Bock et al., *Nucl. Instr and Meth. A* **516** 511 (2004).
[19] W.H. Press et al., *Numerical Recipes in C++* 668 (2002).
[20] S. Chen et al., *IEEE Trans. Neural Networks* **2** 302 (1991).
[21] S. Kirkpatrick et al., *Science* **220** 671 (1983).
[22] N. Metropolis et al., *Journal of Chemical Physics* **21** 1087 (1953).
[23] C.L. Giles et al., *Applied Optics* **26** 4972 (1987).
[24] V. Gorini et al., *Recurrent Fuzzy systems* 3rd International Conference on Fuzzy systems 193 (1994).
[25] C.T. Lin et al., *A Neuro-fuzzy Synergism to intelligent system*, Prentice Hall, N. York (1996).
[26] V.K. Dhar et al., *Nucl. Instr. and Meth. A* **606** 795 (2009).
[27] R.A. Fisher et al., *Annals of Eugenics* **7** 179 (1936).
[28] X. Wang et al., *Trans. of IEEJ* **124**, 842 (2004).
[29] K. Lang et al., *Proc. Connectionist models*, Morgan Kaufmann Publishers Inc: 52 (1998).
[30] D. Barry, *Nonparametric Bayesian Regression*, Ann. Statist. **14** 934 (1986).
[31] T. Hastie et al., *Statist. Science* **1** 297 (1986).
[32] J.H. Friedman, Tech. Rep. 102, *Laboratory for Computational Statistics, Dept. of Statistics, Stanford University* (1990).
[33] L. Breiman, *IEEE Trans. Information Theory* **39** 999 (1993).
[34] L. Breiman et al., *Classification and Regression Trees*, Wadsworth and Brooks, Pacific Grove CA, (1984).
[35] M. Abramovitz and I.A. Stegun, *Handbook of Mathematical Functions*, US Government printing office Washington D.C (1972).
[36] G. A. Carpenter et al., *IEEE Trans. on Neural Networks* **3** 698 (1992).
[37] E.W.M. Lee et al., *Advanced Engineering Informatics* **20** 213 (2006).
[38] T. Denoeux et al., *Neural Network* **6** 351 (1993).
[39] J.C. Jia et al., *Electronic Letters* **31** 1267 (1995).
[40] J. Lee, *Proc. International Joint Conference on Neural Networks* **1** 410 (2003).
[41] C. Lanczos, SIAM Journal on Numerical Analysis, **1** 86 (1964).
[42] W. Bryc, *Appl. Math. Comput.* **127** 365 (2002).
[43] L. Canal, *Computational Statistics and Data Analysis* **48** 803 (2005).