2006

Models for calculating confidence intervals for neural networks

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Models for Calculating Confidence Intervals for Neural Networks

Ashutosh R. Nandeshwar

**Thesis submitted to the
College of Engineering and Mineral Resources
at West Virginia University
in partial fulfillment of the requirements
for the degree of**

Master of Science

in

Industrial Engineering

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ABSTRACT

This research focused on coding and analyzing existing models to calculate confidence intervals on the results of neural networks. The three techniques for determining confidence intervals determination were the non-linear regression, the bootstrapping estimation, and the maximum likelihood estimation. Confidence intervals for non-linear regression, bootstrap estimation, and maximum likelihood were coded in Visual Basic. The neural network used the backpropagation algorithm with an input layer, one hidden layer and an output layer with one unit. The hidden layer had a logistic or binary sigmoidal activation function and the output layer had a linear activation function. These techniques were tested on various data sets with and without additional noise. Out of eight cases studied, non-linear regression and bootstrapping each had the four lowest values for the average coverage probability minus the nominal probability. For the average coverage probabilities minus the nominal probabilities of all data sets, the bootstrapping estimation obtained the lowest values. The ranges and standard deviations of the coverage probabilities over 15 simulations for the three techniques were computed, and it was observed that the non-linear regression obtained consistent results with the least range and standard deviation, and bootstrapping had the largest ranges and standard deviations. The bootstrapping estimation technique gave a slightly better average coverage probability (CP) minus nominal values than the non-linear regression method, but it had considerably more variation in individual simulations. The maximum likelihood estimation had the poorest results with respect to the average CP minus nominal values.

Acknowledgments

I would like to express my sincere gratitude towards Dr. R. C. Creese for selecting me as his graduate research assistant and for his constant guidance in everything. He has been a great inspiration and helped me to see the things with a total different perspective. I don't think it would have been possible to complete my masters this effectively had I not worked under his supervision. Thanks Dr. Creese.

I would also like to thank Dr. S. D. Mohaghegh, for his excellent idea of this research, and his constant support and guidance. His keen interest in this topic has made this thesis possible. I would like to extend my thanks towards Dr. B. Gopalakrishnan for his time and superb support throughout my masters.

I am especially thankful to Dr. R. Chandran of the Plant and Social Sciences Department for his constant motivation and guidance on both professional and personal fronts. I am also thankful to all of my friends here in the U.S.A and in India for showing me the correct path through tough times.

Above all, I would like to thank my parents and family for everything. Words cannot suffice to express what they have done for me.

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Table of Nomenclature

Notations: Also refer Figure 1.3

n	Number of input units.
nob	Number of observations or training pairs.
nh	Number of hidden layer neurons.
noy	Number of output layer neurons.
x_i	Activations of units X_i : For input units X_i , x_i = input signal;
t_k	Target values.
w_{ij}	Weights between the input layer and the hidden layer; w_{0j} Bias term applied to the hidden layer.
v_{jk}	Weights between the hidden layer and the output layer; v_{0k} Bias term applied to the output layer. <i>Note</i> : Bias terms are weights to the connections whose output is always 1.
α	Learning rate.
δ_j, δ_k	Part of error correction weight adjustment

1 Introduction

1.1 Neural Networks

The simple application of Artificial Neural Networks (ANNs) has made them one of the most widespread techniques to predict, forecast, or classify data. Artificial neural networks are also known as neural networks. ANN's capability to detect a pattern or relationship in the given input data is much faster and less labor intensive than conventional methods. Therefore, ANNs are being used as an alternative to traditional models for a range of applications, such as, medical [1, 35], cost estimation [2], ecology [3], coastal research [36], forecasting [41].

1.1.1 What is an Artificial Neural Network?

An artificial neural network (ANN) is an information-processing model that is influenced and motivated by the way the brain works. An ANN is an attempt to represent structure of the brain, which is composed of a large number of highly interconnected processing elements or neurons. Scientists have learned that a brain learns by adjusting the synaptic connections between the neurons. There is a visible similarity between people and ANN, for example, people learn by example and so does ANN. ANNs also adjust the connections between the neurons for learning. If trained with preprocessed data and a proper structure, ANNs may display the capability of generalizing the data and producing good results for unseen data.

There is no universally accepted definition of an ANN, but Online Encyclopædia Britannica© [4] defines it as:

“Computer architecture in which a number of processors are interconnected in a manner suggestive of the connections between neurons in a human brain and which is able to learn by a process of trial and error -- called also neural network.”

1.1.2 Biological Neural Network

A biological neuron has three components that are important in understanding an artificial neural net: *dendrites*, *soma*, and *axon* as mentioned by Laurene Fausett [5]. The input signals are electrical impulses that are transmitted across a synaptic gap. The many dendrites present receive signals from neurons. This incoming information is summed up by soma and then delivered along the neuron's axon to the dendrites at its end. The information will again be passed if the stimulation caused by the signals has exceeded a certain threshold. If a simulation

fails to cross the threshold, it would not be passed further. A biological neuron can be represented as shown in Figure 1.1.

Figure 1.1 A Biological Neuron

1.1.3 Historical Background

With the arrival of modern electronics and computers, attempts to replicate the thinking process was inevitable. Warren McCulloch and Walter Pitts were first to recognize that combining simple neurons into neural system might increase computational power [6, 7]. McCulloch and Pitts developed a neural network for an electric circuit in 1943. Later in their research they dealt with translation and rotation invariant pattern recognition.

In 1949, Donald Hebb designed the first learning law for ANNs and wrote the book *Organization of Behavior* [7]. He presented a theory that the strength of the connection between two neurons should be increased every time they were used or active. Around 1958, John von Newumann, the “father of modern computing,” suggested using telegraph relays or vacuum tubes to emulate simple neuron functions. Soon after that Frank Rosenblatt started working on a class of ANNs called perceptrons. The perceptron was found to be useful in classifying inputs into one class. It is the oldest neural network still in use.

In 1969, Minsky and Papert, published a book titled *Perceptrons*, in which they proved that perceptron was limited and unable to solve the XOR (exclusive-or) problem. The XOR is not linearly separable, while OR and AND are linearly separable. The truth table for XOR is given in Table 1.1. In 1982, John Hopfield developed a number of neural networks based on fixed weights, which brought popular attention to neural nets. Also, optical neural nets by Farhat, Psaltis et al. [1985], and VLSI implementations by Sivilatti, Mahowald, and Mead [1987] were

developed in the 1990s. Faster computational abilities and superior hardware are the reasons for renewed interest in ANN, and today, discussions on ANNs are commonplace.

Table 1.1 The Truth Table for Exclusive-OR (XOR)

a	b	a XOR b
0	0	0
0	1	1
1	0	1
1	1	0

1.1.4 Architecture of a Feed-forward Network

A feed-forward ANN is a straightforward network that sends signals from one layer to another layer, which means the output of one layer does not affect the same layer. The first layer receives the input, and each neuron in a layer is fully connected to all other neurons in the following layer. The output of the last layer is the output of the network. All layers between the input and output layers are called hidden layers. It is a common practice to use either one or two hidden layers, and a single hidden layer was selected as the problems investigated were not complex. A feed forward network with a configuration as one input layer with three inputs, one hidden layer with two nodes, and one output layer with a single output (3-2-1) can be represented as shown in Figure 1.2.

Figure 1.2 Feed-forward Network (3-2-1) Architecture

Figure 1.2 represents a three-two-one feed-forward network structure with three input neurons, two hidden layer neurons, and one output layer neuron. The input layer receives signals as X_1 , X_2 , and X_3 . Random or fixed weights are assigned to the connections between all the neurons in all the layers. The weight matrices are shown in Equation (1). Matrix W denotes the weights between the input layer and the hidden layer, and matrix V denotes the weights between the hidden layer and the output layer.

$$W = \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \\ w_{31} & w_{32} \end{bmatrix}; V = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \quad (1)$$

Matrix W is multiplied with the input signals and then summed up in the hidden layer. An activation function, given in Equation (2), is applied to this summation to give new input signals for the next layer:

$$y = f(x) \quad (2)$$

where,

y = output of the function,

$f()$ = linear identity or non-linear function, and

x = input to the function.

This new information is again fed-forward and multiplied by the weights between hidden and output layer, i.e., matrix V . This multiplied signal is again sent through the activation function to give the output or result of the network. A feed-forward network for one hidden layer is depicted in Figure 1.3.

n Number of input units
 nh Number of hidden layer neurons
 x_i Activation of units X_i
 For input units X_i
 x_i = input signal
 w_{ij} Weights between the input layer and the hidden layer
 v_{jk} Weights between the hidden layer and the output layer
 z_in_j Input to the hidden layer:

$$z_in_j = \sum_{i=1}^n w_{ij} \cdot x_i$$

z_out_j Output of the hidden neurons:

$$z_out_j = f(z_in_j)$$

y_in_k Input to the output layer:

$$y_in_k = \sum_{j=1}^{nh} v_{jk} \cdot z_out_j$$

Note: If there is only one output unit, then subscript k is removed

y_out_k Output of the network:

$$y_out_k = f(y_in_k)$$

Figure 1.3 A Feed-forward Network with One Hidden Layer [5]

1.1.5 Activation Function

Activation functions are needed to introduce nonlinearity into the network. Without nonlinearity, hidden units would not be and more powerful than just plain perceptrons (which do not have any hidden units, just input and output units). A linear function of linear functions is always a linear function. However, it is the capability to represent nonlinear functions that makes multilayer networks so powerful. For backpropagation learning, the activation function must be differentiable, and it is helpful if the function is bounded.

(i) Identity Activation Function

For the input layer identity, activation function is used as given in Equation (3) and shown in Figure 1.4. It is a common practice to use the same activation function for all the neurons in a layer. An identity activation function is typically used for the output and input layer.

$$f(x) = x \text{ for all } x \quad (3)$$

Figure 1.4 Identity Activation Function

(ii) *Binary Step Function*

The binary step function is also known as threshold function. The output of this function is either bipolar (1 or -1) or binary (1 or 0). This function applies a simple rule, that is, if the input exceeds its threshold, then the output is positive, otherwise it is negative. The binary step function is given in Equation (4) and depicted in Figure 1.5.

$$f(x) = \begin{cases} 1 & \text{if } x \geq \theta; \\ 0 & \text{if } x < \theta. \end{cases} \quad (4)$$

Figure 1.5 Binary Step Activation Function

(iii) *Binary Sigmoid Function*

This function is also called logistic function with an output range from zero to one. This is the most common activation function used and this function was used for the hidden layer. It is in the form given in Equation (5) and is illustrated in Figure 1.6.

$$f(x) = \frac{1}{1 + e^{(-x)}} \quad (5)$$

Figure 1.6 Logistic Activation Function

(iv) *Bipolar Sigmoid Function*

The most common form of bipolar sigmoid function is given in Equation (6) and is depicted in Figure 1.7. The range commonly used is -1 to 1 and therefore it is called a bipolar sigmoid function.

$$f(x) = \frac{1 - e^{-x}}{1 + e^{-x}} \quad (6)$$

Figure 1.7 Bipolar Activation Function

(v) *Hyperbolic Tangent Function*

TanH has a similar sigmoid shape to the logistic function, but values are spread through the interval $[-1, 1]$, rather than $[0, 1]$. This function is given by Equation (7), and it takes the shape shown in Figure 1.8.

$$f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} \quad (7)$$

Figure 1.8 Hyperbolic Tangent (tanh) Function

The most common of activation function used in the construction of ANNs for the hidden layer is the binary sigmoid function and tanh function. With sigmoid units, a small change in the weights will usually produce a change in the outputs, which makes it possible to tell whether that change in the weights is good or bad. Also, the sigmoid function is global in the sense that it

divides the feature space into two halves, one where the response is approaching one and another where it is approaching zero. For the output layer, usually a linear function is used [5].

1.1.6 Network Learning

The brain updates itself whenever it receives a new pattern. This updating helps the brain to solve a problem related to that pattern. ANNs are developed to make an attempt to imitate the brain which is the reason ANNs are sometimes called machine-learning algorithms [8].

However, in the case of ANNs, updating occurs only for the weights used in the network and not the whole network. An ANN learns new patterns by adjusting these weights connected between all the layers.

The learning procedure, also known as a training algorithm, and the architecture of an ANN determine its learning ability. The architecture and the training algorithm may vary from requirement to requirement but mostly they fall in two major categories – supervised (reinforcement learning) and unsupervised learning.

(i) *Supervised (Reinforcement Learning)*

In supervised learning, the learning rule is provided with the training set consisting of an input and output or target sample set as given in Equation (8). The inputs are applied to the network to calculate the network outputs, which are then compared to the targets. After completion of that step, the learning rule is used to adjust the weights of the network to decrease the error between the network outputs and the targets:

$$\{X_1, T_1\}, \{X_2, T_2\}, \{X_3, T_3\}, \dots, \{X_{nob}, T_{nob}\} \quad (8)$$

where,

X = input matrix,

T = target or output matrix, and

nob = number of observation or samples.

(ii) *Unsupervised Learning*

In this approach, no sample targets or outputs are provided to the network against which the network can measure its performance for given inputs. The network modifies the weights in response to network inputs only. As is mentioned in the Matlab neural network

toolbox online documentation [9], the network categorizes the input patterns into a finite number of classes.

As stated in the online documentation on neural networks by West Virginia University [10], the Hopfield net, the Hamming net, the Bidirectional Associative Memory (BAM), the Delta rule, and the backpropagation algorithm are considered to be supervised learning networks. The Adaptive Resonance Theory (ART) by Carpenter and Grossberg and Kohonen's self-organizing maps are unsupervised learning networks [10].

The backpropagation algorithm is the most known and widely used learning procedure. Two reasons for its popularity in the neural network fraternity are the robustness and stability of the network. There is a vast literature available on the backpropagation algorithm and the backpropagation algorithm was used as the learning procedure.

1.1.7 Backpropagation Algorithm

The limitation to solve a wide variety of problems using single-layer neural networks was an important factor in the decrease of interests in neural networks in the 1970s. The discovery of the backpropagation or the generalized delta rule training methods for multi-layer networks by D. E. Rumelhart, G. E. Hinton, and R. J. Williams [11] helped rejuvenate neural network interest.

The term backpropagation refers to the manner in which a backward pass of error to each internal neuron within the network is used to calculate weight gradients for that neuron. The learning of the network is accomplished by alternately propagating forward the activations and propagating backward the instantaneous errors. The network weights are moved along the negative of the gradient of the performance function.

The backpropagation algorithm is shown in Figure 1.9 and it consists of these important steps:

- (i) initializing of the weights,
- (ii) executing the feed-forward network,
- (iii) back propagating of the error and adjustment of the weights, and
- (iv) repeating of these steps until the difference between the target and the network output values is within an acceptable range.

Algorithm:

Step 0. Initialize weights to small random values.

Step 1. Repeat steps 2-8 until the stopping condition is false.

Step 2. Repeat steps 3-7 for $m=1$ to nob :

Step 3. Each hidden neuron ($Z_j, j=1, \dots, nh$) sums its weighted input signals:

$$z_in_j = w_{0j} + \sum_{i=1}^n w_{ij}.x_i.$$

Output signal of the hidden neurons:

$$z_out_j = f(z_in_j).$$

Step 4. Each output neuron ($Y_k, k=1, \dots, noy$) sums its weighted input signals:

$$y_in_k = v_{0k} + \sum_{j=1}^{nh} v_{jk}.z_out_j.$$

Note: If there is only one output unit then subscript k is removed

Output of the network:

$$y_out_k = f(y_in_k).$$

Step 5. Each output layer neuron computes its error information:

$\delta_k = (t_k - y_out_k).f'(y_in_k)$, then it calculates its weight correction term:

$\Delta v_{jk} = \alpha.\delta_k.z_out_j$, then it calculates its bias correction term:

$\Delta v_{0k} = \alpha.\delta_k$, and then δ_k is sent back to the hidden layer.

Step 6. Each hidden neuron sums its delta inputs:

$\delta_in_j = \sum_{k=1}^{noy} \delta_k.v_{jk}$, then it calculates its error information term:

$\delta_j = \delta_in_j.f'(z_in_j)$, then it calculates its weight correction term:

$\Delta w_{ij} = \alpha.\delta_j.x_i$, and then it calculates its bias correction term:

$\Delta w_{0j} = \alpha.\delta_j$.

Step 7. Each hidden layer neuron updates its bias and weights:

$$w_{ij}(new) = w_{ij}(old) + \Delta w_{ij}$$

Each output layer neuron updates its bias and weights:

$$v_{jk}(new) = v_{jk}(old) + \Delta v_{jk}$$

Step 8. Check the stopping condition.

Figure 1.9 Steps of the Backpropagation Algorithm [5]

The derivation of the learning rule is adopted from Laurene Fausett's book, *Fundamentals of Neural Networks* [7] given as follows. The error to be minimized is

$E = 0.5 \sum_k [t_k - y_{out_k}]^2$. By using the chain rule, we have

$$\begin{aligned} \frac{\partial E}{\partial V_{jk}} &= \frac{\partial}{\partial V_{jk}} 0.5 \sum_k [t_k - y_{out_k}]^2 = \frac{\partial}{\partial V_{jk}} 0.5 \sum_k [t_k - f(y_{in_k})]^2 \\ &= -[t_k - y_{out_k}] \frac{\partial}{\partial V_{jk}} f(y_{in_k}) = -[t_k - y_{out_k}] f'(y_{in_k}) \frac{\partial}{\partial V_{jk}} f(y_{in_k}) \\ &= -[t_k - y_{out_k}] f'(y_{in_k}) z_{out_j} \end{aligned}$$

Define: $\delta_k = [t_k - y_{out_k}] f'(y_{in_k})$

$$\begin{aligned} \frac{\partial E}{\partial W_{ij}} &= - \sum_k [t_k - y_{out_k}] \frac{\partial}{\partial W_{ij}} y_{out_k} = - \sum_k [t_k - y_{out_k}] f'(y_{in_k}) \frac{\partial}{\partial W_{ij}} y_{in_k} \\ &= - \sum_k \delta_k V_{jk} \frac{\partial}{\partial W_{ij}} z_{out_j} = - \sum_k \delta_k V_{jk} f'(z_{in_j}) [x_i] \end{aligned}$$

Define: $\delta_j = \sum_k \delta_k V_{jk} f'(z_{in_j})$

Using this chain rule the gradients or partial derivatives of error with respect to the weights were found. With this gradient the weight correction terms were found and the old weights were updated. This process of finding error information terms and updating of weights is called as backpropagation.

1.2 Need of Confidence Intervals for Neural Networks

It is a common perception that ANN is a “black box” that is able to predict an output pattern when it recognizes the input pattern. The desired output or result is entirely based on the behavior of the network, neither the user is ever sure of the results. Nevertheless, ANNs are used widely because of their capability of picking random or sudden changes in the pattern. Results of the networks suffer, however from uncertainty due to improper preparation of data and design of a neural network. Unfortunately, ANN models do not provide assurance, accuracy, or reliability of their output.

D. Lowe and K. Zapart [28] stated that the application of neural network approaches to the real world problems has now approached to a situation where they are being considered for the functionality of key embedded components in safety-critical and mission-critical systems.

They also noted that in critical situations the ability of ANNs to classify, forecast, or regress was not adequate. The ANNs must quantify the minimum additional knowledge to produce confidence intervals, which are necessary to quantify the accuracy or reliability of the neural network performance.

The ability to estimate the uncertainty of predictions is important for many reasons. For example, in process control, when designing controllers and verifying their performance, it is useful to know the accuracy of the model used by the controller. Model accuracy is an important factor for model selection. J. Schumann et. al. [27] mention testing the practical feasibility of a neural network-based controller for aircraft at NASA, for manned F-15 active aircraft based at Dryden Flight Research Center, as well as for a C-17 transport aircraft. On-line trained neural networks within the flight controller can adapt to sudden damage of a control surface to prevent fatal accidents.

J. Schumann, P. Gupta, and S. Nelson [27] states that the main criticism against inclusion of on-line trained neural networks in safety-critical applications has been their non-determinism. Therefore, it is very important that the predictions of the neural networks provide some information on the reliability and the confidence intervals on the output of the neural networks and can provide a precision check.

S. L. Ho et. al. [41] used ANNs for time-series forecasting of the solder paste deposition process, and they constructed confidence intervals on the output of the neural networks using non-linear regression. They noted that process control using neural networks with confidence bounds provided more quality information for better decision making and continuous improvement.

1.2.1 Confidence Interval

A confidence interval is a range of values that has a specified probability of containing the parameter being estimated from a given set of sample data as given in V. J. Easton et. al. [28]. The width of the confidence interval gives us some idea of how uncertain we are about the estimated or unknown parameter. A wide interval may indicate that more data should be collected before anything very definite can be said about the parameter.

The most widely used confidence intervals are the 95% and 99% confidence intervals, which have 0.95 and 0.99 probabilities of containing the parameter respectively. If the user

selects a 95% confidence level, which can also be stated as $(1 - \alpha)$ where α is acceptable risk of being wrong and equals to 0.05, confidence level then it would mean that if the same population is sampled on numerous occasions and confidence interval estimates are made on each occasion, the resulting intervals would bracket the true population parameter in approximately 95% of the cases. A confidence interval has the specified probability of containing the parameter if the sample data on which it is based is the only information available about the value of the parameter.

1.3 Research Method

This research was carried out as given in the following steps:

- (i) *Literature search*: There are four main techniques available to compute the confidence intervals: non-linear regression (NLR), bootstrapping (boot), maximum likelihood estimation (MLE), and Bayesian estimation. Only NLR, bootstrap, and MLE were coded in a programming language and analyzed, as Bayesian estimation was too complex to be coded.
- (ii) *Develop a neural network model*: A basic multi-layer perceptron feed-forward network with the backpropagation algorithm for weight adjustment was developed. A model was developed that would train and test the given data. The output neuron or the output unit and the number of hidden layers were limited to one.
- (iii) *Coding confidence interval models*: Three different models, NLR, bootstrap, and MLE, were coded in Visual Basic programming language to provide good user interface.
- (iv) *Detailed analysis*: These models were tested and analyzed on different data sets. Additional noise was added to test the models for errors other than the errors in the original data.
- (v) *Conclusion*: Results on the different options for calculating confidence intervals on neural networks with reliability were presented.

2 Literature Review

2.1 Introduction

A literature search was done to analyze the existing techniques for computing the confidence intervals of the output of neural networks. *Fundamentals of Neural Networks* by Laurene Fausett [5, 7] was studied to learn more about neural networks and their applications. *Computer Systems That Learn* by S. M. Weiss and C. A. Kulikowski [12] gave a mathematical view on neural networks. Papers were collected from the *IEEE Transactions on Neural Networks*, ScienceDirect® by Elsevier, and various authors' personal WebPages.

The techniques available to compute confidence intervals on neural networks were: non-linear regression (NLR), bootstrapping, the maximum-likelihood estimation (MLE), multilinear regression (MLR), and the Bayesian inference. However, the application of the MLR technique was use only once [37], therefore, it was not included in this research. The Bayesian inference estimation technique was complex and excluded from the research. The results for the base case were compared with linear regression, non-linear regression, bootstrapping, and the maximum-likelihood is

2.1.1 Non-linear Regression (NLR)

G. Chryssolouris, M. Lee, and A. Ramsey [16] were among the first to derive an estimate of a neural network's accuracy as an empirical modeling tool. They defined confidence interval as : “*a prediction of the range of the output of a model where the actual value exists*”. A brief background of calculating confidence interval for parameterized models with and without noisy data was presented. They have extended the confidence interval calculation for neural networks and also provided an example of the method. These data were not available for this research. The authors assumed that the error was normally distributed. The authors successfully observed that 85% of predictions by the neural network were within confidence intervals.

L. H. Ungar, R. D. D. Veaux, and E. Rosengarten [17] compared the ability of non-linear regression and Bayesian estimation to provide accurate confidence intervals. The authors also examined the coverage probabilities of the confidence intervals with computational costs and practical implementation. The paper focused on a feed-forward network and backpropagation algorithm with sigmoidal function as its activation function. This paper presented a comparison of non-linear regression and the Bayesian estimation techniques on the data generated using sine

wave function with Gaussian noise with standard deviation of one, and a function as given in Equation (9). The authors concluded that the Bayesian method of model estimation should be tried on more data before it can be trusted. The results from this paper of actual coverage probabilities (CP) for nominal 95% confidence intervals on 1000 test data points are given in Table 2.1. CP is the probability that the target (true value) of an input pattern lies within the confidence intervals. The observed mean CP should be near the “nominal” value of confidence level if the confidence estimation technique is performing well. The mean CP is a measure of global performance, i.e., the average quality of the uncertainty estimate. The CP can be calculated by determining whether the true parameter values lie within the confidence regions and confidence intervals.

$$y = (10\sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5 + \varepsilon) / 25 \quad (9)$$

Table 2.1 Actual Coverage Probabilities for Nominal 95% Confidence Intervals- L. H. Ungar et al [17]

	Non-linear Regression		Bayesian	
	CP	CP-95	CP	CP-95
Sine wave	98.8	3.8	98.4	3.4
Equation (9)	100.0	5.0	100.0	5.00

R. Shao, E. B. Martin, J. Zhang, and A. J. Morris [14] discuss and analyze non-linear regression as a tool to calculate confidence intervals. However, the authors are critical of the distribution of the training data used by G. Chryssolouris, M. Lee, and A. Ramsey. They present a new, or as they have termed it “a novel,” method of computing confidence bounds on predictions from a feed-forward neural network with determined data structure. The authors [14] state that “*this novel approach not only calculates the accuracy of the neural network but it also incorporates the influence of the training data density.*”

R.D. De Veaux, J.Schumi, J. Schweinsberg, and L.H. Ungar [13] state that it is possible to reduce the number of parameters needed for the calculation of confidence intervals by stopping the training algorithm prior to convergence of the network. The authors also claimed that the non-linear regression method for the calculation of confidence intervals is promising in theory, but it works poorly in practice. The authors presented a new technique of using weight

decay, and they conclude by noting that using a weight decay constant as a regularizer, accurate function approximations are obtained.

L. Yang, T. Kavli, M. Carlin, S. Clausen, and P. F. M. de Groot [15] used non-linear regression and analyzed it over a 10-dimensional function with changing parameters, such as level of noise, the size of the training set, the number of training epochs, and by adding irrelevant inputs. They developed a method to estimate the bias of the coverage of confidence intervals. This bias then can be applied to correct the confidence bounds. However, they agreed that the standard non-linear regression confidence bound estimation algorithm gave satisfactory results.

S. L. Ho et. al. [41] applied a non-linear regression technique to estimate confidence bounds for time-series forecasting of a solder paste deposition process using neural networks. They ran simulation tests for two data sets with different nominal values (95% and 90%), and they concluded that these confidence intervals gave satisfactory coverage percentages as compared to the nominal confidence levels.

The original algorithm for non-linear regression as a confidence interval estimator [16, 19, 38-41] assumes that the distribution of the error for the neural network is normal. Neural networks can be considered as a non-linear system given as $f(x; \theta^*)$ with output y , where x is the set of inputs, θ^* represents the true values of the set of parameters, and θ for the function that models the system. The error ε associated with the function in modeling the system is assumed to be independently and identically distributed with variance σ^2 , where the distribution has the form $N(0, \sigma^2)$. With n observations, Equation (10) represents the system:

$$y_i = f(x_i; \theta^*) + \varepsilon_i, \quad i=1, 2, \dots, n. \quad (10)$$

The least-squares estimate of θ^* is $\hat{\theta}$, which is obtained by minimizing the error function given in Equation (11). The backpropagation algorithm is used to minimize error function in neural networks. The predicted output from the model is $\hat{y}_i$, which can be represented in Equation (12).

$$S(\theta) = \sum_{i=1}^n [y_i - f(x_i; \theta)]^2 \quad (11)$$

$$\hat{y}_i = f(x_i; \hat{\theta}) \quad (12)$$

If the model is able to predict values close to the actual values, then $\hat{\theta}$ is close to the true value of the set of parameters θ^* . A Taylor expansion is used to approximate $f(x; \hat{\theta})$ in terms of $f(x; \theta^*)$. This expansion is given in Equation (13).

$$f(x_i; \hat{\theta}) \approx f(x_i; \theta^*) + f_0^T \cdot (\hat{\theta} - \theta^*) \quad (13)$$

where,

$$f_0^T = \left(\frac{\partial f(x_i; \theta^*)}{\partial \theta_1^*}, \frac{\partial f(x_i; \theta^*)}{\partial \theta_2^*}, \dots, \frac{\partial f(x_i; \theta^*)}{\partial \theta_p^*} \right) \text{ and } p \text{ is the number of parameters.}$$

Using Equation (10) and (13), the difference between the true value of y of the system and the predicted value $\hat{y}$ can be calculated as given in Equation (14). The expected value of this difference is given in Equation (15). The subscript value used in Equation (15) is to denote the set of points other than those used for the least-squares estimation of θ^* .

$$\begin{aligned} y_0 - \hat{y}_0 &\approx y_0 - f(x_0; \theta^*) - f_0^T \cdot (\hat{\theta} - \theta^*) \\ &= \varepsilon_0 - f_0^T \cdot (\hat{\theta} - \theta^*) \end{aligned} \quad (14)$$

$$E[y_0 - \hat{y}_0] \approx E[\varepsilon_0] - f_0^T E[(\hat{\theta} - \theta^*)] \approx 0. \quad (15)$$

The variance can be expressed as given in Equation (16) because of the statistical independence between $\hat{\theta}$ and ε_0 .

$$\text{var}[y_0 - \hat{y}_0] \approx \text{var}[\varepsilon_0] + \text{var}[f_0^T \cdot (\hat{\theta} - \theta^*)]. \quad (16)$$

For an error ε_0 with a normal distribution and with a mean of zero and a variance of $\sigma^2 (N(0, \sigma^2 I_n))$, the distribution of $\hat{\theta} - \theta^*$ can be approximated to have the distribution $N_p(0, \sigma^2 [F \cdot (\hat{\theta})^T F \cdot (\hat{\theta})]^{-1})$. The $F \cdot (\hat{\theta})$ is the Jacobian matrix consisting of first derivatives in the form shown in Equation (17), where the single period denotes the matrix with first-order differential terms.

$$F(\hat{\theta}) = \frac{\partial f(x, \hat{\theta})}{\partial \hat{\theta}} = \begin{bmatrix} \frac{\partial f_1(x_1, \hat{\theta})}{\partial \hat{\theta}_1} & \frac{\partial f_1(x_1, \hat{\theta})}{\partial \hat{\theta}_2} & \cdots & \frac{\partial f_1(x_1, \hat{\theta})}{\partial \hat{\theta}_p} \\ \frac{\partial f_2(x_2, \hat{\theta})}{\partial \hat{\theta}_1} & \cdots & \cdots & \frac{\partial f_2(x_2, \hat{\theta})}{\partial \hat{\theta}_p} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_n(x_n, \hat{\theta})}{\partial \hat{\theta}_1} & \frac{\partial f_n(x_n, \hat{\theta})}{\partial \hat{\theta}_2} & \cdots & \frac{\partial f_n(x_n, \hat{\theta})}{\partial \hat{\theta}_p} \end{bmatrix} \quad (17)$$

$$\text{var}[y_0 - \hat{y}_0] \approx \sigma^2 + \sigma^2 f_0^T (F^T \cdot F)^{-1} f_0. \quad (18)$$

Equation 18 gives the unbiased estimator of σ^2 and using Equation (19), the Student t -distribution is given in Equation (20). Equation (21) gives the confidence interval $100^*(1 - \alpha)$ for the predicted value $\hat{y}$.

$$s^2 = \frac{\|y - f(x, \hat{\theta})\|^2}{n - p} \quad (19)$$

$$t_{n-p} \sim \frac{y_0 - \hat{y}_0}{\sqrt{\text{var}[y_0 - \hat{y}_0]}} \approx \frac{y_0 - \hat{y}_0}{\sqrt{s^2 + s^2 f_0^T (F^T \cdot F)^{-1} f_0}} \approx \frac{y_0 - \hat{y}_0}{s(1 + f_0^T (F^T \cdot F)^{-1} f_0)^{\frac{1}{2}}} \quad (20)$$

$$\hat{y}_0 \pm t_{n-p}^{\alpha/2} s(1 + f_0^T (F^T \cdot F)^{-1} f_0)^{\frac{1}{2}} \quad (21)$$

Rivals and Personnaz [18, 39, and 40] use the least squares estimation term instead of NLR. The calculation of the inverse of the matrix $F^T F$ is a known problem in the literature, as the values of the matrix F nearly become singular. Rivals and Personnaz [39, 40] provide an alternate solution as discussed below.

Rivals and Personnaz mention that a statement on rank deficiency of F cannot be made. The estimation of whether confidence interval can be estimated accurately or not should be decided on the need of inverse of $F^T F$. The most accurate estimation was performed using F 's singular value decomposition (SVD) $F = U \Sigma V^T$. They provided equations to obtain the computer version of $(F^T F)^{-1}$ in the form of Equation (22).

$$\widehat{(F^T F)^{-1}} = \widehat{V} \widehat{(\Sigma^T \Sigma)^{-1}} \widehat{V}^T \text{ with } \begin{cases} \left[\widehat{(\Sigma^T \Sigma)^{-1}} \right]_{ii} = \frac{1}{(\widehat{\sigma}_i)^2} \text{ for } i = 1 \text{ to } q \\ \left[\widehat{(\Sigma^T \Sigma)^{-1}} \right]_{ij} = 0 \quad \forall i \neq j \end{cases} \quad (22)$$

where q (p as used in G. Chryssoulouris [16]) is the number of parameters a neural network has.

The absolute error on the i^{th} singular value is bounded by Equation (23).

$$\left| \sigma_i - \widehat{\sigma}_i \right| \leq \sigma_1 \varepsilon \quad \text{for } i = 1 \text{ to } q \quad (23)$$

where ε is the computer unit rounded off ($\varepsilon = 10^{-16}$ for usual computers).

The relative error on the smallest singular values is bounded by Equation (24).

$$\left| \frac{\sigma_q - \widehat{\sigma}_q}{\sigma_q} \right| \leq \frac{\sigma_1}{\sigma_q} \varepsilon = \kappa(F) \varepsilon \quad (24)$$

It can be seen that the absolute error was directly related to the condition number $\kappa(F)$ of F , which is the ratio of its largest to its smallest singular value. The relative error on the smallest singular value may be 100% if $\kappa(F)$ reaches $1/\varepsilon = 10^{16}$.

Therefore, Rivals and Personnaz recommend discarding neural networks with $\widehat{\kappa(F)} > 10^8$ as Equation (22) involves calculating the inverse of the squared Jacobian matrix, and hence, the inverse of the computed squared singular values. The inverse of the matrix $(F^T F)$ can only be calculated with precision when $\widehat{\kappa(F)} \ll 10^8$. Also, the precision of $\kappa(F)$ itself is excellent when $\widehat{\kappa(F)}$ is below 10^8 .

The rank of Jacobian matrix can be estimated as the number of computer singular values that are larger than the threshold of $\widehat{\sigma}_1 \varepsilon$, as given in Equation (25).

$$\hat{r} = \text{card} \left\{ \widehat{\sigma}_i > \widehat{\sigma}_1 \varepsilon, i = 1 \text{ to } q \right\} \quad (25)$$

Rivals and Personnaz suggest an alternate way to calculate the inverse than Equation(22), which does not deal with the computation of the inverse of the Jacobian matrix. When $r = q$, the diagonal elements of the $H = F(F^T F)^{-1} F^T$ can be calculated using Equation (26).

$$\widehat{h}_{kk} = \sum_{i=1}^{\widehat{r}} (\widehat{u}_{ki})^2 \quad \text{for } k = 1 \text{ to } N \quad (26)$$

where $\widehat{r}$ is calculated using Equation (25).

As Equation (26) does not require the inverse of the square of possibly inaccurate small singular values, it is less sensitive to the ill-conditioning of F than $(F^T F)^{-1}$.

Two additional tests are performed on values which are of interest for the computation of CI's and are related to the orthogonal projection matrix H on the range of F . If F is of full rank, since H is a projection matrix, Equation (27) and (28) should be satisfied.

$$\text{trace}(H) = \sum_{k=1}^N h_{kk} = \text{rank}(H) = q \quad (27)$$

$$\frac{1}{N} \leq h_{kk} \leq 1 \text{ for } k = 1 \text{ to } N \quad (28)$$

Rivals and Personnaz mentioned the importance of verifying Equation (27) and (28), since for an input x^k , belonging to the training set, the expression of the CI is precisely given by Equation (29), rather than Equation (21).

$$\widehat{y}_k \pm t_{N-q}^{\alpha} s \sqrt{h_{kk}} \quad (29)$$

They caution on the usefulness of the CIs. “If (27) or (28) are not satisfied, even if the network has not been diagnosed to overfit by a test on the singular values, the computation of the CIs is meaningless.” All cases studied in this research satisfied both the conditions.

Although, this model assumes that error associated with modeling is normally distributed, Shao et. al. [14] mention the importance of including actual error in the confidence intervals, as the width of the confidence intervals is in proportion to the standard deviation of the error vector. Therefore, Shao et. al. suggest multiplying the CIs by the ratio of the prediction error to the standard deviation of the whole vector by λ . This correction factor can be calculated using Equation (30).

$$\lambda_i = \frac{|y_i - \widehat{y}_i|}{std(|y_i - \widehat{y}_i|)}, i = 1, 2, \dots, n \quad (30)$$

where n is the number of predicted points.

Thus, the modified confidence intervals can be given by Equation

$$\hat{y}_k \pm t_{N-q}^{\alpha} \lambda_k s \sqrt{h_{kk}} \quad (31)$$

Since the paper published by G. Chryssoulouris [16], various researchers studied non-linear regression to calculate the confidence intervals on the output of neural networks. Coverage probability (CP) was used as a tool to test the accuracy of this estimation by L. H. Ungar [17]. Rivals and Personnaz [18] reported a different way to estimate the calculation terms as the method reported by G. Chryssoulouris [16] created problems in the calculations.

2.1.2 Bootstrap Estimation

A book by Efron and Tibshirani on bootstrapping [20] affirms that confidence interval can be obtained by using a resampling technique such as bootstrapping. T. Heskes [30] states that bootstrapping is based on the idea that the available data set is nothing but a particular realization of some unknown probability distribution. Instead of sampling over the true distribution, which is obviously impossible, an empirical distribution is defined, according to Heskes [30].

The bootstrap is a computer-based method for assigning measures of accuracy to statistical estimates. Bootstrapping will provide a nonparametric confidence interval for any population estimate. This process involves creating a large number of bootstrap samples by repeatedly resampling (with replacement) the original dataset in a random order, each with probability of $1/n$, where n is the number of samples. By resampling with replacement it, is indicated that the same data row can be used repeatedly to generate a bootstrap sample if a random number matching that row is selected. Each bootstrap sample is used as a training set. An illustration on bootstrap resampling is provided in Table 2.2 and the data used are taken from McKim [46] (also appeared in K. N. Lankalpalli and R. C. Creese [21]). To illustrate bootstrap sampling with replacement, two bootstrap samples are generated by creating random number between one and 23 as shown in Table 2.2.

Table 2.2 Bootstrap Resampling Example [46]

	Original Data			Bootstrap Sample Set 1				Bootstrap Sample Set 2			
	Flow	Head	Actual Price	Random Number	Flow	Head	Actual Price	Random Number	Flow	Head	Actual Price
S.N.	gpm	inches	\$		gpm	inches	\$		Gpm	inches	\$
1	100	700	25,584	9	300	2000	36,660	19	600	700	31,668
2	100	1200	28,296	22	700	700	43,668	12	400	1200	31,860
3	100	2000	32,160	20	600	1200	34,008	19	600	700	31,668
4	200	700	25,584	21	600	2000	39,240	11	400	700	28,908
5	200	1200	28,296	18	500	2400	39,240	5	200	1200	28,296
6	200	2000	32,160	18	500	2400	39,240	11	400	700	28,908
7	300	700	27,924	23	700	1200	34,008	12	400	1200	31,860
8	300	1200	30,936	16	500	1200	31,860	10	300	2400	39,240
9	300	2000	36,660	8	300	1200	30,936	2	100	1200	28,296
10	300	2400	39,240	7	300	700	27,924	7	300	700	27,924
11	400	700	28,908	14	400	2400	39,240	8	300	1200	30,936
12	400	1200	31,860	14	400	2400	39,240	19	600	700	31,668
13	400	2000	36,660	16	500	1200	31,860	17	500	2000	36,660
14	400	2400	39,240	2	100	1200	28,296	16	500	1200	31,860
15	500	700	28,908	5	200	1200	28,296	7	300	700	27,924
16	500	1200	31,860	16	500	1200	31,860	18	500	2400	39,240
17	500	2000	36,660	17	500	2000	36,660	9	300	2000	36,660
18	500	2400	39,240	9	300	2000	36,660	13	400	2000	36,660
19	600	700	31,668	22	700	700	43,668	2	100	1200	28,296
20	600	1200	34,008	23	700	1200	34,008	14	400	2400	39,240
21	600	2000	39,240	10	300	2400	39,240	22	700	700	43,668
22	700	700	43,668	15	500	700	28,908	2	100	1200	28,296
23	700	1200	34,008	5	200	1200	28,296	5	200	1200	28,296

Baxt and White [22] have successfully used bootstrapping to compute confidence intervals for clinical input variable effects in a network to identify the presence of acute myocardial infarction. They took 19 input variables and one binary output variable, which would predict if a patient has myocardial infarction. The authors generated 1000 sets of 706 input-target pairs. After training these 1000 sets using backpropagation, they found the sample means and examined the network statistically. The authors claimed that they are the first to statistically validate observed relationships between the input information processed by an ANN and its target. They also claim that bootstrapping is not limited by network architecture and is applicable to most network constructs. They found that one of the indicators or input variables of infarction previously identified as statistically significant was in fact statistically insignificant.

G. Papadopoulos et. al. [23], R. Tibshirani [24], and R. Dybowski et. al. [25] discuss the use of bootstrapping to calculate confidence intervals for neural networks. G. Papadopoulos simulated three artificial data sets (120 input-target pairs for training) and one real data set (369 input-target pairs for training) [23]. Moreover, the authors added noisy data, which had been treated as a function of the inputs. The number of bootstrap samples used in G. Papadopoulos et.al. [23] was 20. Tibshirani [24] states that the number of bootstrap samples or number for retraining the network is typically between 20 and 200, but he used 20 samples. The data set used in [24] had 111 input-target pairs or observations. The author concluded that the bootstrap methods provided the most accurate estimates of the standard errors of the predicted value.

Bhide and Piovoso [42] studied the bootstrap technique for generating appropriate statistic for the confidence interval on the output of the neural networks. Also, W. Y. Goh et.al. [43] used the bootstrap estimation technique to calculate the confidence intervals using recurrent neural networks. The bootstrap pairs sampling algorithm [24] is given as follows:

```

begin
let  $\{(x^{(1)}, t^{(1)}), \dots, (x^{(N)}, t^{(N)})\}$  be the true sample S;
for  $b = 1$  to  $B$  do
    randomly sample (with replacement)  $N(x, t)$  -pairs from S;
    let  $\{(x^{(*b,1)}, t^{(*b,1)}), \dots, (x^{(*b,N)}, t^{(*b,N)})\}$  be the random sample;
    derive regression function  $f(x; \hat{\theta}^{(*b,N)})$  from training set
         $\{(x^{(*b,1)}, t^{(*b,1)}), \dots, (x^{(*b,N)}, t^{(*b,N)})\}$ ;
endfor
The bootstrap estimate of standard error of  $f(x; \hat{\theta})$ , which is a function of  $x$ , is given by

$$\hat{SE}_{boot}(f(x; \cdot)) = \sqrt{\frac{1}{B} \left[ \sum_{b=1}^B f(x; \hat{\theta}^{(*b)}) - f_{boot}(x; \cdot) \right]^2},$$

where  $f_{boot}(x; \cdot) = \sum_{b=1}^B \frac{f(x; \hat{\theta}^{*b})}{B}$ .

```

Assuming a normal distribution for $f(x; \hat{\theta})$ over the space of all possible $\hat{\theta}$, the 95% bootstrap confidence interval for $f(x)$ can be given in Equation (32).

$$f(x; \hat{\theta}) \pm t_{0.025, [B]} \cdot \widehat{SE}_{boot}(f(x; \cdot)) \quad (32)$$

Using bootstrapping, a realization of some unknown probability distribution of the data and a nonparametric confidence interval for any population estimate was found.

2.1.3 Maximum Likelihood (ML) Estimation

Dybowski and Roberts in [25] discuss the idea of using maximum likelihood estimators (MLE) for the calculation of confidence bounds. The definition of maximum likelihood estimation as given in R.E. Walpole et.al. [26] as follows.

“Given independent observations $x_1, x_2, \dots, x_n$ from a probability density function (continuous case) or probability mass function (discrete case) $f(x, \theta)$ the maximum likelihood estimator $\hat{\theta}$ is that which maximizes the likelihood function

$$L(x_1, x_2, \dots, x_n, \theta) = f(x_1, \theta) \cdot f(x_2, \theta) \cdot \dots \cdot f(x_n, \theta) ”$$

For discrete cases, the maximum likelihood estimator is one that results in a maximum value of joint probability or maximizes the likelihood of the sample. The notion of maximum likelihood extends to the estimation of parameters of continuous distribution too. Differentiating the probability density or mass function and setting the derivative to zero should give the maximum value.

G. Papadopoulos et. al.[25], state the methodology for incorporating the maximum likelihood estimation for neural networks. They say if a feed-forward neural network $f(x; \hat{\theta})$ is trained on a dataset $\{x^{(1)}, t^{(1)}, \dots, x^{(N)}, t^{(N)}\}$ by minimizing $Err(\theta)$ (given in Equation (34)), where θ are the network weights, it can be shown that the resulting network approximates the mean value for t conditioned x ,

$$f(x; \hat{\theta}) \approx E[t|x] \quad (33)$$

the approximation becoming equality if N goes to infinity and $f(x; \hat{\theta})$ has unlimited flexibility. Therefore, a feed-forward network trained via $Err(\theta)$ can be regarded as a regression function.

$$Err(\theta) = \frac{1}{2} \sum_{n=1}^N \left[f(x^{(n)}; \hat{\theta}) - t^{(n)} \right]^2 \quad (34)$$

The variance of t associated with output $f(x; \hat{\theta})$ is given, as in Equation (35). A second neural network $\hat{\sigma}^2(x; \hat{u})$ using squared residuals $(f(x; \hat{\theta}) - t)^2$ as the target values for the sum-of-squares function given in Equation (36) so that $Var[t|x] \approx \hat{\sigma}^2(x; \hat{u})$.

$$Var[t|x] = E[(f(x;\hat{\theta}) - t)^2 | x]. \quad (35)$$

$$\frac{1}{2} \sum_{n=1}^N \left\{ \hat{\sigma}^2(x^{(n)}; \mathbf{u}) - [f(x^{(n)}; \hat{\theta}) - t^{(n)}]^2 \right\}^2 \quad (36)$$

By assuming a Gaussian distribution for t , given in Equation (37), the confidence interval for t about $f(x; \hat{\theta})$ can be obtained.

$$p(t|x) = \frac{1}{\sqrt{2\pi\hat{\sigma}(x; \hat{\mathbf{u}})}} \exp \left\{ \frac{-(f(x; \hat{\theta}) - t)^2}{2\hat{\sigma}^2(x; \hat{\mathbf{u}})} \right\} \quad (37)$$

By training a separate neural network for the error terms, the variance on the predicted output was estimated and hence the confidence intervals were computed.

2.2 Summary

The literature search provided important views in the existing research in the area of confidence interval computation. It was noted that even though this area is relatively new, various researchers are attempting to develop with better techniques or modifications. The primary techniques for constructing confidence intervals existing in the literature were found to be non-linear regression, bootstrap algorithm, maximum-likelihood, and approximate Bayesian approach.

The researchers used different approaches with various data sets and parameters, leaving little ground for direct comparisons. Although some researchers were able to tell which techniques were actually better than others in some aspects, no author was able to recommend a single approach applicable to any condition. Artificial neural networks are commonly known as “black boxes” and are not able to explain the results and give assurances on the results. However, many authors in the literature claim that confidence intervals can be constructed on the results of neural networks under specified assumptions.

2.3 Research Objective

The primary objective of the research was to model, compare, and analyze non-linear regression, bootstrapping, and MLE in the literature on constructing confidence intervals for the outputs of neural networks. As mentioned earlier, it is very important to have confidence intervals on the outputs of the “black box” model. However, this field of calculating confidence

intervals on the outputs of neural networks is relatively new and research is an ongoing process. Therefore, it is imperative that the existing methods of calculating the confidence intervals should be tested and analyzed as much as possible on different scenarios.

This research was conducted to explore different options on constructing the confidence intervals available in the literature. Even though the literature provides some insight about these techniques, a more detailed and organized study was required. This research attempted to provide an easy-to-use neural network model for any application with confidence intervals on the output.

3 Model Development

3.1 Development of an Artificial Neural Network Model

An artificial neural network model with feed-forward architecture was developed using backpropagation algorithm for updating the weights developed by Laurene Fausett [5]. The backpropagation algorithm can be depicted in Figure 3.1. The number of hidden layers and output neurons were limited to one for ease of calculation.

Figure 3.1 Flowchart of the Backpropagation Algorithm

Equation (38) was used to generate a data set of 250 points with X being randomly selected between 0 and 1. There is no recommended rule for selecting the number of neurons in the hidden layer, but they are generally selected more than the number of input parameters. Too many hidden neurons may result in a failure to generalize properly, and too few hidden neurons may result in a failure to achieve a low average error. Therefore, the number of hidden neurons should be chosen after some trial and error. For this specific problem, the number of neurons in the hidden layer was selected as two because the problem was not complex.

$$y = 2X_1^2 + 3X_2^3 + 4X_3 + X_4^{1/2} + 4X_5 \quad (38)$$

The stopping condition generally used is either based on the Mean Square Error (MSE) or the number of iterations. The number of iterations, also called as epochs, is the number of times the error is back propagated and weights are updated. The flexible number of iterations helps to avoid the problem of overfitting, which means that the model has become too powerful to model the associated noise with the data. The scaling of the input and output variables was necessary as the sigmoidal activation function was used which limits the values between zero and one.

3.1.1 Scaling

The binary sigmoidal activation function, $y = 1/(1 + \exp(-x_i))$, ensures that the output of any neuron is between 0 and 1, which causes the problem of restricting the output to between 0 and 1, when the actual output may not be in that range. Researchers came up with this idea of scaling the input data set that can be used by the neural network and the output must be scaled back to give the output in the original comparable form. The data used in this research were scaled between 0.1 and 0.9 using Equation (39), as given in [21] and scaling back of the data was done by using Equation (40).

$$val_{scaled} = \frac{0.8 * val_{org} + 0.1 * val_{max} - 0.9 * val_{min}}{val_{max} - val_{min}} \quad (39)$$

where,

val_{scaled} = value to be scaled

val_{org} = original value

val_{max} = maximum value of the same data row of the value to be scaled

val_{min} = minimum value of the same data row of the value to be scaled

$$val_{new} = \frac{0.9 * val_{min} - 0.1 * val_{max} + val_{scaled} * (val_{max} - val_{min})}{0.8} \quad (40)$$

where,

val_{new} = Value to be scaled back

For example, if we have to scale the first value (100) from Table 2.2, it would be done as given in Equation (41). The maximum and minimum values in the data set are 700 and 100 respectively. If the value to be scaled is the minimum value of that data set, the scaled value is 0.1, which is the minimum value of the scale (0.1, 0.9).

$$val_{scaled} = \frac{0.8 * 100 + 0.1 * 700 - 0.9 * 100}{700 - 100} = 0.1 \quad (41)$$

3.1.2 Neural Network Model Results

From the 250 data sets generated using Equation(38), 175 were used for training and the remaining 75 were used for testing the network. The data used are presented in Appendix A. Using two neurons in the hidden layer and 20, 30, and 40 epochs, the network was trained and the results are shown in Figure 3.2. The R^2 between the actual and model output for training data obtained were 0.31, 0.63, and 0.96 for 20, 30, and 40 iterations, respectively. It can be seen that the R^2 value increases with an increase in the number of iterations or epochs, and therefore, there is a decrease in MSE with an increase in the number of iterations. However, it should be noted that the number of epochs may not necessarily reduce the error in the predicted values as it also depends on the starting random weights.

Figure 3.2 MSE for Training and Test Data, and R-square for Training and Test Data Using 20, 30, and 40 Epochs

3.1.3 Random Weight Initialization

Although the usual practice is to assign small random numbers as starting weights, D. Nguyen and B. Widrow [44] developed a new algorithm, known as the Nguyen-Widrow initialization (NWI) method. It is a simple modification of the common random weight initialization, which allows for gives much faster learning by the neural network. This initialization of weights was used throughout the research.

The approach is based on a geometrical analysis of the response of the hidden neurons to a single input; the analysis is extended to the case of several inputs by using Fourier transformations. The weights from hidden units to the output units and biases on the output units are initialized to random values between -0.5 and 0.5.as is commonly the case.

This initialization of the weights from input to output units is done to improve the hidden units' ability to learn. This is accomplished by distributing the initial weights and biases so that for each input pattern, it is likely that the net input to one of the hidden units will be in the range in which that hidden neuron will learn most readily. This method is described as follows:

n number of input units

p number of hidden units

β scale factor, given as:

$$\beta = 0.7(p)^{1/n} = 0.7\sqrt[n]{p}$$

The procedure consists of the following steps:

For each hidden unit ($j=1, \dots, p$):

Initialize its weight vector (from the input units):

(old)=random number between -0.5 and 0.5 (or between $-\gamma$ and γ).

Compute $\|V_{ij}(old)\| = \sqrt{V_{1j}(old)^2 + V_{2j}(old)^2 + \dots + V_{nj}(old)^2}$

Reinitialize weights:

$$v_{ij} = \frac{\beta v_{ij}(old)}{\|V_{ij}(old)\|}$$

set- bias:

$$v_{0j} = \text{random number between } -\beta \text{ and } \beta$$

A neural network was tested by using the Nguyen-Widrow initialization method and without using it. Data from McKim [46] was used for this test. Ten simulations were run with the parameters given in Table 3.1. Mean squared errors (MSE) for these simulations are shown in Table 3.2 and Figure 3.3.

Table 3.1 Parameters for Neural Network to Test Nguyen-Widrow Initialization

Hidden Neurons	2
Iterations	50
Activation function (Input-Hidden)	Sigmoid
Activation function (Hidden-Output)	Linear
Learning rate	0.2
Observations for training	19
Observations for test	4

Table 3.2 Mean Squared Error (MSE) with and without Nguyen-Widrow Initialization

Simulation Number	MSE with-NWI (Millions)	MSE without-NWI (Millions)
1	161	566
2	220	340
3	172	380
4	183	445
5	137	540
6	348	355
7	161	290
8	307	434
9	210	362
10	359	431
Average	226	414
Range	137-359	290-566

Figure 3.3 MSE and Average MSE for Neural Networks with and without NWI

It can be seen from Table 3.2 and Figure 3.3 that neural network with NWI outperform the neural network without NWI. In only one of the ten cases were the MSE values approximately equal. The average MSE for the neural networks with NWI is 45% lower than the average MSE for the neural networks without NWI. A brief manual of this NN program is given in Appendix E.

3.2 Development of Confidence Interval for Linear Regression

A simple linear regression model is given in Equation (42).

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i \quad (42)$$

where,

Y_i is the dependent or response variable in the i^{th} trial ($i=1, \dots, n$)

X_i is the independent variable

β_0 and β_1 are parameters to be estimated

ε_i is the normally distributed error term with expected value to be zero and variance σ^2

The parameters β_0 and β_1 are estimated by minimizing the sum of the squared residuals as given in Equation (43).

$$\sum_{i=1}^n e_i^2 = \sum_{i=1}^n (Y_i - \hat{Y}_i)^2 \quad (43)$$

where $\hat{Y}_i$ is the predicted value using estimated parameters β_0 and β_1 . The MSE or error mean square given by Equation (44) is an unbiased indicator of σ^2 .

$$MSE = \frac{\sum_{i=1}^n e_i^2}{n-2} \quad (44)$$

Confidence intervals for linear regression are based on the estimated variance of $\hat{Y}_h$, the predicted value for observation h [45]. This variance is given by Equation (45).

$$\sigma^2 \{ \hat{Y}_h \} = \sigma^2 \left[\frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right] \quad (45)$$

When MSE is substituted for σ^2 , the estimated variance of $\hat{Y}_h$, $s^2 \{ \hat{Y}_h \}$, can be calculated by Equation (46).

$$s^2 \left\{ \widehat{Y}_h \right\} = MSE \left[\frac{1}{n} + \frac{(X_h - \bar{X})^2}{\sum (X_i - \bar{X})^2} \right] \quad (46)$$

Confidence intervals with $1-\alpha$ confidence for $E\{\widehat{Y}_h\}$ can be calculated by using Equation(47), and the confidence interval for individual observation is given by Equation (48).

$$\widehat{Y}_h \pm t_{1-\alpha/2}^{n-2} s \left\{ \widehat{Y}_h \right\} \quad (47)$$

$$\widehat{Y}_h \pm t_{1-\alpha/2}^{n-2} \left[s^2 \left\{ \widehat{Y}_h \right\} + MSE \right]^{1/2} \quad (48)$$

3.2.1 Linear Regression Confidence Intervals for Tree Data Set [46]

The tree data set obtained from SAS's website [47] had 104 rows and three columns. The three columns (variables) were rootstock, trunk girth, and weight of the tree, and the data is in Table A-2. In the 1930's, the weights and trunk girths were measured for eight specimens from each of thirteen rootstocks for a total of 104 tree specimens. These data were collected to determine if the girth and/or rootstock of the trees were useful in predicting the weight of trees. As the rootstock was not a continuous variable, it was excluded from this research. This data table can be found in Table A-2. Out of 104 observations, 80 were used for training and 24 for testing. Regression summary and the ANOVA table on these data are given in Table 3.3.

The estimated variance $s^2 \left\{ \widehat{Y}_h \right\}$ for the first observation ($X_h = 406$) in e Figure 3.2 was calculated using Equation 46. Substituting $MSE = 29,644$, $n = 80$, $\bar{X} = 395$ and $\sum (X_i - \bar{X})^2 = 376,758$ in Equation(46), $s^2 \left\{ \widehat{Y}_h \right\} = 380.22$ was obtained. The confidence intervals for mean and confidence intervals for the individual observations were calculated using Equation (47) and (48) respectively, as shown in Figure 3.2 with $t_{0.975}^{78} = 1.665$.

Using the coefficients found during the regression analysis, predicted values were calculated. The predicted values and calculations of confidence intervals are shown in Figure 3.4. The trunk girth vs. weight plotted with the confidence curves is shown in Figure 3.5. The coverage probability for this confidence interval (individual) was 92.31%, covering 96 points for a nominal probability of 95%. For 90% probability the coverage probability, was 82.69% covering 86 points, with $|CP-90|\%$ of 7.31%.

Table 3.3 Regression Analysis and ANOVA for Tree Data [46]

Regression Statistics			
Multiple R	0.92		
R Square	0.85		
Adjusted R Square	0.85		
Standard Error	172.18		
Observations	80.00		
ANOVA			
	<i>df</i>	<i>SS</i>	<i>MS</i>
Regression	1	13412097	13412097
Residual	78	2312255	29644.29
Total	79	15724351	
		<i>Coefficients</i>	<i>Standard Error</i>
Intercept		-1270.16	112.44
X Variable 1		5.97	0.28

	A	B	C	D	E	F	G	H	I	J	K
1	TrunkGirth	Weight	PredictedWeight	Smean	Sind			LCImean	UCImean	LCIInd	UCIInd
2	406	1094	1152.25	19.50	173			1120	1185	864	1441
3	405	1241	1146.29	19.46	173			1114	1179	858	1435
4	385	1017	1026.96	19.45	173			995	1059	739	1315
5	351	726	824.09	22.85	174			786	862	535	1113
6	465	1658	1504.28	27.51	174			1458	1550	1214	1795
7	450	1288	1414.78	24.68	174			1374	1456	1125	1704
8	375	790	967.29	20.04	173			934	1001	679	1256
9	460	1751	1474.45	26.53	174			1430	1519	1184	1764
10	452	1499	1426.71	25.04	174			1385	1468	1137	1716
11	478	1571	1581.84	30.23	175	Total	104	1532	1632	1291	1873
12	405	1023	1146.29	19.46	173	obs used Training	80	1114	1179	858	1435
13	424	1177	1259.65	20.91	173	mean	395	1225	1294	971	1548
14	205	251	-47.02	56.64	181	SSETR	2,312,255	-141	47	-349	255
15	425	1488	1265.62	21.02	173	dof	78	1231	1301	977	1554
16	390	944	1056.79	19.30	173	MSETR	29,644	1025	1089	768	1345
17	343	733	776.36	24.14	174	Clevel	95	736	817	487	1066
18	404	1084	1140.32	19.42	173	Tdist	1.665	1108	1173	852	1429
19	395	952	1086.62	19.25	173	RsqrTR	0.853	1055	1119	798	1375
20	226	278	78.28	51.14	180	RsqrTe	0.806	-7	163	-221	377
21	299	506	513.84	33.08	175	Should've covered	99	459	569	222	806
22	463	1838	1492.35	27.12	174	covered (indiv)	96	1447	1537	1202	1782
23	334	610	722.66	25.74	174	CP (indiv)	92.31%	680	766	433	1012
24	438	1197	1343.18	22.73	174			1305	1381	1054	1632
25	410	1035	1176.12	19.71	173			1143	1209	888	1465

Figure 3.4 Calculations of Confidence Intervals for Linear Regression in a Spreadsheet

Figure 3.5 Trunk Girth vs. Weight for the Tree Data [46] using Regression Predicted Weight Values Given By Dots, Actual Weight Values Given By Stars, and Solid Lines 95% Confidence Curves

3.3 Development of Confidence Interval via Non-linear Regression

Constructing confidence interval via non-linear regression is a straightforward process except for obtaining values for the elements in the Jacobian matrix, F (Equation 16) and f_0^T matrices. The F and f_0^T contain the derivatives of the output with respect to the parameters used to estimate y . This calculation of the elements of F and f_0^T matrices was adopted from [16]. Two terms defined by the authors in [16] are $net_j^{[\beta]}$ and $layer^{[\beta]}$ given in Equation (49) and (50) respectively. The $net_j^{[\beta]}$ is summation of the outputs from the nodes of layer $\beta - 1$ entering node j in layer β . The $layer^{[\beta]}$ is the response of layer β for a given set of inputs, which is the summation of $net_j^{[\beta]}$ functions for layer β .

$$net_j^{[\beta]} = \left(\sum_{i=1}^n w_i^{[\beta-1]} zout_i^{[\beta-1]} \right) - b_j \quad (49)$$

where,

n = Number of nodes in layer $\beta - 1$, and

b_j = Bias term of node j

$$\text{layer}^{[\beta]} = \sum_{i=1}^m \text{net}_j^{[\beta]} \quad (50)$$

where,

m = Number of nodes in layer β

Equation (51) expresses the derivative of the output y with respect to the weights and the biases, $\frac{\partial y}{\partial w_\gamma^{[\alpha]}}$, where γ is the specific weight value of layer α . The terms used in Equation (51),

$\frac{\partial y}{\partial \text{net}^{[m]}}$, $\frac{\partial \text{net}^{[m]}}{\partial \text{layer}^{[m-1]}}$, $\frac{\partial \text{layer}^{[m-1]}}{\partial \text{layer}^{[m-2]}}$, $\frac{\partial \text{layer}^{[\alpha+2]}}{\partial \text{net}_\gamma^{[\alpha+1]}}$, $\frac{\partial \text{net}^{[\alpha+1]}}{\partial w_\gamma^{[\alpha]}}$ are given in Equation (52), (53), (54), (55)

and (56) respectively.

$$\frac{\partial y}{\partial w_\gamma^{[\alpha]}} = \frac{\partial y}{\partial \text{net}^{[m]}} \frac{\partial \text{net}^{[m]}}{\partial \text{layer}^{[m-1]}} \frac{\partial \text{layer}^{[m-1]}}{\partial \text{layer}^{[m-2]}} \dots \frac{\partial \text{layer}^{[\alpha+3]}}{\partial \text{layer}^{[\alpha+2]}} \frac{\partial \text{layer}^{[\alpha+2]}}{\partial \text{net}_\gamma^{[\alpha+1]}} \frac{\partial \text{net}^{[\alpha+1]}}{\partial w_\gamma^{[\alpha]}} \quad (51)$$

$$\frac{\partial y}{\partial \text{net}^{[m]}} = \begin{cases} 1 & \text{if the output neuron has linear activation function,} \\ y(1-y) & \text{if the output neuron has sigmoidal activation function.} \end{cases} \quad (52)$$

$$\frac{\partial \text{net}^{[m]}}{\partial \text{layer}^{[m-1]}} = \sum_{i=1}^n \frac{\partial \text{net}^{[m]}}{\partial \text{net}_i^{[m-1]}} \quad (53)$$

$$\frac{\partial \text{layer}^{[m-1]}}{\partial \text{layer}^{[m-2]}} = \sum_{j=1}^p \left(\sum_{i=1}^n \frac{\partial \text{net}_j^{[m-1]}}{\partial \text{net}_i^{[m-2]}} \right) \quad (54)$$

Where,

p = Number of nodes in layer $m - 1$.

$$\frac{\partial \text{layer}^{[\alpha+2]}}{\partial \text{net}_\gamma^{[\alpha+1]}} = \sum_{i=1}^p \frac{\partial \text{net}_j^{[\alpha+2]}}{\partial \text{net}_\gamma^{[\alpha+1]}} \quad (55)$$

$$\frac{\partial \text{net}^{[\alpha+1]}}{\partial w_\gamma^{[\alpha]}} = \text{zout}_\gamma^{[\alpha]} \quad (56)$$

A general form of $\frac{\partial \text{net}_\lambda^{[\phi+1]}}{\partial \text{net}_\zeta^{[\phi]}}$ is given in Equation(57), where ϕ is an arbitrary layer, λ is an arbitrary node in layer $\phi+1$, ζ is an arbitrary node in layer ϕ , and A is the number of nodes in layer ϕ .

$$\frac{\partial \text{net}_\lambda^{[\phi+1]}}{\partial \text{net}_\zeta^{[\phi]}} = \sum_{a=1}^A \left\{ w_a^{[\phi]} \text{zout}_a^{[\phi]} (1 - \text{zout}_a^{[\phi]}) \right\} \quad (57)$$

3.3.1 Steps for Finding Confidence Intervals Using Non-Linear Regression

The steps to find confidence interval using non-linear regression are given as follows:

1. Split the data into training and test data sets.
2. Scale the data.
3. Train the network using the training data set.
4. Calculate s^2 using Equation (19) for the training data. (Page 19)
5. Predict the test data.
6. Find first order partial derivatives of output with respect to the parameters (weights), i.e., matrices F and f_0 using Equations (49) to(57). (Pages 33-34-Code given in Appendix C)
7. Calculate the SVD of F and diagonal elements of the H matrix as given on pages 19 and 20.
8. Select appropriate confidence level and respective t-distribution value.
9. Calculate the correction factor λ given by Equation (30).
10. Calculate confidence intervals for the training and test data using Equation (31). (Page 21)

3.3.2 Validation of the NLR model

This model was developed on the information presented by Chryssolouris et al [16]. However, calculating the matrix is a complex process and calculating its inverse is often impossible if the matrix becomes singular. Therefore, the method described in Rivals and Personnaz [39, 40] was used. The data presented in Chryssolouris et.al. [16] could not be found after a thorough search and hence this model was not able to be validated.

The major problem with the technique presented in Chryssolouris et.al. [16] is the values in the $F^T.F$ matrix. Sometimes the values are so small that the matrix becomes singular and the inverse of the matrix cannot be calculated. Therefore, the confidence interval cannot be

predicted or instability occurs, which can make the confidence intervals several orders of magnitude too wide in extreme cases [13]. As noted in R.D. De Veaux et.al .[13], non-linear regression methods are prone to cause several problems when applying to small samples. The ratio of the number of weights vs. training data is very important.

One more problem with the NLR technique is the number of degrees of freedom, which is the (number of observations – number of parameters). The number of parameters, total number of weights and biases, can exceed the number of observations, and that is not appropriate for these calculations. However, the advantage of this method is that it gives results quickly, and it does not require higher computational powers.

3.4 Development of Confidence Interval via Bootstrap Estimation

The development of a confidence interval using bootstrap estimation is a straightforward process. The main problem with this method is that it is computationally expensive. The steps involved in this technique were given in Section 2.1.2. The bootstrap estimation algorithm requires that the model be retrained B times, which is the number of bootstrap samples. Typically B is in the range $20 \leq B \leq 200$ [24]. This method doesn't require matrix inversion or the existence of derivatives, and it can be shown that [24] the bootstrap pairs sampling estimate (as $B \rightarrow \infty$) agrees with the standard least squares formula $[x_i^T (X^T X)^{-1} x_i \hat{\sigma}^2]^{1/2}$, X denoting the design matrix having rows x_i .

3.4.1 Validation of Bootstrapping Model

For validation purposes, the method given in R. Tibshirani [24] was used. This method requires calculating the standard deviation estimators for 25 simulations. In this example, four input Gaussian variables with mean zero and variance one were used. This predictor set was generated once and then fixed for all 25 simulations. The value y was generated as given in Equation (58). There were 100 observations in each training set. The architecture used for training was 4-2-1.

$$y = 3f(2x_1 + 4x_2 + 3x_3 + 3x_4) + 3f(2x_1 + 4x_2 - 3x_3 + 3x_4) + \varepsilon \quad (58)$$

where $f(\cdot)$ is sigmoidal function given as $f(x) = \frac{1}{1 + \exp(-x)}$ and ε is Gaussian with a mean of zero and standard deviation of 0.7.

Table 3.4 Median Standard Error and Standard Deviation for 25 Simulations.

Simulation Number	Median of Standard error	Standard Deviation of Predicted	MSE Training
1	1.69	1.67	1.30
2	1.66	1.67	1.32
3	1.76	1.68	1.29
4	1.73	1.68	1.37
5	1.81	1.57	1.50
6	1.65	1.66	1.43
7	1.82	1.42	1.93
8	1.70	1.54	1.61
9	1.70	1.45	1.89
10	1.65	1.66	1.35
11	1.73	1.67	1.34
12	1.72	1.66	1.30
13	1.74	1.68	1.29
14	1.65	1.66	1.30
15	1.74	1.65	1.38
16	1.64	1.53	1.71
17	1.74	1.39	1.96
18	1.69	1.58	1.51
19	1.83	1.59	1.51
20	1.71	1.47	1.79
21	1.80	1.65	1.32
22	1.74	1.56	1.59
23	1.75	1.59	1.50
24	1.71	1.66	1.30
25	1.75	1.55	1.51
Median	1.73	1.65	

Let $\hat{s}_{ik}$ be the estimated standard deviation of $f(x; \hat{\theta})$ for the k^{th} simulated sample. The median over the training cases of the estimated standard deviation of $\hat{y}_i$ for the k^{th} simulated sample is given by $se_k \equiv \text{median}_i(\hat{s}_{ik})$. Let s_i be the actual standard deviation of $f(x; \hat{\theta})$. The

median of the actual values of the standard deviation was found to be 1.65 and se_k calculated over 25 simulated samples was 1.73, which is very close to the actual standard deviation. For the example given by R. Tibshirani [24], the actual standard deviation was found to be 0.86, and for the bootstrap sampling (se_k), it was found to be 0.96. Since the values of standard deviation were close, the developed model was treated as a valid model. The median of the standard errors and actual standard deviation values are given in Table 3.4.

3.5 Development of Confidence Interval via Maximum-likelihood Estimation (MLE)

As mentioned by Papadopoulos et. al. [23] there are two sources of uncertainty – noise variance σ_v^2 and uncertainty variance σ_m^2 . The data noise is modeled as additive Gaussian independently, identically distributed (i.i.d.) errors with zero mean and variance σ_v^2 . The independently, identically distributed are those variables that have the same probability distribution as any of the others and are mutually independent. The later uncertainty variance, σ_m^2 , is referred to as the model uncertainty variance. In case of the ANNs, the model certainty is due to weight misspecification.

As further explained by Papadopoulos et.al.[23], these two sources of uncertainties are assumed to be independent, and the total prediction variance is calculated as $\sigma_{total}^2 = \sigma_v^2 + \sigma_m^2$. Under maximum-likelihood training, a separate network is used to obtain the input independent estimate of σ_m^2 . The data noise variance σ_v^2 is calculated using the standard formula to calculate the variance in the data. The steps to calculate the confidence interval are given as follows:

1. Split the data into training and test data.
2. Scale the data.
3. Train the network.
4. Calculate σ_v^2 for the data used to predict the output.
5. Scale the values back.
6. Calculate the errors ($y_{out} - target$) for each data set.
7. Scale the data again.

8. Train a separate network using the same inputs used in step three with target values as $(y_{out} - target)^2$.
9. Approximating the target values of the network from step six as σ_m^2 , the total noise variance σ_{total}^2 can be calculated.
10. Scale the data back.
11. Select an appropriate confidence level and respective student t-distribution value.
12. Use $y_{out_k} - t \sigma_{total}^2 \leq f(x) \leq y_{out_k} + t \sigma_{total}^2$ to find confidence intervals for the training data [31].
13. Repeat steps two to 12 for the test data.

3.5.1 Validation of the MLE model

The MLE model was developed based on the information mentioned by J. G. Carney, P. Cunningham, and U. Bhagwan [31] and R. Dybowski [32]. Carney et.al.[31] provided important insight over the information for predicting confidence intervals using MLE. The authors test the models using Equation (60). However, Carney et al. [31] did not have sufficient information to validate this model. The authors provided information only on the efficiency of the model. Dybowski [32] provided the basic information needed to construct the confidence intervals, but did not have information on the validation of the model nor does the give any example for comparison.

3.6 Comparison of Confidence Intervals for Linear Regression and Neural Networks

Computations of confidence intervals for linear regression were discussed in Section 3.2. Tree data [47] were used to compute the confidence intervals, and to recall the coverage probability for individual observations was 92.31% for linear regression with 95% nominal probability and 82.69% CP with 90% nominal probability. The same data were used to compute confidence intervals using the above discussed techniques. The neural network and confidence interval parameters are given in Table 3.5.

Table 3.5 Neural Network and Confidence Interval Parameters for 95% Nominal Probability

Number of Observations For Training	80
Number of Observations For Testing	24
Number of Hidden Neurons	2
Number of Iterations	500
Total Number of Parameters	7
Degrees of Freedom	73
t-Distribution Value	1.99
Activation Function Between Input and Hidden	Sigmoid
Activation Function Between Hidden and Output	Linear

The details of the results obtained from neural network and the confidence estimating techniques is listed in Table 3.6 and Table 3.7. According to the CP-95 values, linear regression has the least difference from the nominal probability. Confidence curves obtained via all the techniques and by linear regression are superimposed on one graph, shown in Figure 3.9. Confidence curves obtained via non-linear regression (NLR) with (NLR-wCF) and without the correction factor for neural networks are shown in Figure 3.6. Although linear regression had the best CP-95 value among all the techniques, bootstrapping was the best CP-90 value.

Table 3.6 Results Obtained by Neural Network and Confidence Estimation Techniques with 95% Probability

Total Observations	104	Observations for Training	80		
Training MSE	1,416,605	Test MSE	883,801		
Training R-sq	0.91	Test R-sq	0.85		
Nominal (%)	95	Points should've covered	99		
	NLR	NLR-wCF	Boot	MLE	LR
Points Covered by CIs	89	104	102	88	96
Points Not covered by CIs	15	0	2	16	8
CP (%)	85.58%	100.00%	98.08%	84.62%	92.31%
CP - Nominal (%)	9.42%	-5.00%	-3.08%	10.38%	2.69%

Table 3.7 Results Obtained by Neural Network and Confidence Estimation Techniques with 90% Probability

Total Observations	104	Observations for Training		80	
Training MSE	1,416,605	Test MSE		883,801	
Training R-sq	0.91	Test R-sq		0.85	
Nominal (%)	90	Points should've covered		94	
	NLR	NLR-wCF	Boot	MLE	LR
Points Covered by CIs	85	104	93	85	86
Points Not covered by CIs	19	0	11	19	18
CP (%)	81.73%	100.00%	89.42%	81.73%	82.69%
CP - Nominal (%)	8.27%	-10.00%	0.58%	8.27%	-7.31%

Figure 3.6 Trunk Girth vs. Weight Using Neural Networks with Confidence Curves via Non-Linear Regression-with and without the Correction Factor (CF) with Confidence Level 95%

Both fitted line and actual data points for NLR with the CF are shown in Figure 3.6. Confidence intervals obtained without the CF are wide for initial trunk girth values, then narrow around the high data density area. Confidence intervals obtained using the CF cover all the points, hence, obtaining coverage probability of 100%. Figure 3.7 shows the confidence curves

obtained using the bootstrap estimation technique. Bootstrap spreads out when the data density is low and narrow when data density is high.

Confidence curves obtained using the maximum likelihood estimation (MLE) technique are shown in Figure 3.8. Results obtained by MLE were quite close to results obtained by NLR without the CF with CP of 84.62%. MLE failed to obtain spread like NLR and bootstrapping but it obtained CP similar to NLR. The spread was constant similar to the spread obtained by linear regression.

It should be noted that all these techniques assume that the predicted output is very close to the actual values, which was not a case in this example. All the curves are superimposed in one graph and shown in Figure 3.9. The spread obtained by bootstrapping was very close to the expectation. Linear regression and MLE obtained a constant spread for all data points. For 90% probability, linear regression obtained $|CP-90|$ of 7.31%, which was close to the CP-90 obtained by NLR and MLE.

Figure 3.7 Trunk Girth vs. Weight Using Neural Networks with Confidence Curves Using Bootstrap with Confidence Level 95%

Figure 3.8 Trunk Girth vs. Weight Using Neural Networks with Confidence Curves Using MLE with Confidence Level 95%

Figure 3.9 Confidence Curves Obtained via All Techniques

4 Assessing Confidence Estimation Techniques

4.1 Introduction

The assessment of the confidence estimation techniques was done by following the methods suggested by R.D. De Veaux et.al.[13], G. Papadopoulos et.al.[23], J. R. Donaldson et.al.[33], and J. T. G. Hwang et.al.[34]. The estimation techniques were the non-linear regression, bootstrapping, and maximum likelihood estimation. The coverage probability (CP) of the confidence intervals was computed to assess the confidence estimation techniques. CP is evaluated by calculating the percentage of target (original y) data points that lie within the confidence interval range on the predicted data. Therefore, CP is the probability that the true value lies within the confidence interval [23]. The performance of a confidence measure can be assessed in practice by estimating the observed CP and comparing it with the nominal value. Also, a confidence estimation technique will be good if the CP value is close to the nominal value.

It should be noted that for the maximum likelihood estimation technique, the results could vary depending on the number of epochs used for training the residuals as target values. The literature does not provide any information on how long the residuals are trained. Moreover, the number of hidden layer neurons can also be changed for the residual training, and the literature again fails to provide the information.

Various data sets from the literature were used to assess the estimation techniques. Fifteen simulations were taken for each estimation technique and then mean CP was calculated. All the techniques assume that the error or noise in the data or in the weights is Gaussian distributed, except NLR, which uses the correction factor as explained in Section 2.1.1. If the correction factor is used, it results in coverage of all the actual points, hence, obtaining a CP of 100%. However, the comparing criterion of this research was based on coverage probabilities, therefore, the NLR estimation technique without the correction factor was used.

Four different cases were studied for the assessment of these confidence estimation techniques. For Case A, a synthetic data set was created using a polynomial equation with five input variables, one output variable, and it had 250 data points. Case B was taken from McKim [46], which had two input and one output variables. The input variables were flow of pumps in gpm and head in inches and the output variable was the actual cost of the pump. This data set had 23 observations.

Synthetic data presented in J. G. Carney [31], which had 1000 observations for training and 1000 observations for testing with one input and output variable, was for Case C. Tree data [46] used for Case D was the same data set previously used to compare the techniques. This data set had trunk girth of the tree as an input variable, weight of the tree as an output variable, and had 104 observations.

4.2 Case Studies

4.2.1 Case A

A data set with 250 rows with five input variables using Equation (59) was generated. This data set was without any noise, and it was easy to train. Out of 250 data points, 175 were used for training and 75 were used for testing. The data set used is given in Table A-1 of Appendix A. The values of X were generated randomly, ranging from zero to one. The neural net architecture was 5-2-1. The learning rate was kept constant, as 0.2 and 100 epochs were sufficient for a good fit for the training and test data. Usually preferred, sigmoid activation function for the hidden layer and linear activation function for the output layer were selected. The details of training and confidence interval calculation parameters are given in Table 4.1. The number of bootstrap samples used was 20, which is the lower limit of samples recommended [24] but good enough for complicated problems such as neural networks.

$$y = 2x_1^2 + 3x_2^3 + 4x_3 + x_4^{1/2} + 4x_5 \quad (59)$$

Table 4.1 Neural Network and Confidence Interval Parameters for Case A

Number of Observations For Training	175
Number of Observations For Testing	75
Number of Inputs	5
Number of Hidden Neurons	2
Learning Rate	0.2
Number of Iterations	100
Total Number of Parameters	15
Degrees of Freedom	160
Activation Function Between Input And Hidden	Sigmoid
Activation Function Between Hidden And Output	Linear

For Case A at the 95% confidence interval, NLR obtained the best average $|CP-95|$ of 0.76%. Bootstrap estimation obtained an average $|CP-95|$ of 3.29% over 15 simulations, whereas MLE obtained, average $|CP-95|$ of 3.45% with the coverage of 232 points inside the confidence intervals. Table 4.2 gives the summary for this case study. These programs were run on a computer with a Pentium 4, 2.20 GHz processor and 640 MB RAM. Results for all the 15 simulations for nominal probability of 95% are given in Table C-1 of Appendix C. Results for 90% nominal probability are summarized in Table 4.3. When the confidence level or nominal probability was 90%, bootstrap was found to be the best of the three techniques with the average CP-90 of 6.91%. Results for this confidence level are given in Table C-2. Standard deviation (SD) of all the CPs obtained over 15 simulations was also computed and given in Table 4.2 and Table 4.3. It can be seen that bootstrapping had the highest SD over 15 simulations and NLR had the lowest SD.

Table 4.2 Results for Case A: Average Taken Over 15 Simulations for 95% Confidence Level

		Non-linear Regression	Bootstrapping	MLE
1	Total Points Used	250	250	250
2	Nominal	95%	95%	95%
3	Expected Coverage	238	238	238
4	Covered Points	239	241	232
5	Average CP (%)	95.63%	96.37%	92.88%
6	Average $ CP - 95 $ (%)	0.76%	3.29%	3.45%
7	Range	94.00-96.80	90.00-100.00	89.20-100.00
8	SD of CPs	0.61	3.57	3.14

Table 4.3 Results for Case A: Average Taken Over 15 Simulations for 90% Confidence Level

		Non-linear Regression	Bootstrapping	MLE
1	Total Points Used	250	250	250
2	Nominal	90%	90%	90%
3	Expected Coverage	225	225	225
4	Covered Points	205	220	200
5	Average CP (%)	82.13%	88.16%	80.16%
6	Average $ CP - 90 $ (%)	7.87%	6.91%	12.51%
7	Range	80.80-86.80	73.20-99.20	74.40-100.00
8	SD of CPs	1.43	8.48	8.27

4.2.2 Case B

For case B, cost data were taken from McKim [46], which are also given in Table 2-1. These data contained two input variables and one output variable with 23 data rows. Out of 23 data rows, the first 19 were used for training and the remaining four for testing. The number of hidden layer neurons was two with 10 degrees of freedom, which were used in calculations of non-linear regression. The net architecture was 2-2-1, and no excess noise was added. Detailed training and confidence interval parameters are given in Table 4.4. Summary of the results obtained for Case B are given in Table 4.5.

Table 4.4 Neural Network and Confidence Interval Parameters for Case B

Number of Observations For Training	19
Number of Observations For Testing	4
Number of Inputs	2
Number of Hidden Neurons	2
Learning Rate	0.2
Number of Iterations	200
Total Number of Parameters	9
Degrees of Freedom	10
Activation Function Between Input and Hidden	Sigmoid
Activation Function Between Hidden and Output	Linear

Table 4.5 Results for Case B: Average Taken Over 15 Samples for 95% Confidence Level

		Non-linear Regression	Bootstrap	MLE
1	Total Points Used	23	23	23
2	Nominal	95%	95%	95%
3	Expected Coverage	22	22	22
4	Covered Points	22	22	21
5	Average CP (%)	95.65%	94.20%	90.72%
6	Average CP – 95 (%)	0.65%	1.67%	4.62%
7	Range	95.65-95.65	91.30-95.65	82.61-95.65
8	SD of CPs	0.00	2.12	3.98

For Case B, bootstrapping and NLR obtained average $|CP-95|$ of 0.65% and 1.67% respectively, whereas MLE had average $|CP-95|$ of 4.62%. Figure 4.1 show the obtained confidence intervals by all the techniques for the nominal probability of 95%. The results for all simulations are given in Table C-3 of Appendix C. Results obtained for Case B with nominal probability of 90% are given in Table 4.6. For 90% nominal probability, NLE and bootstrap obtained average $|CP-95|$ of 2.17% and 2.35%, respectively. MLE obtained the worst average $|CP-95|$ of 8.55%. The results for all simulations are given in Table C-4.

Table 4.6 Results for Case B: Average Taken Over 15 Samples for 90% Confidence Level

		Non-linear Regression	Bootstrap	MLE
1	Total Points Used	23	23	23
2	Nominal	90%	90%	90%
3	Expected Coverage	21	21	21
4	Covered Points	21	21	19
5	Average CP (%)	92.17%	90.14%	84.64%
6	Average $ CP - 90 $ (%)	2.17%	2.35%	8.55%
7	Range	91.30-95.65	82.61-95.65	73.91-95.65
8	SD of CPs	1.80	3.06	7.86

Figure 4.1 Confidence Intervals by all the Techniques for Case B

4.2.3 Case C

The data for Case C were taken from J. G. Carney et.al.[31]. Here, the input vector contains only a single value, and the inputs were uniformly drawn at random from the interval [0, 2]. The target values were generated using (60) and (61). One thousand data were used for training and 1000 were used for testing the models. The net architecture was 1-3-1, which was trained using 200 epochs. This case was complex compared to the other cases; hence an additional hidden neuron was used. Training and confidence interval parameters are given in Table 4.7, and Table 4.8 summarizes the results for the models.

$$y = 4.26(e^{-x} - 4e^{-2x} + 3e^{-3x}) + \varepsilon(x) \quad (60)$$

$$\langle \varepsilon^2(x) \rangle = -0.1(e^{-18x} - e^{-4x}) \quad (61)$$

As it is shown in Table 4.8, bootstrapping calculated better confidence intervals than the NLR and MLE, with average |CP-95| of 3.80%. The results obtained by the MLE and NLR technique were almost the same with average |CP-95| of 5.02% and 4.98% respectively. Although, bootstrapping provided the best results of the three techniques, it should be noted that bootstrapping requires high computational powers for large data sets, as in this case, which it took approximately 45 minutes to predict confidence intervals for 15 simulations. However, time taken by other techniques is minimal. Results for all the 15 simulations are given in Table C-5 of Appendix C. Results obtained for 90% nominal probability are given in Table 4.9. When the intervals were calculated using 90%, bootstrap failed to achieve good results with average |CP-90| of 7.09%, and NLR obtained much better average |CP-90| of 3.38%. The results for all simulations are given in Table C-6. Confidence curves obtained by all the techniques for the 11th simulation are shown in Figure 4.2.

Table 4.7 Neural Network and Confidence Interval Parameters for Case C

Number of Observations for Training	1000
Number of observations for testing	1000
Number of inputs	1
Number of Hidden Neurons	3
Learning Rate	0.2
Number of iterations	200
Total Number of parameters	10
Degrees of Freedom	990
Activation function between input and hidden	Sigmoid
Activation Function Between Hidden And Output	Linear

Table 4.8 Results for Case C: Average Taken Over 15 Samples for 95% Confidence Level

		Non-linear Regression	Bootstrap	MLE
1	Total Points Used	2000	2000	2000
2	Nominal	95%	95%	95%
3	Expected Coverage	1900	1900	1900
4	Covered Points	1800	1973	1986
5	Average CP (%)	90.02%	98.64%	99.32%
6	Average CP – 95 (%)	4.98%	3.80%	5.02%
7	Range	89.75-90.35	93.85-100.00	89.75-100.00
8	SD of CPs	0.19	1.84	2.65

Table 4.9 Results for Case C: Average Taken Over 15 Samples for 90% Confidence Level

		Non-linear Regression	Bootstrap	MLE
1	Total Points Used	2000	2000	2000
2	Nominal	90%	90%	90%
3	Expected Coverage	1800	1800	1800
4	Covered Points	1732	1942	1982
5	Average CP (%)	86.62%	97.09%	99.11%
6	Average CP – 90 (%)	3.38%	7.09%	9.55%
7	Range	86.00-87.05	91.05-99.90	86.70-100.00
8	SD of CPs	0.28	2.60	3.43

Figure 4.2 Confidence Curves Obtained by all Techniques for Case C at 95% Confidence Level

It clearly can be seen from Figure 4.2 that MLE greatly overestimated variance and obtained very wide intervals. Bootstrapping also overestimated the confidence intervals, in particular for the values of x greater than 0.5, whereas NLR underestimated the confidence level for the values of x less than 0.8.

4.2.4 Case D

The data for case D was taken from SAS's Website [45] as explained in Section 3.2. There were 104 observations, one output variable, and one input variable in the dataset. The neural network and confidence interval parameters are given in Table 4.10, and the results are summarized in Table 4.11 (95%) and Table 4.12 (90%). In this case, bootstrap was better than the NLR and the MLE techniques with $|CP-95|$ of 4.18%. Results from this case are given in Table C-7 and Table C-8 of Appendix C. For 90% nominal probability, again bootstrap was better than NLR and the MLE with $|CP-90|$ of 5.12%. All of the technique gave relatively poor results for case D compared to the other three cases.

Table 4.10 Neural Network and Confidence Interval Parameters for Case D

Number of Observations For Training	80
Number of Observations For Testing	24
Number of Inputs	1
Number of Hidden Neurons	2
Learning Rate	0.2
Number of Iterations	300
Total Number of Parameters	7
Degrees of Freedom	73
Activation Function Between Input And Hidden	Sigmoid
Activation Function Between Hidden And Output	Linear

Table 4.11 Results for Case D: Average Taken Over 15 Samples for 95% Confidence Level

		Non-linear Regression	Bootstrap	MLE
1	Total Points Used	104	104	104
2	Nominal	95%	95%	95%
3	Expected Coverage	99	99	99
4	Covered Points	90	102	97
5	Average CP (%)	86.73%	97.69%	93.53%
6	Average CP – 95 (%)	8.27%	4.18%	6.81%
7	Range	85.58-91.35	88.46-100.00	83.65-100.00
8	SD of CPs	1.59	3.77	7.26

Table 4.12 Results for Case D: Average Taken Over 15 Samples for 90% Confidence Level

		Non-linear Regression	Bootstrap	MLE
1	Total Points Used	104	104	104
2	Nominal	90%	90%	90%
3	Expected Coverage	94	94	94
4	Covered Points	85	97	95
5	Average CP (%)	81.86%	93.14%	90.96%
6	Average CP – 90 (%)	8.14%	5.12%	9.71%
7	Range	81.73-83.65	83.65-100.00	77.88-100.00
8	SD of CPs	0.50	4.97	10.04

5 Results and Conclusion

The non-linear regression, the bootstrapping estimation, and the maximum likelihood estimation were identified as techniques for predicting confidence intervals on the output of the neural networks. These techniques were modeled in Visual Basic to analyze them further by testing on various data sets. All three techniques were tested on artificial and real data sets.

To assess these techniques, the coverage probability was calculated over 15 samples and the average was taken. The average of the absolute values of (CP-95) for all cases are given in Table 5.1 and Figure 5.1. For a nominal probability of 95%, the bootstrapping estimation (3.23%) was slightly better than the NLR technique (3.67%), and the NLR was better than the MLE (4.98%). However the bootstrapping method had significantly higher standard deviations in its estimates than the NLR method. Table 5.2 and Figure 5.2 indicated slightly better results for the bootstrapping method at |CP-90%| when comparing averages but worse results when comparing standard deviations.

On the basis of average coverage probability minus nominal probability, out of the eight cases (95 and 90), NLR and bootstrap were better for four cases. Also, bootstrapping was never the worst of all the techniques in the eight cases. However, when the ranges and standard deviation (SD) of the CP for all simulations were considered, NLR had the least range SD and was consistent with the coverage probability. Coverage probability ranges for bootstrapping were not consistent, as bootstrapping involves the training of the bootstrap samples, and the coverage probabilities depend upon the training of each sample. The random weight initialization for each training session was always different and caused the variation in the training of each bootstrap sample.

After examining these results, recommending which technique should be used depends on the need of the user. If consistency is the primary criterion, the non-linear regression technique should be used as it had the smallest ranges, and its average CP values were within one-half percentage point of the bootstrapping method, and this difference was statistically not significant. If coverage probability is the primary criterion, bootstrapping can be used in the instances where the difference between non-linear regression and bootstrap is statistically significant and bootstrap has better CP-nominal probability. T-tests were conducted to test if the average |CP-95| and average |CP-90| obtained by NLR and bootstrap were statistically different, given in Appendix F. For average |CP-95|, for all the cases, the t-statistics were significant at the 0.05

and 0.1 critical alpha level. Therefore, the null hypothesis for all cases and critical alpha level of 0.05 and 0.1 was rejected, and it was concluded that there was significant difference between the average |CP-95| obtained by NLR and bootstrap, as given in Table F-1. For the average |CP-90|, the null hypothesis was accepted for Case A and Case B and it was rejected for Case C and Case D, at critical alpha level of 0.05 and 0.1. Therefore, it was concluded that there was no significant difference in the average |CP-90| obtained by NLR and bootstrap for Case A and Case B, as given Table F-2.

Table 5.1 Values of (CP-95) for Each Case

	Average CP-95 (%)							Lowest CP-95	Lowest SD
	NLR		Bootstrap		MLE				
	Avg	SD	Avg	SD	Avg	SD			
Case A	0.76%	0.61	3.29%	3.57	3.45%	3.14	NLR	NLR	
Case B	0.65%	0.00	1.67%	2.12	4.62%	3.98	NLR	NLR	
Case C	4.98%	0.19	3.80%	1.84	5.02%	2.65	Boot	NLR	
Case D	8.27%	1.59	4.18%	3.77	6.81%	7.26	Boot	NLR	
Average	3.67%	0.60	3.23%	2.82	4.98%	4.26	Boot	NLR

Figure 5.1 CP – 95 Results for Each Technique for Respective Data Sets Shown in this Order: NLR, Bootstrapping, and MLE

Table 5.2 Values of (CP-90) for Each Case

	Average CP-90 (%)							Lowest CP-90	Lowest SD
	NLR		Bootstrap		MLE				
	Avg	SD	Avg	SD	Avg	SD			
Case A	7.87%	1.43	6.91%	8.48	12.51%	8.27	Boot	NLR	
Case B	2.17%	1.80	2.35%	3.06	8.55%	7.86	NLR	NLR	
Case C	3.38%	0.28	7.09%	2.60	9.55%	3.43	NLR	NLR	
Case D	8.14%	0.50	5.12%	4.97	9.71%	10.04	Boot	NLR	
Average	5.39%	1.00	5.37%	4.78	10.08%	7.40	Boot	NLR

Figure 5.2 CP – 90 Results for Each Technique for Respective Data Sets Shown in this Order: NLR, Bootstrapping and MLE

The time taken for calculation was also a criterion to judge the performance of these models. The situations where the confidence intervals are most important are in mission-critical or safety-critical situations. Therefore, the time needed to calculate the confidence intervals ideally should be small. Bootstrapping estimation took a large amount of time for each run, as it was trained B times, where B is the number of bootstrap samples. The MLE model also took more time than the non-linear regression, as two nets are trained for the calculation of the confidence intervals. The non-linear regression was the fastest, as it is trained only once, and it

obtained more consistent results in all cases and was the best method in one-half of the cases studied.

5.1 Future Study

The focus of this research was to model, analyze, and compare three popular confidence estimation techniques on the output of neural networks. This research was limited to four cases studied for each technique. The following future studies are suggested for this research:

1. If possible, refine the non-linear regression technique so that the problem of singular matrix or a large matrix does not occur.
2. Develop a better methodology than the coverage probability to compare the results calculated by the confidence estimation techniques, as CP involves using different nominal probabilities to compare the techniques.
3. Develop a rationale for choosing the training parameters for the NN with residuals as target values for the maximum likelihood estimation as,
4. Determine the effect of more hidden neurons in a layer and more layers upon the output of the network.

The most critical problem faced in this research was of the computation of the inverse of the Jacobian matrix; hence, if possible, refinement of the existing non-linear regression technique should be done. Different nominal probabilities (95% and 90%) were used in this research to compare the techniques using the coverage probability technique, which demands extra time and efforts. Therefore, a better method to compare the techniques in a single run would save time and effort.

6 References

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Appendix A Data Tables

Table A-1 The Data Used for Developing Neural Network in Section 3.2.1-

S.N.	x ₁	x ₂	x ₃	x ₄	x ₅	Actual y
1	0.0239	0.2281	0.2837	0.9457	0.6764	4.8494
2	0.1571	0.5192	0.5285	0.7370	0.6364	5.9876
3	0.6795	0.6443	0.8955	0.3714	0.9198	9.5968
4	0.9631	0.2735	0.3764	0.1937	0.7892	7.0193
5	0.8691	0.4995	0.4351	0.0631	0.7287	6.7905
6	0.4740	0.4804	0.8204	0.6564	0.9313	8.5989
7	0.1256	0.6800	0.1080	0.0453	0.2924	2.7894
8	0.3469	0.6336	0.5620	0.1417	0.6948	6.4071
9	0.1467	0.5378	0.8104	0.5658	0.0556	4.7262
10	0.7358	0.8559	0.8393	0.5282	0.7486	10.0420
11	0.2762	0.1367	0.7559	0.4707	0.8531	7.2822
12	0.6781	0.7725	0.7578	0.2065	0.5496	7.9863
13	0.6267	0.0449	0.0119	0.0594	0.7131	3.9293
14	0.1339	0.3106	0.5082	0.2049	0.7556	5.6334
15	0.5132	0.1146	0.3071	0.9322	0.2545	3.7428
16	0.2137	0.3644	0.9563	0.6002	0.1824	5.5661
17	0.0397	0.3595	0.8112	0.2297	0.4008	5.4701
18	0.8914	0.8178	0.4779	0.0551	0.2130	6.2285
19	0.5203	0.2147	0.8441	0.1063	0.3700	5.7536
20	0.9312	0.3654	0.3229	0.6691	0.8939	7.5658
21	0.1268	0.6412	0.7021	0.3286	0.2128	5.0560
22	0.4048	0.7625	0.6609	0.7150	0.8542	8.5634
23	0.8937	0.7554	0.8679	0.8709	0.0785	7.6090
24	0.8071	0.4231	0.3670	0.3018	0.0260	3.6514
25	0.0426	0.7968	0.3431	0.7370	0.6933	6.5253
26	0.2718	0.4407	0.4416	0.7126	0.2619	4.0625
27	0.2627	0.9230	0.3075	0.0553	0.0480	4.1544
28	0.7823	0.5018	0.7328	0.8124	0.1230	5.9276
29	0.0192	0.7359	0.1902	0.0783	0.1991	3.0333
30	0.8913	0.8169	0.8083	0.0748	0.3980	8.3226
31	0.0134	0.6790	0.7415	0.8339	0.3749	6.3185

Table A-1 The Data Used for Developing Neural Network in Section 3.2.1-Cont'd

S.N.	x ₁	x ₂	x ₃	x ₄	x ₅	Actual y
32	0.0734	0.4884	0.9802	0.7821	0.7508	8.1685
33	0.3949	0.8804	0.2933	0.1133	0.6062	6.2937
34	0.7339	0.4585	0.7351	0.4932	0.7389	7.9643
35	0.7656	0.0137	0.6070	0.7290	0.0064	4.4799
36	0.3444	0.7594	0.2260	0.4149	0.7128	5.9503
37	0.8015	0.3532	0.9486	0.2659	0.2815	6.8527
38	0.6184	0.8659	0.5598	0.7140	0.0068	5.8240
39	0.6136	0.6239	0.7199	0.4452	0.5346	7.1668
40	0.0948	0.3264	0.4926	0.1900	0.0998	2.9277
41	0.1180	0.9481	0.2577	0.8953	0.1227	5.0521
42	0.3469	0.4105	0.0513	0.0285	0.5911	3.1869
43	0.5559	0.9643	0.4943	0.6764	0.5592	8.3444
44	0.9051	0.6873	0.2058	0.6894	0.1003	4.6675
45	0.3950	0.5173	0.3644	0.2676	0.2310	3.6262
46	0.6230	0.2508	0.2118	0.9758	0.1386	3.2128
47	0.4411	0.8772	0.3807	0.6505	0.4002	6.3442
48	0.7975	0.4668	0.0856	0.5023	0.6999	5.4278
49	0.8092	0.3320	0.9264	0.3814	0.4807	7.6654
50	0.2221	0.1583	0.6054	0.1641	0.2355	3.8794
51	0.9471	0.4417	0.4604	0.8783	0.1391	5.3875
52	0.9126	0.8013	0.9857	0.7792	0.0232	8.1276
53	0.9093	0.9862	0.7828	0.5770	0.9999	12.4218
54	0.5680	0.7294	0.1067	0.3431	0.6226	5.3126
55	0.5209	0.9931	0.0804	0.4290	0.4198	6.1361
56	0.6801	0.8100	0.2017	0.9051	0.4014	5.8832
57	0.3100	0.9004	0.8872	0.8204	0.1096	7.2752
58	0.6777	0.1640	0.1855	0.3466	0.4621	4.1113
59	0.9112	0.1917	0.6855	0.0547	0.4423	6.4267
60	0.3117	0.9877	0.4843	0.3650	0.3965	7.2122
61	0.2280	0.0467	0.1026	0.9404	0.2700	2.5646
62	0.2951	0.2270	0.1909	0.5251	0.3857	3.2405
63	0.2512	0.6615	0.3822	0.5652	0.3585	4.7090
64	0.1628	0.0218	0.7591	0.9421	0.4239	5.7553
65	0.8647	0.4620	0.3933	0.3864	0.4532	5.7985

Table A-1 The Data Used for Developing Neural Network in Section 3.2.1-Cont'd

S.N.	x ₁	x ₂	x ₃	x ₄	x ₅	Actual y
66	0.6335	0.5478	0.6324	0.0639	0.1765	4.7845
67	0.9811	0.5597	0.4834	0.0639	0.8187	7.9126
68	0.7080	0.1566	0.9612	0.2189	0.7393	8.2838
69	0.7386	0.4789	0.0463	0.9596	0.2925	3.7556
70	0.3404	0.3797	0.9975	0.2679	0.9131	8.5558
71	0.8566	0.7577	0.0272	0.2721	0.2793	4.5204
72	0.3696	0.9260	0.0232	0.5718	0.0189	3.5792
73	0.5100	0.5620	0.6927	0.3615	0.0258	4.5278
74	0.2969	0.0253	0.6400	0.3067	0.7892	6.4468
75	0.8339	0.9618	0.6412	0.3240	0.0971	7.5821
76	0.0684	0.6194	0.6557	0.8244	0.5986	6.6475
77	0.9727	0.5761	0.1997	0.7980	0.3587	5.5930
78	0.6869	0.8771	0.3365	0.1055	0.4638	6.4941
79	0.3473	0.9077	0.0337	0.2185	0.3502	4.4881
80	0.3200	0.3063	0.7559	0.1178	0.4499	5.4575
81	0.3940	0.7924	0.5717	0.1294	0.6936	7.2240
82	0.6238	0.6501	0.5776	0.3082	0.2359	5.4118
83	0.8650	0.0365	0.6956	0.2370	0.9106	8.4079
84	0.2149	0.4066	0.5051	0.2656	0.8267	6.1368
85	0.1775	0.6390	0.3491	0.9226	0.2894	4.3601
86	0.2020	0.0233	0.9229	0.7632	0.2136	5.5011
87	0.9238	0.3293	0.1232	0.6243	0.3323	4.4262
88	0.2562	0.3846	0.6441	0.5276	0.2604	4.6464
89	0.9465	0.6304	0.5181	0.9919	0.1338	6.1468
90	0.5620	0.3794	0.9842	0.6549	0.3658	7.0046
91	0.8507	0.8384	0.8734	0.1001	0.5907	9.3880
92	0.1984	0.5782	0.4140	0.5404	0.8026	6.2603
93	0.6868	0.8578	0.3759	0.7524	0.7593	8.2448
94	0.2944	0.9174	0.6105	0.1310	0.6146	7.7518
95	0.1202	0.3986	0.6082	0.2452	0.3633	4.6000
96	0.3092	0.1226	0.3854	0.3724	0.5265	4.4548
97	0.1859	0.4205	0.6849	0.9640	0.4316	5.7401
98	0.9842	0.2275	0.4219	0.2407	0.9888	8.1059
99	0.2862	0.3026	0.6762	0.1097	0.5313	5.4082

Table A-1 The Data Used for Developing Neural Network in Section 3.2.1-Cont'd

S.N.	x_1	x_2	x_3	x_4	x_5	Actual y
100	0.3964	0.1493	0.4643	0.7676	0.9578	6.8887
101	0.0071	0.8208	0.8392	0.5430	0.0840	6.0881
102	0.8158	0.3934	0.9404	0.4607	0.2343	6.8912
103	0.2749	0.0008	0.5066	0.9608	0.4835	5.0919
104	0.4890	0.1120	0.6724	0.8636	0.2614	5.1469
105	0.1810	0.9914	0.3332	0.9942	0.6214	7.8042
106	0.1079	0.8806	0.4427	0.5065	0.3362	5.8988
107	0.8181	0.6815	0.8889	0.2395	0.3648	7.7920
108	0.5097	0.3612	0.8775	0.0385	0.4585	6.2014
109	0.4348	0.2717	0.5575	0.5584	0.8244	6.7130
110	0.3425	0.9309	0.8669	0.8539	0.3047	8.2653
111	0.7452	0.0928	0.5085	0.5488	0.3653	5.3491
112	0.3319	0.0906	0.4034	0.2624	0.8145	5.6063
113	0.0407	0.5712	0.6190	0.0699	0.4435	5.0764
114	0.6785	0.6325	0.0723	0.3515	0.0855	2.9040
115	0.1224	0.7119	0.2399	0.6785	0.5409	5.0595
116	0.0773	0.5078	0.5643	0.6446	0.7030	6.2772
117	0.6357	0.0396	0.6937	0.1212	0.2191	4.8075
118	0.7104	0.2313	0.2838	0.6047	0.7401	5.9198
119	0.7296	0.0281	0.1633	0.5545	0.5701	4.7427
120	0.7405	0.3688	0.1491	0.8700	0.8939	6.3522
121	0.6587	0.4608	0.6283	0.4940	0.7414	7.3429
122	0.6300	0.8905	0.1533	0.7308	0.2405	5.3428
123	0.4181	0.1814	0.8571	0.9921	0.3026	6.0025
124	0.4075	0.0294	0.4287	0.5155	0.5689	5.0405
125	0.3004	0.7691	0.7138	0.2311	0.1105	5.3233
126	0.4735	0.2910	0.8175	0.2037	0.1535	4.8579
127	0.9722	0.9219	0.8917	0.6238	0.4208	10.2802
128	0.4668	0.7926	0.5638	0.5911	0.6917	7.7209
129	0.8029	0.9061	0.1782	0.7836	0.4943	7.0969
130	0.1191	0.7769	0.7423	0.6156	0.7220	8.0770
131	0.4114	0.2153	0.7511	0.6300	0.5954	6.5481
132	0.7276	0.7320	0.7102	0.6282	0.4134	7.5220
133	0.2569	0.3297	0.6233	0.9762	0.2045	4.5389

Table A-1 The Data Used for Developing Neural Network in Section 3.2.1-Cont'd

S.N.	x ₁	x ₂	x ₃	x ₄	x ₅	Actual y
134	0.5201	0.7981	0.5460	0.4931	0.7296	7.8709
135	0.0844	0.9684	0.5018	0.4287	0.0943	5.7775
136	0.1304	0.2845	0.4544	0.2136	0.9012	5.9878
137	0.7163	0.7403	0.5449	0.2579	0.0409	5.0939
138	0.6686	0.5257	0.3850	0.0464	0.3138	4.3407
139	0.2552	0.6929	0.9831	0.6398	0.7074	8.6901
140	0.2494	0.6695	0.7755	0.9577	0.7273	8.0145
141	0.0931	0.6636	0.1045	0.3358	0.1434	2.4649
142	0.5527	0.4078	0.4254	0.7132	0.7351	6.3009
143	0.8479	0.1602	0.6971	0.0533	0.1590	5.1055
144	0.1886	0.3155	0.2074	0.5268	0.1944	2.4988
145	0.8582	0.0152	0.3994	0.2757	0.4730	5.4876
146	0.5354	0.5035	0.1505	0.1208	0.4132	3.5587
147	0.5329	0.6784	0.6925	0.5082	0.2088	5.8226
148	0.5740	0.5394	0.2210	0.5600	0.9368	6.5090
149	0.2175	0.2864	0.3200	0.2001	0.9305	5.6145
150	0.5359	0.1086	0.3636	0.1453	0.2174	3.2833
151	0.0119	0.4085	0.4363	0.2094	0.7796	5.5261
152	0.7644	0.1965	0.1484	0.7671	0.8295	5.9789
153	0.0674	0.2795	0.3926	0.0248	0.1376	2.3531
154	0.6001	0.7814	0.7365	0.2785	0.6445	8.2034
155	0.5402	0.8785	0.0665	0.5590	0.7503	6.6326
156	0.7044	0.9223	0.4359	0.4430	0.6627	8.4063
157	0.6319	0.2204	0.9289	0.5939	0.5202	7.3974
158	0.6073	0.4399	0.0490	0.4452	0.9869	5.8036
159	0.1536	0.9651	0.4113	0.2516	0.0902	5.2514
160	0.1905	0.7917	0.5573	0.5785	0.0322	4.6798
161	0.0420	0.8044	0.0564	0.9220	0.9976	6.7411
162	0.7442	0.6157	0.9454	0.5453	0.5918	8.6949
163	0.4474	0.9662	0.9673	0.0853	0.7087	10.1020
164	0.1288	0.5301	0.2301	0.5638	0.5983	4.5445
165	0.4196	0.8213	0.2681	0.8713	0.3679	5.4915
166	0.6343	0.2961	0.9048	0.0549	0.1813	5.4612
167	0.1907	0.4504	0.2713	0.5807	0.6317	4.7210

Table A-1 The Data Used for Developing Neural Network in Section 3.2.1-Cont'd

S.N.	x ₁	x ₂	x ₃	x ₄	x ₅	Actual y
168	0.5135	0.1835	0.5221	0.2426	0.2151	3.9876
169	0.9579	0.9167	0.3560	0.3826	0.9830	10.1209
170	0.2054	0.9116	0.2765	0.5485	0.6124	6.6535
171	0.8182	0.3308	0.4105	0.8696	0.3685	5.4959
172	0.9750	0.8725	0.6025	0.1045	0.8472	10.0155
173	0.3113	0.2304	0.3960	0.7194	0.1274	3.1724
174	0.4886	0.0289	0.0229	0.3573	0.7044	3.9847
175	0.2581	0.1801	0.6694	0.6382	0.6542	6.2441
176	0.1128	0.6585	0.0555	0.4213	0.5148	3.8123
177	0.1402	0.2739	0.8277	0.3332	0.9574	7.8188
178	0.0337	0.0412	0.1765	0.4780	0.7614	4.4454
179	0.8596	0.8034	0.7434	0.3772	0.2451	7.6021
180	0.3910	0.4500	0.8571	0.1771	0.9643	8.2858
181	0.3812	0.0335	0.4742	0.9616	0.3131	4.4204
182	0.0932	0.7859	0.3164	0.6562	0.9324	7.2789
183	0.6427	0.5295	0.7836	0.1365	0.9827	8.7062
184	0.8294	0.1850	0.3612	0.0970	0.3930	4.7227
185	0.3806	0.9405	0.4711	0.7344	0.3295	6.8443
186	0.9313	0.7566	0.7370	0.2105	0.5830	8.7730
187	0.3264	0.8321	0.8396	0.4447	0.6439	8.5421
188	0.4405	0.3639	0.4695	0.4465	0.6871	5.8276
189	0.6709	0.6583	0.0355	0.6759	0.8252	6.0206
190	0.4836	0.1906	0.6240	0.6970	0.5428	5.9906
191	0.1842	0.0782	0.8574	0.1993	0.8308	7.2687
192	0.3924	0.3597	0.5523	0.7894	0.2094	4.3832
193	0.0327	0.8136	0.3620	0.9500	0.8606	7.4826
194	0.2393	0.6213	0.4343	0.2957	0.7943	6.2922
195	0.9090	0.3484	0.2768	0.9190	0.2461	4.8296
196	0.8749	0.7321	0.0916	0.9134	0.2724	5.1198
197	0.5651	0.9125	0.1096	0.3481	0.1310	4.4704
198	0.3391	0.6068	0.4231	0.9952	0.6479	6.1816
199	0.3286	0.5211	0.3222	0.3325	0.0500	2.7058
200	0.8462	0.9062	0.5152	0.5494	0.0233	6.5594
201	0.0476	0.7180	0.0509	0.4954	0.0118	2.0701

Table A-1 The Data Used for Developing Neural Network in Section 3.2.1-Cont'd

S.N.	x ₁	x ₂	x ₃	x ₄	x ₅	Actual y
202	0.4931	0.3284	0.1354	0.8006	0.7770	5.1368
203	0.8645	0.2591	0.6253	0.0123	0.4648	6.0181
204	0.8264	0.5410	0.4129	0.7736	0.2639	5.4281
205	0.3900	0.7750	0.9228	0.1586	0.9456	9.5727
206	0.5144	0.6677	0.0217	0.3597	0.2637	3.1637
207	0.9533	0.2478	0.8995	0.1411	0.7346	8.7750
208	0.5291	0.6454	0.3536	0.5909	0.0597	3.7880
209	0.4940	0.0885	0.4985	0.8502	0.7788	6.5215
210	0.0896	0.1014	0.1736	0.1966	0.9558	4.9803
211	0.4932	0.2320	0.4239	0.4991	0.2663	3.9914
212	0.6681	0.4161	0.4060	0.1667	0.8554	6.5625
213	0.0439	0.6841	0.1388	0.8801	0.6208	4.9409
214	0.3526	0.9460	0.8034	0.1935	0.7740	9.5377
215	0.4857	0.1074	0.0688	0.7523	0.7981	4.8105
216	0.4901	0.6029	0.0443	0.9058	0.6762	4.9713
217	0.1889	0.2873	0.5162	0.5899	0.7016	5.7816
218	0.5348	0.5360	0.9350	0.0104	0.8186	8.1508
219	0.1610	0.0418	0.8916	0.1728	0.2197	4.9126
220	0.5544	0.3034	0.1748	0.6127	0.3957	3.7633
221	0.5053	0.4064	0.7773	0.9292	0.1089	5.2206
222	0.5106	0.8627	0.8675	0.5647	0.3349	8.0086
223	0.1902	0.7687	0.2353	0.8232	0.2655	4.3453
224	0.8050	0.5386	0.5477	0.2707	0.1147	4.9347
225	0.4309	0.4760	0.8922	0.2891	0.8811	8.3256
226	0.1322	0.7747	0.5724	0.1743	0.8014	7.3427
227	0.8862	0.1516	0.8259	0.9947	0.7942	9.0585
228	0.8577	0.6988	0.8926	0.1442	0.0134	6.4986
229	0.9791	0.7953	0.6163	0.8461	0.3546	8.2297
230	0.9920	0.8411	0.4349	0.3904	0.2068	6.9450
231	0.6576	0.6502	0.7534	0.5948	0.7933	8.6476
232	0.9582	0.3646	0.2848	0.5764	0.5002	5.8808
233	0.2932	0.7870	0.2097	0.0027	0.3066	3.7510
234	0.0651	0.2372	0.9718	0.1690	0.3072	5.5755
235	0.9474	0.6717	0.6880	0.2959	0.0241	6.0966

Table A-1 The Data Used for Developing Neural Network in Section 3.2.1-Cont'd

S.N.	x₁	x₂	x₃	x₄	x₅	Actual y
236	0.8553	0.6513	0.1895	0.5220	0.8510	7.1761
237	0.6433	0.9528	0.9217	0.1119	0.3222	8.7330
238	0.9234	0.6475	0.7131	0.1951	0.8499	9.2132
239	0.8055	0.8589	0.4852	0.4797	0.3707	7.3146
240	0.5252	0.2896	0.3573	0.5916	0.3944	4.4008
241	0.0918	0.8950	0.3130	0.4616	0.9318	7.8265
242	0.1734	0.6991	0.0159	0.9045	0.5308	4.2228
243	0.2934	0.1362	0.8896	0.2738	0.8035	7.4756
244	0.5374	0.9794	0.4441	0.3150	0.4848	7.6721
245	0.1378	0.6899	0.4213	0.6860	0.9035	7.1505
246	0.7730	0.3125	0.3326	0.8647	0.5728	5.8385
247	0.1304	0.3856	0.7780	0.5945	0.0144	4.1466
248	0.9500	0.5251	0.6080	0.1306	0.8014	8.2386
249	0.0328	0.5564	0.7400	0.8584	0.9934	8.3791
250	0.2637	0.4944	0.1119	0.5518	0.0026	1.7028

Table A-2 Tree Data Set [47]-

Obs. No.	Rootstock	Trunk Girth	Weight
1	I	358	760
2	I	375	821
3	I	393	928
4	I	394	1009
5	I	360	766
6	I	351	726
7	I	398	1209
8	I	362	750
9	II	409	1036
10	II	406	1094
11	II	487	1635
12	II	498	1517
13	II	438	1197
14	II	465	1244
15	II	469	1495
16	II	440	1026
17	III	376	912
18	III	444	1398
19	III	438	1197
20	III	467	1613
21	III	448	1475
22	III	478	1571
23	III	457	1506
24	III	456	1458
25	IV	389	944
26	IV	405	1241
27	IV	405	1023

Table A-2 Tree Data Set [47]-Cont'd

Obs. No.	Rootstock	Trunk Girth	Weight
28	IV	392	1067
29	IV	327	693
30	IV	395	1085
31	IV	427	1242
32	IV	385	1017
33	V	404	1084
34	V	416	1151
35	V	479	1381
36	V	442	1242
37	V	347	673
38	V	441	1137
39	V	464	1455
40	V	457	1325
41	VI	376	800
42	VI	314	606
43	VI	375	790
44	VI	399	853
45	VI	334	610
46	VI	321	562
47	VI	363	707
48	VI	395	952
49	VII	266	414
50	VII	241	335
51	VII	380	885
52	VII	401	1012
53	VII	296	489
54	VII	315	616
55	VII	358	788

Table A-2 Tree Data Set [47]-Cont'd

Obs. No.	Rootstock	Trunk Girth	Weight
56	VII	343	733
57	IX	231	375
58	IX	250	410
59	IX	219	335
60	IX	275	560
61	IX	205	251
62	IX	213	272
63	IX	266	478
64	IX	226	278
65	X	299	506
66	X	381	882
67	X	362	737
68	X	372	772
69	X	369	827
70	X	368	821
71	X	408	1149
72	X	410	1035
73	XII	431	1609
74	XII	465	1658
75	XII	484	1789
76	XII	527	2375
77	XII	463	1556
78	XII	412	1418
79	XII	514	2266
80	XII	522	2508
81	XIII	387	1052
82	XIII	414	1167
83	XIII	387	981

Table A-2 Tree Data Set [47]-Cont'd

Obs. No.	Rootstock	Trunk Girth	Weight
84	XIII	390	944
85	XIII	327	737
86	XIII	424	1392
87	XIII	421	1326
88	XIII	382	1052
89	XV	448	1258
90	XV	435	1304
91	XV	451	1290
92	XV	450	1288
93	XV	428	1176
94	XV	424	1177
95	XV	482	1331
96	XV	469	1490
97	XVI	452	1499
98	XVI	412	1412
99	XVI	425	1488
100	XVI	460	1751
101	XVI	464	1937
102	XVI	457	1823
103	XVI	463	1838
104	XVI	473	1817

Appendix B VBA Code for the NN-CI Program

```
Option Compare Database
```

```
Option Explicit
```

```
Private Sub cmbCItech_AfterUpdate()  
Select Case Me.cmbCItech  
Case 1 ' Non-linear regression  
    Me.txtbootsamples.Visible = False  
    Me.Label15.Visible = False  
Case 2 ' Bootstrap  
    Me.txtbootsamples.Visible = True  
    Me.Label15.Visible = True  
Case 3 'MLE  
    Me.txtbootsamples.Visible = False  
    Me.Label15.Visible = False  
End Select  
End Sub
```

```
Private Sub cmdCalculate_Click()  
On Error GoTo errorhandler
```

```
Dim i As Long, j As Long, k As Long  
Dim IParrscaled() As Double, minvalX() As Double, maxvalX() As  
Double  
Dim matcal As New cMathLib  
IParrscaled() = pmtsIP()(0) 'Input array  
minvalX() = pmtsIP()(1)  
maxvalX() = pmtsIP()(2)  
Dim OParrscaled() As Double, minvalY() As Double, maxvalY() As  
Double  
OParrscaled() = pmtsOP()(0) 'Output array  
minvalY() = pmtsOP()(1)  
maxvalY() = pmtsOP()(2)  
Dim novars As Long, noobs As Long, noitrs As Long, alpha As
```

```

Double, nohn As Byte, Cilevel As Double
novars = Forms("frm_Main").lstIPFlds.ItemsSelected.Count
noobs = Forms("frm_Main").txtNOB
noitrs = Forms("frm_Main").txtNoIti
nohn = Forms("frm_Main").txtNOHLN
alpha = Forms("frm_Main").txtAlpha
Cilevel = Me.cmbCilevel
Dim wts() As Variant, V() As Double, W() As Double, Ypred() As
Double, YpredSB() As Double

'Input array for Training
Dim IParrTRScaled() As Double
ReDim IParrTRScaled(noobs - 1, novars - 1)
For i = 0 To noobs - 1
    For j = 0 To novars - 1
        IParrTRScaled(i, j) = IParrscaled(i, j)
    Next j
Next i

'Output array for Training
Dim OParrTRScaled() As Double
ReDim OParrTRScaled(noobs - 1, 0)
For i = 0 To noobs - 1
    OParrTRScaled(i, 0) = OParrscaled(i, 0)
Next i

'Input array for Testing
Dim IParrTEScaled() As Double
ReDim IParrTEScaled(totNoRecs - noobs - 1, novars - 1)
For i = noobs To totNoRecs - 1
    For j = 0 To novars - 1
        IParrTEScaled(i - noobs, j) = IParrscaled(i, j)
    Next j
Next i

'Output array for Testing
Dim OParrTEScaled() As Double
ReDim OParrTEScaled(totNoRecs - noobs - 1, 0)
For i = noobs To totNoRecs - 1

```

```

        OParrTEScaled(i - noobs, 0) = OParrscaled(i, 0)
Next i
'-----
'intFileHandle = FreeFile
'Open wkfolderpath & ExtractFilename(wkbkpathnname) & ".txt" For
Output As #intFileHandle
'-----
'''log file
    Dim FileNo As Byte
    FileNo = FreeFile ' file no for log
    Open LogFile For Append As #FileNo
'----
Dim T_dist_Val As Double
Select Case Me.cmbCItech
Case 1 ' Non-linear regression
    Call CloseWarning
    Dim sigmaSQ As Double, sigma As Double, dof_NLR As Long
    Dim TotNoParams As Long
    TotNoParams = (nohn * (novars + 2)) + 1
    For i = 0 To noobs - 1
        'Debug.Print saved_Output(i)
        sigmaSQ = sigmaSQ + (saved_Output_SB(i) - Yorg_saved(i))
^ 2
    Next i
    If noobs <= (nohn * (novars + 2) + 1) Then
        sigma = Sqr(sigmaSQ)
        dof_NLR = 1
    Else
        dof_NLR = noobs - TotNoParams
        sigma = Sqr(sigmaSQ / dof_NLR)
    End If
    'Debug.Print sigma
    Dim JacobianMatTR() As Double: ReDim JacobianMatTR(noobs - 1,
TotNoParams - 1)
    Dim JacobianMatTE_trans() As Double: ReDim
JacobianMatTE_trans(totNoRecs - noobs - 1, TotNoParams - 1)

```

```

    Dim JacobianMatAll() As Double: ReDim
JacobianMatAll(totNoRecs - 1, TotNoParams - 1)
    Dim ZsTR() As Double: ReDim ZsTR(noobs - 1, nohn - 1)
    Dim ZsTE() As Double: ReDim ZsTE(totNoRecs - noobs - 1, nohn
- 1)
    ZsTR = returnZs(IParrTRScaled, saved_W, saved_V, 1, 0)
    '*****Jacobian matrix
format*****'
'dy/dw0 dy/dv01 dy/dv02 dy/dv03 dy/dw1 dy/dw2 dy/dw3 dy/dv11
dy/dv12 dy/dv13 dy/dv21 dy/dv22 dy/dv23
    '*****Jacobian matrix
format*****'
    Dim Rows As Long, n As Long
    'Jacobian matrix for Training data
    For Rows = 0 To noobs - 1
        JacobianMatTR(Rows, 0) = 1
        For j = 0 To nohn - 1
            'calc for V-bias V01 V02 V03
            JacobianMatTR(Rows, j + 1) = saved_W(j + 1) *
ZsTR(Rows, j) * (1 - ZsTR(Rows, j))
            'calc for W--- W1 W2 W3
            JacobianMatTR(Rows, nohn + j + 1) = ZsTR(Rows, j) *
(1 - ZsTR(Rows, j))
        Next j
        n = 0
        For i = 0 To novars - 1
            For j = 0 To nohn - 1
                JacobianMatTR(Rows, 2 * nohn + 1 + n) = saved_W(j
+ 1) * ZsTR(Rows, j) * (1 - ZsTR(Rows, j)) * IParrTRScaled(Rows,
i)
                n = n + 1
            Next j
        Next i
    Next Rows
    'JacobianMatrix for test data
    ZsTE = returnZs(IParrTEScaled, saved_W, saved_V, 1, 0)

```

```

n = 0
For Rows = 0 To totNoRecs - noobs - 1
    JacobianMatTE_trans(Rows, 0) = 1
    For j = 0 To nohn - 1
        'calc for V-bias V01 V02 V03
        JacobianMatTE_trans(Rows, j + 1) = saved_W(j + 1) *
ZsTE(Rows, j) * (1 - ZsTE(Rows, j))
        'calc for W--- W1 W2 W3
        JacobianMatTE_trans(Rows, nohn + j + 1) = ZsTE(Rows,
j) * (1 - ZsTE(Rows, j))
    Next j
    n = 0
    For i = 0 To novars - 1
        For j = 0 To nohn - 1
            JacobianMatTE_trans(Rows, 2 * nohn + 1 + n) =
saved_W(j + 1) * ZsTE(Rows, j) * (1 - ZsTE(Rows, j)) *
IParrTEScaled(Rows, i)
            n = n + 1
        Next j
    Next i
Next Rows
For Rows = 0 To noobs - 1
    For j = 0 To TotNoParams - 1
        JacobianMatAll(Rows, j) = JacobianMatTR(Rows, j)
    Next j
Next Rows
For Rows = noobs To totNoRecs - 1
    For j = 0 To TotNoParams - 1
        JacobianMatAll(Rows, j) = JacobianMatTE_trans(Rows -
noobs, j)
    Next j
Next Rows
    '*****Check the condition
number*****
    Dim SVD_res() As Variant, sing_val_mat() As Double,
U_sing_val_mat() As Double, V_sing_val_mat() As Double

```

```

SVD_res = SVDF(JacobianMatAll) 'finding the SVD for Z or
Jacobian Matrix
U_sing_val_mat = SVD_res()(0)
sing_val_mat = SVD_res()(1)
V_sing_val_mat = SVD_res()(2)

Dim CondNo As Double ' condition number
If MinMaxVector(sing_val_mat) <> 0 Then
CondNo = MinMaxVector(sing_val_mat, False) /
MinMaxVector(sing_val_mat)
End If
Dim rhat As Long ' estimated rank of Jacobian matrix
Dim eps As Double, tol As Double
eps = 2 ^ (-52) 'Floating-point relative accuracy
tol = MinMaxVector(sing_val_mat, False) * eps
For i = 0 To UBound(sing_val_mat, 1)
    If sing_val_mat(i) > tol Then
        rhat = rhat + 1
    End If
Next i
'note that if CondNo > 10^8 and rhat < TotNoParams the CIs
are useless
.....

'    Dim JacotransJacoInv() As Double
'    Dim SigmaTransSigmaInv() As Double: ReDim
SigmaTransSigmaInv(TotNoParams - 1, TotNoParams - 1)

'    If CondNo > 10 ^ 8 Or rhat < TotNoParams Then
'        MsgBox "Warning: An error might be generated because-
Condition number of Jacobian matrix = " & CondNo & vbCrLf & _
'        "Rank of Jacobian matrix is = " & rhat & " and Total no
of parameters are =" & TotNoParams & vbCrLf, vbInformation,
Prog_TTitle
'    End If
'*****Logging

```

```

data*****
    Print #FileNo, "CondNo=" & CondNo
    Print #FileNo, "Rhat=" & rhat
    Print #FileNo, "TotNoParams=" & TotNoParams
    Print #FileNo, "Sigma_NLR=" & sigma
'*****Logging data
end*****

    Dim DiagHatmatrix() As Double: ReDim DiagHatmatrix(totNoRecs
- 1)

    For i = 0 To totNoRecs - 1
        For j = 0 To TotNoParams - 1
            DiagHatmatrix(i) = DiagHatmatrix(i) +
U_sing_val_mat(i, j) ^ 2
        Next j
    Next i
    'PrintMatrixHere matcal.Transpose(DiagHatmatrix)
    Dim SE_NLR() As Double
    ReDim SE_NLR(totNoRecs - 1)

'    Dim t1() As Double, t2() As Double: ReDim t2(0, TotNoParams
- 1)
'    Dim t3() As Double
    Dim Y_LB_NLR() As Double: ReDim Y_LB_NLR(totNoRecs - 1)
    Dim Y_UB_NLR() As Double: ReDim Y_UB_NLR(totNoRecs - 1)
'    Dim Y_LB_SB() As Double, Y_UB_SB() As Double
    If noobs <= TotNoParams Then
        dof_NLR = noobs
    Else
        dof_NLR = noobs - TotNoParams
    End If
    'Calculating CI for data
    T_dist_Val = T_dist(CIlevel, dof_NLR, True)
    For Rows = 0 To totNoRecs - 1

```

```

        SE_NLR(Rows) = sigma * Sqr(DiagHatmatrix(Rows))
    Next Rows
'    Dim SE_NLR_SB() As Double
'    SE_NLR_SB = postmnx(SE_NLR, minvalY(0), maxvalY(0))
    For Rows = 0 To totNoRecs - 1
        'SE_NLR(Rows) = sigma * SE_NLR(Rows)
        Y_LB_NLR(Rows) = saved_Output_SB(Rows) - T_dist_Val *
SE_NLR(Rows)
        Y_UB_NLR(Rows) = saved_Output_SB(Rows) + T_dist_Val *
SE_NLR(Rows)
        'sending NLR values to final matrix
        AllResults(Rows, 2) = SE_NLR(Rows)
        AllResults(Rows, 3) = Y_LB_NLR(Rows)
        AllResults(Rows, 4) = Y_UB_NLR(Rows)
    Next Rows
    Send2ResultsTbl "Results", "SE_NLR", AllResults, 2
    Send2ResultsTbl "Results", "YLB_NLR", AllResults, 3
    Send2ResultsTbl "Results", "YUB_NLR", AllResults, 4
    Call GetWarning
    MsgBox "Non-linear regression CI calculated", vbInformation,
Prog_TTitle
Case 2 ' Bootstrap
    Call CloseWarning
    Dim BootSamples As Byte
    BootSamples = Me.txtbootsamples
    Dim Xarry_boot() As Double, Yarry_boot() As Double
    ReDim Xarry_boot(noobs - 1, novars - 1): ReDim
Yarry_boot(noobs - 1, 0)
    Dim sample_no(), Ypred_boot() As Double, predY() As Double,
predYSB() As Double
    ReDim Ypred_boot(noobs - 1, BootSamples - 1)
    Dim BootstrapNos() As Double: ReDim BootstrapNos(BootSamples
- 1, totNoRecs - 1)
    'calculating CI for training data
    For i = 0 To BootSamples - 1
        sample_no = get_bootstrap_rnd_nos(noobs)

```



```

For j = 0 To noobs - 1
    For k = 0 To novars - 1
        Xarry_boot(j, k) = IParrTRScaled(sample_no(j), k)
    Next k
    Yarry_boot(j, 0) = OParrTRScaled(sample_no(j), 0)
    BootstrapNos(i, j) = sample_no(j)
Next j
wts() = train_NN(Xarry_boot(), Yarry_boot(), noobs,
novars, noitrs, alpha, nohn, BTEactFNIPH, BTEactFNHOP)
V() = wts()(0)
W() = wts()(1)
predY() = returnY(Xarry_boot(), W(), V(), BTEactFNIPH,
BTEactFNHOP)
predYSB() = postmnx(predY(), minvalY(0), maxvalY(0))
For j = 0 To noobs - 1
    Ypred_boot(j, i) = predYSB(j)
Next j
Next i
Dim meanY_boot() As Double: ReDim meanY_boot(noobs - 1)
Dim SE_boot() As Double: ReDim SE_boot(totNoRecs - 1)
'Dim SE_AllBoot_AllObs() As Double: ReDim
SE_AllBoot_AllObs(totNoRecs - 1, BootSamples - 1)
For j = 0 To noobs - 1
    meanY_boot(j) = 0
    For i = 0 To BootSamples - 1
        meanY_boot(j) = meanY_boot(j) + Ypred_boot(j, i)
    Next i
    meanY_boot(j) = meanY_boot(j) / BootSamples '<< Notice
that mean is calculated by dividing sum w no of boot samples, and
in case of test sum would be less resulting lower mean
    SE_boot(j) = 0
    For i = 0 To BootSamples - 1
        SE_boot(j) = SE_boot(j) + (Ypred_boot(j, i) -
meanY_boot(j)) ^ 2
    Next i

```

```

        SE_boot(j) = Sqr((1 / (BootSamples - 1)) * SE_boot(j))
    Next j
'    Dim Y_org_pred() As Double, Y_org_pred_SB() As Double
'    Y_org_pred() = returnY(IParrTRScaled(), saved_W(),
saved_V(), BTEactFNIPH, BTEactFNHOP)
'    predYSB() = postmnx(Y_org_pred(), minvalY(0), maxvalY(0))

' Code for NN starts
Option Compare Database
Option Explicit
Public TblSelected As Boolean
Public counterwksht As Long

Private Sub cmdCI_Click()
DoCmd.OpenForm "frm_CI_params"
End Sub

Private Sub cmdExport_Click()
counterwksht = counterwksht + 1
On Error GoTo errorhandler1
Dim strOPFilename As Variant
Dim obj1 As Object
Dim wb As Object
Dim ws As Object
If flsAppRunning("Excel") Then
Set obj1 = GetObject(, "Excel.Application")
Else
Set obj1 = CreateObject("Excel.Application")
End If
strOPFilename = obj1.GetSaveAsFilename(, "Excel files (*.xls), *.xls", , "Select the file
name/location")
If strOPFilename = "" Or strOPFilename = False Then

```

```

    MsgBox "Not a valid filename, try again", vbCritical, Prog_Title
    GoTo errorhandler1
End If
DoCmd.TransferSpreadsheet acExport, acSpreadsheetTypeExcel9, "Results", strOPFilename
Set wb = obj1.Workbooks.Open(strOPFilename)
Set ws = wb.Worksheets("Results")
ws.Name = "sim" & counterwksht
wb.Save
wb.Close
Set ws = Nothing
Set wb = Nothing
Set obj1 = Nothing
MsgBox "Results exported to " & strOPFilename & " succesfully!", vbInformation
Exit Sub 'if there is no error exit the sub
errorhandler1:
If Err.Number <> 0 Then
    Dim msg As String
    msg = "Error # " & Str(Err.Number) & " was generated by " _
        & Err.Source & Chr(13) & Err.Description
    MsgBox msg, vbCritical, Prog_Title & "-Error", Err.HelpFile, Err.HelpContext
End If
Set ws = Nothing
Set wb = Nothing
Set obj1 = Nothing
End Sub

Private Sub cmdTest_Click()
    Call CloseWarning
    Dim IParr() As Variant, strSQL As String, noobs As Long, IPTEarrScaled() As Double
    noobs = Me.txtNOB
    Dim IParrscaled() As Double

```

```

IParrscaled() = pmtsIP()(0)
Dim IPfldsSelected As Byte
IPfldsSelected = Me.lstIPFlds.ItemsSelected.Count
ReDim IPTEarrScaled(totNoRecs - noobs - 1, IPfldsSelected - 1)
Dim i As Long, j As Long
For i = noobs To totNoRecs - 1
    For j = 0 To IPfldsSelected - 1
        IPTEarrScaled(i - noobs, j) = IParrscaled(i, j)
    Next j
Next i
Dim OParrscaled() As Double, minvalY() As Double, maxvalY() As Double
minvalY() = pmtsOP()(1)
maxvalY() = pmtsOP()(2)
Dim Ypred() As Double
Ypred() = returnY(IPTEarrScaled(), saved_W(), saved_V(), BTEactFNIPH, BTEactFNHOP)
Dim YpredSB() As Double
YpredSB() = postmnx(Ypred, minvalY(0), maxvalY(0))
TeMSE = 0
For i = 0 To UBound(Ypred)
    TeMSE = TeMSE + (Yorg_saved(i + noobs) - YpredSB(i)) ^ 2
    saved_Output(i + noobs) = Ypred(i)
    saved_Output_SB(i + noobs) = YpredSB(i)
    AllResults(i + noobs, 1) = YpredSB(i) 'Sending Ypred vals to Allresults matrix
Next i
'*****"Sending values to results table
Send2ResultsTbl "Results", "Yorg", AllResults, 0
Send2ResultsTbl "Results", "YPred", AllResults, 1
'sending values done
'*****Logging data*****
Dim FileNo As Byte
FileNo = FreeFile

```

```

    Open LogFile For Append As #FileNo
    Print #FileNo, "TeMSE=" & TeMSE
    Close FileNo

    *****Logging data end*****

    'Call sendvals2XL(wkbkpathnname, YpredSB, noobs + 2, totNoRecs + 1, col2sendData2,
    wkshtname)
    Call GetWarning
    MsgBox "Test Complete!", vbInformation, Prog_Title
    If IsFormOpen("frmChart") Then
        DoCmd.Close acForm, "frmChart"
        DoCmd.OpenForm "frmChart", acNormal
        Forms("frmchart").Requery
    Else
        DoCmd.OpenForm "frmChart", acNormal
        Forms("frmchart").Requery
    End If
    Me.cmdCI.Enabled = True
End Sub

Private Sub cmdTrain_Click()
    Call CloseWarning
    'If Me.txtwkshtname = "" Or Me.txtcolnumber = "" Then
    '    MsgBox "Worksheet name or column number is missing", vbCritical, Prog_Title
    '    Exit Sub
    'End If
    'wkbkpathnname = Me.txtwkbkpathname
    'wkshtname = Me.txtwkshtname
    'col2sendData2 = val(Me.txtcolnumber)
    inputflds = ""
    If Me.lstIPFlds.ItemsSelected.Count = 0 Then
        MsgBox "You have not selected any input field, please select one.", vbCritical, Prog_Title
    
```

```

Exit Sub
End If
If Me.lstOPflds.ItemsSelected.Count = 0 Then
    MsgBox "You have not selected any output field, please select one.", vbCritical, Prog_Title
Exit Sub
End If
Dim inputarr() As Variant, outputarr() As Variant
Dim noobs As Long, noIrs As Long, nohn As Byte, alpha As Double, intsSelected As Long
Dim blNW As Boolean 'Nguyen-widrow initilization
intsSelected = Me.lstIPFlds.ItemsSelected.Count
noobs = Me.txtNOB
noIrs = Me.txtNoIti
nohn = Me.txtNOHLN
alpha = Me.txtAlpha
BTEactFNIPH = Me.cmbActFnIPH
BTEactFNHOP = Me.cmdActFnHOP
strSelectedTblName = Me.lstTbls
blNW = Me.cmbNW
Dim cn As New ADODB.Connection
Dim rs As ADODB.Recordset
Set rs = New ADODB.Recordset
Set cn = CurrentProject.Connection
Dim strSQL As String
inputflds = get_input_flds(Me.lstIPFlds)
strSQL = "SELECT " & inputflds & " FROM " & strSelectedTblName & ";"
rs.Open strSQL, cn, 1
totNoRecs = rs.RecordCount
ReDim saved_Output(totNoRecs - 1)
ReDim saved_Output_SB(totNoRecs - 1)
ReDim AllResults(totNoRecs - 1, 13)
ReDim Yorg_saved(totNoRecs - 1)

```

```

inputarr = rs.GetRows(totNoRecs)
Dim inputarrDbl() As Double, IParrscaled() As Double, matcal As New cMathLib
inputarrDbl = mat_transpose_getrows(inputarr())
'Debug.Print NumberOfDimensions(inputarrDbl())
pmtsIP() = premnx(inputarrDbl)
Dim minvalIP_arr() As Double, maxvalIP_arr() As Double, IParrTRScaled() As Double
IParrscaled() = pmtsIP()(0) 'Input array
minvalIP_arr() = pmtsIP()(1)
maxvalIP_arr() = pmtsIP()(2)
'PrintMatrixHere matcal.Transpose(IParrscaled)
Dim i As Long, j As Long
ReDim IParrTRScaled(noobs - 1, intsSelected - 1)
For i = 0 To noobs - 1
    For j = 0 To intsSelected - 1
        IParrTRScaled(i, j) = IParrscaled(i, j)
    Next j
Next i
'For i = 0 To UBound(arrB, 1)
'    Debug.Print arrB(i) & " " & arrC(i)
'Next i
rs.Close
OPFId = Me.lstOPflds
strSQL = "SELECT " & OPFId & " FROM " & strSelectedTblName & ";"
rs.Open strSQL, cn
outputarr = rs.GetRows(totNoRecs)
Dim OParrscaled() As Double
outputarrDbl = mat_transpose_getrows(outputarr())
'Sending Yorg values to the Final array
For i = 0 To totNoRecs - 1
    AllResults(i, 0) = outputarrDbl(i, 0)
    Yorg_saved(i) = outputarrDbl(i, 0)

```

Next i

pmtsOP() = premnx(outputarrDbl)

Dim minvalOP() As Double, maxvalOP() As Double, OParrTRScaled() As Double

OParrscaled() = pmtsOP()(0) 'Target Array

minvalOP() = pmtsOP()(1)

maxvalOP() = pmtsOP()(2)

'PrintMatrixHere matcal.Transpose(OParrscaled)

ReDim OParrTRScaled(noobs - 1, 0)

For i = 0 To noobs - 1

 OParrTRScaled(i, 0) = OParrscaled(i, 0)

Next i

'For i = 0 To UBound(OParrScaled, 1)

'Debug.Print OParrScaled(i)

'Next i

Dim wts() As Variant, V() As Double, W() As Double, Ypred() As Double

wts() = train_NN(IParrTRScaled(), OParrTRScaled(), noobs, intsSelected, noIrs, alpha, nohn,
BTEactFNIPH, BTEactFNHOP, bINW)

V() = wts()(0)

W() = wts()(1)

Ypred() = returnY(IParrTRScaled(), W(), V(), BTEactFNIPH, BTEactFNHOP)

Dim YPred_SB() As Double

YPred_SB() = postmnx(Ypred(), minvalOP(0), maxvalOP(0))

TrMSE = 0

For i = 0 To UBound(Ypred)

 TrMSE = TrMSE + (Yorg_saved(i) - YPred_SB(i)) ^ 2

 saved_Output(i) = Ypred(i)

 saved_Output_SB(i) = YPred_SB(i)

 AllResults(i, 1) = YPred_SB(i) 'Sending Ypred vals to Allresults matrix

Next i

'Call sendvals2XL(wkbkpathnname, YPred_SB, 2, noobs + 1, col2sendData2, wkshtname)


```
*****Logging data*****
```

```
LogFile = WkFolderPath & strSelectedTblName & ".txt"
```

```
Dim FileNo As Byte
```

```
FileNo = FreeFile
```

```
Open LogFile For Output As #FileNo
```

```
Print #FileNo, "W"
```

```
PrintMatrix matcal.Transpose(W), FileNo
```

```
Print #FileNo, "V"
```

```
PrintMatrix matcal.Transpose(V), FileNo
```

```
Print #FileNo, "TrMSE=" & TrMSE
```

```
Close FileNo
```

```
*****Logging data end*****
```

```
saved_W = W
```

```
saved_V = V
```

```
rs.Close
```

```
Set rs = Nothing: Set cn = Nothing
```

```
DoCmd.RunSQL "DELETE * FROM Results;" ' Cleaning the results table
```

```
Call resetAutoNum("Results", "OBsNo")
```

```
Call GetWarning
```

```
MsgBox "Training Complete!", vbInformation, Prog_Title
```

```
Me.cmdTest.Enabled = True
```

```
End Sub
```

```
Private Sub cmdWkShtName_Click()
```

```
wkbkpathnname = GetOpenFile("C:\Thesis Work", "Select file to output")
```

```
Me.txtwkbkpathname = wkbkpathnname
```

```
'Dim wkshtnames() As String
```

```
'wkshtnames = Getwkshtnames()
```

```
'Dim i As Long
```

```

For i = 0 To UBound(wkshtnames, 1)
'   Debug.Print wkshtnames(i)
Next i
End Sub

```

```

Private Sub Form_Load()
Dim cnn As New ADODB.Connection
Dim cat As New ADOX.Catalog
Set cnn = CurrentProject.Connection
Set cat.ActiveConnection = cnn
Dim tbl As ADOX.Table
With Me.lstTbls
    For Each tbl In cat.Tables
        If tbl.Type = "TABLE" Then
            .AddItem Item:=tbl.Name
        End If
    Next
End With
Set cnn = Nothing
Set cat = Nothing
Me.cmdTest.Enabled = False
Me.cmdTrain.Enabled = False
Me.cmdCI.Enabled = False
End Sub

```

```

Private Sub lstIPFlds_AfterUpdate()
Dim varItem As Variant, ctrl1 As Control
Set ctrl1 = Me.lstIPFlds
Dim intI As Long, intNumColumns As Long
With ctrl1
    intNumColumns = .ListCount

```

```

If TblSelected Then
    For intI = 0 To intNumColumns - 1
        Me.lstOPflds.AddItem Item:=.ItemData(intI)
    Next intI
    TblSelected = False
End If

intNumColumns = .ItemsSelected.Count
For Each varItem In .ItemsSelected
    If IsValThere(Me.lstOPflds, .ItemData(varItem)) Then
        Me.lstOPflds.RemoveItem Index:=.ItemData(varItem)
    End If
Next varItem

intNumColumns = .ListCount

Dim strval As String
For intI = 0 To intNumColumns - 1
    strval = .ItemData(intI)
    If Not IsItemSelected(Me.lstIPFlds, strval) And Not IsValThere(Me.lstOPflds, strval) Then
        Me.lstOPflds.AddItem Item:=.ItemData(intI)
    End If
Next intI

End With
End Sub

Private Sub lstTbls_AfterUpdate()
If Not table_name_exists(Me.lstTbls) Then
    MsgBox "Table with name " & Me.lstTbls & " does not exists. Please select a table",
vbCritical, Prog_Title
    Forms!frm_main!lstTbls.SetFocus
Exit Sub
End If
strSelectedTblName = Me.lstTbls
TblSelected = True

```

```

Me.cmdTrain.Enabled = True
Dim cnn As New ADODB.Connection
Dim rs As ADODB.Recordset
Dim fld As ADODB.Field
Set cnn = CurrentProject.Connection
Set rs = New ADODB.Recordset
Me.lstIPFlds.SetFocus
rs.Open strSelectedTblName, cnn, , , adCmdTable
Call clear_list(Me.lstIPFlds)
With Me.lstIPFlds
    For Each fld In rs.Fields
        .AddItem Item:=fld.Name
    Next fld
End With
rs.Close
Set cnn = Nothing
Set rs = Nothing
Set fld = Nothing
Call clear_list(Me.lstOPflds)
End Sub

```

Appendix C Simulation Results

Table C-1 Simulation Results for Case A with Nominal Probability of 95%

	Non-linear Regression		Bootstrap		MLE	
Simulation	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)
1	239	95.60	245	98.00	230	92.00
2	239	95.60	243	97.20	228	91.20
3	240	96.00	226	90.40	224	89.60
4	242	96.80	245	98.00	230	92.00
5	238	95.20	239	95.60	231	92.40
6	241	96.40	250	100.00	232	92.80
7	239	95.60	245	98.00	250	100.00
8	239	95.60	237	94.80	235	94.00
9	240	96.00	239	95.60	228	91.20
10	239	95.60	250	100.00	231	92.40
11	238	95.20	226	90.40	250	100.00
12	235	94.00	225	90.00	223	89.20
13	239	95.60	250	100.00	228	91.20
14	239	95.60	250	100.00	231	92.40
15	239	95.60	244	97.60	232	92.80
Avg	239	95.63	241	96.37	232	92.88

Table C-2 Simulation Results for Case A with Nominal Probability of 90%

	Non-linear Regression		Bootstrap		MLE	
Simulation	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)
1	206	82.40	228	91.20	193	77.20
2	203	81.20	219	87.60	191	76.40
3	205	82.00	191	76.40	188	75.20
4	205	82.00	231	92.40	192	76.80
5	207	82.80	206	82.40	197	78.80
6	203	81.20	248	99.20	193	77.20
7	204	81.60	229	91.60	250	100.00
8	217	86.80	208	83.20	207	82.80
9	202	80.80	213	85.20	189	75.60
10	207	82.80	242	96.80	194	77.60
11	206	82.40	183	73.20	250	100.00
12	203	81.20	192	76.80	186	74.40
13	203	81.20	248	99.20	193	77.20
14	205	82.00	244	97.60	192	76.80
15	204	81.60	224	89.60	191	76.40
Avg	205	82.13	220	88.16	200	80.16

Table C-3 Simulation Results for Case B with Nominal Probability of 95%

		Non-linear Regression		Bootstrap		MLE	
Simulation	MSE Training	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)
1	652,950	22	95.65	22	95.65	22	95.65
2	753,655	22	95.65	21	91.30	19	82.61
3	690,692	22	95.65	22	95.65	21	91.30
4	783,757	22	95.65	22	95.65	22	95.65
5	839,712	22	95.65	21	91.30	22	95.65
6	690,745	22	95.65	22	95.65	20	86.96
7	880,970	22	95.65	22	95.65	21	91.30
8	737,897	22	95.65	21	91.30	21	91.30
9	752,819	22	95.65	22	95.65	20	86.96
10	783,204	22	95.65	22	95.65	20	86.96
11	815,248	22	95.65	21	91.30	21	91.30
12	854,376	22	95.65	21	91.30	21	91.30
13	686,712	22	95.65	22	95.65	22	95.65
14	696,833	22	95.65	22	95.65	21	91.30
15	689,696	22	95.65	22	95.65	20	86.96
Avg	753,951	22	95.65	22	94.20	21	90.72

Table C-4 Simulation Results for Case B with Nominal Probability of 90%

		Non-linear Regression		Bootstrap		MLE	
Simulation	MSE Training	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)
1	652,950	21	91.30	21	91.30	22	95.65
2	753,655	22	95.65	19	82.61	18	78.26
3	690,692	21	91.30	20	86.96	21	91.30
4	783,757	22	95.65	20	86.96	22	95.65
5	839,712	21	91.30	21	91.30	22	95.65
6	690,745	21	91.30	21	91.30	18	78.26
7	880,970	21	91.30	21	91.30	17	73.91
8	737,897	21	91.30	21	91.30	19	82.61
9	752,819	21	91.30	21	91.30	18	78.26
10	783,204	21	91.30	21	91.30	19	82.61
11	815,248	21	91.30	21	91.30	19	82.61
12	854,376	21	91.30	21	91.30	19	82.61
13	686,712	21	91.30	21	91.30	22	95.65
14	696,833	21	91.30	20	86.96	18	78.26
15	689,696	22	95.65	22	95.65	18	78.26
Avg	753,951	21	92.17	21	90.14	19	84.64

Table C-5 Simulation Results for Case C with Nominal Probability of 95%

		Non-linear Regression		Bootstrap		MLE	
Simulation	MSE Training	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)
1	0.01148	1807	90	1933	97	2000	100
2	0.01384	1797	90	1983	99	2000	100
3	0.01397	1795	90	1963	98	2000	100
4	0.01223	1804	90	2000	100	2000	100
5	0.01350	1802	90	1999	100	2000	100
6	0.01140	1806	90	1987	99	2000	100
7	0.02401	1796	90	1877	94	2000	100
8	0.01170	1802	90	2000	100	2000	100
9	0.01221	1801	90	1915	96	2000	100
10	0.01317	1799	90	1995	100	2000	100
11	0.01131	1802	90	1997	100	2000	100
12	0.02711	1797	90	1974	99	2000	100
13	0.01254	1797	90	1998	100	2000	100
14	0.01263	1797	90	1978	99	1795	90
15	0.01201	1803	90	1994	100	2000	100
Avg	0.01421	1800	90	1973	99	1986	99

Table C-6 Simulation Results for Case C with Nominal Probability of 90%

		Non-linear Regression		Bootstrap		MLE	
Simulation	MSE Training	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)
1	0.01148	1732	87	1886	94	2000	100
2	0.01384	1737	87	1946	97	2000	100
3	0.01397	1738	87	1925	96	2000	100
4	0.01223	1729	86	1998	100	2000	100
5	0.01350	1741	87	1993	100	2000	100
6	0.01140	1733	87	1950	98	2000	100
7	0.02401	1724	86	1821	91	2000	100
8	0.01170	1731	87	1995	100	2000	100
9	0.01221	1732	87	1857	93	2000	100
10	0.01317	1737	87	1957	98	2000	100
11	0.01131	1734	87	1983	99	2000	100
12	0.02711	1720	86	1932	97	2000	100
13	0.01254	1736	87	1982	99	2000	100
14	0.01263	1734	87	1943	97	1734	87
15	0.01201	1728	86	1960	98	2000	100
Avg	0.01421	1732	87	1942	97	1982	99

Table C-7 Simulation Results for Case D with Nominal Probability of 95%

		Non-linear Regression		Bootstrap		MLE	
Simulation	MSE Training	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)
1	17,013	90	87	92	88	91	88
2	19,449	89	86	104	100	87	84
3	21,885	91	88	103	99	104	100
4	20,484	91	88	104	100	104	100
5	17,002	89	86	104	100	104	100
6	17,118	89	86	104	100	90	87
7	19,964	89	86	104	100	104	100
8	17,789	90	87	94	90	104	100
9	17,759	90	87	104	100	87	84
10	17,827	89	86	104	100	104	100
11	17,053	91	88	104	100	104	100
12	26,580	95	91	100	96	92	88
13	19,992	89	86	99	95	104	100
14	22,350	92	88	104	100	90	87
15	17,405	89	86	100	96	90	87
Avg	19,311	90	87	102	98	97	94

Table C-8 Simulation Results for Case D with Nominal Probability of 90%

		Non-linear Regression		Bootstrap		MLE	
Simulation	MSE Training	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)	Covered Points	Coverage Probability (%)
1	17,013	85	82	89	86	85	82
2	19,449	85	82	99	95	85	82
3	21,885	85	82	96	92	104	100
4	20,484	85	82	104	100	104	100
5	17,002	85	82	96	92	104	100
6	17,118	85	82	99	95	85	82
7	19,964	85	82	102	98	104	100
8	17,789	85	82	87	84	104	100
9	17,759	85	82	103	99	83	80
10	17,827	85	82	99	95	104	100
11	17,053	85	82	97	93	104	100
12	26,580	87	84	97	93	84	81
13	19,992	85	82	91	88	104	100
14	22,350	85	82	102	98	81	78
15	17,405	85	82	92	88	84	81
Avg	19,311	85	82	97	93	95	91

Appendix D Gradient or First Order Derivatives Calculation Code

```
deltatmp = 1
For Rows = 0 To totNoRecs - 1
  For j = 0 To nohn - 1
    GradientW(j + 1) = AllZs(Rows, j) * deltatmp
    DelHid(j) = saved_W(j + 1) * deltatmp
    DelHid(j) = DelHid(j) * actfunction_der(AllZs(Rows, j), BTEactFNIPH)
  Next j
  GradientW(0) = 1
  For j = 0 To nohn - 1
    For i = 0 To novars - 1
      GradientV(i, j) = IParrFull(Rows, i) * DelHid(j)
    Next i
    GradientVb(j) = DelHid(j)
  Next j
  tmpXX = Put_grads_vector(GradientW, GradientV, GradientVb, novars, TotNoParams,
nohn)
  'PrintMatrixHere tmpXX
  '*****Jacobian matrix format*****
'dy/dw0 dy/dw1 dy/dw2 dy/dw3 dy/dv01 dy/dv02 dy/dv03 dy/dv11 dy/dv12 dy/dv13 dy/dv21
dy/dv22 dy/dv23
  For i = 0 To TotNoParams - 1
    JacobianMatAll(Rows, i) = tmpXX(i)
  Next i
Next Rows
```

Appendix E Program Manual

There are various input boxes and drop-down lists where the neural network parameters are specified and the data table is selected. The inputs to the program are (see Figure E-1):

1. Number of observations used for training (remaining observations of the data set will be used for testing)
2. Number of hidden layer neurons
3. Number of iterations
4. Learning rate
5. Usage of Nguyen-Widrow random weight initialization,
6. Activation function for the hidden layer
7. Activation function for the output layer
8. Data table
9. Input fields (variables)
10. Output field (variable)

The screenshot shows a window titled "Neural Network Parameters" with a blue title bar and standard Windows window controls. The window contains the following elements:

- Number of observations:** A text box containing the value "19".
- Number of Hidden Layer neurons:** A text box containing the value "2".
- Number of Iterations:** A text box containing the value "150".
- Learning Rate:** A text box containing the value "0.2".
- Use Batch Update:** A dropdown menu with "True" selected.
- Use Nguyen-Widrow initialization?:** A dropdown menu with "True" selected.
- Select activation function for Input and Hidden layer:** A dropdown menu with "Sigmoid" selected.
- Select activation function for Hidden and Output layer:** A dropdown menu with "Linear" selected.
- Select data table:** A dropdown menu that is currently empty.
- Select Input fields:** A large empty rectangular box.
- Select output field:** A large empty rectangular box.
- Buttons:** Four buttons at the bottom: "Train the NN", "Test the NN", "Calculate CI", and "Export".

Figure E-1 Main Screen of the Program

The possible values of these inputs are given in Table E-1. It should be noted that these possible values are just recommendations or tested values with this program. Experiments can be done using different values with the inputs– number of iterations, number of hidden layer neurons, learning rate, and activation functions.

Table E-1 Inputs and the Possible Values to the Program

Input	Possible Values	Data Type
Number of observations used for training	About 80-90% of the total number of observations in the data set	Integer
Number of hidden layer neurons	From 1 to 15 based on the complexity of the data	Integer
Number of iterations	>10	Integer
Learning rate	Between 0.1 and 0.9	Double
Usage of Nguyen-Widrow random weight initialization	True/False	Boolean
Activation function for the hidden layer	Linear/Sigmoid/Bi-polar Sigmoid/Tanh	Text
Activation function for the output layer	Linear/Sigmoid/Bi-polar Sigmoid/Tanh	Text
Data table	Different data tables in the database	Text
Input fields (variables) and	Fields in the data table	Text
Output field (variable)	Fields in the data table	Text

After the input fields are selected, the button “Train the NN” can be used. Once the training is complete, a message box with the information that the training is complete will pop up. After completion of training, “Test the NN” button can be used. Testing should be fast compared to the training and after completion of testing, a message box with the information that “Test is complete” will pop up. Clicking “OK” on this message box will generate two plots of actual data vs. the output of the NN as shown in Figure E-2. The plot on the left side is a scatter plot between actual data and the output of the NN. The plot on the right side is a line plot with two different series of actual data points and the output of the NN. This window will also show **Mean Squared Error (MSE)** for the training and the test data set.

Once the training and the testing of the NN is complete, confidence intervals can be computed using the “Calculate CI” button. Clicking this button will bring one more window, where the confidence interval estimation technique and the confidence level should be selected. This screen is shown in Figure E-3.

Figure E-2 Plots Generated by the Program

Figure E-3 shows the "Parameters for CI" form. It includes three dropdown menus for configuration: "Select the technique to calculate CI" (set to "Non-Linear Regression"), "Select confidence level (%)" (set to "95"), and "Want the correction factor?" (set to "False"). A "Calculate" button is positioned at the bottom of the form.

Figure E-3 Confidence Intervals Parameters Form

For the non-linear regression technique, there is an option of using a correction factor (by default, this value is set to false). If bootstrapping as a technique is selected, then there is an option of entering the number of bootstrapping samples. Generally, this value should be greater than 20. After calculation of the intervals, a message box pops up and the results should be saved in the "Results" table. This program will create a text file with the name of the data table selected in the same folder where this file is kept. This text file will have the final weights, training and test MSE, and the condition number and r^2 for the non-linear regression technique.

Appendix F T-test for the Means of NLR and Bootstrap

T-tests were conducted to test if the average |CP-90| and |CP-95| obtained by NLR and bootstrap were equal for critical alpha levels of 0.05 and 0.1. The tests conducted are shown in Figure F-1 [48]. The test results for $\alpha=0.05$ and $\alpha=0.1$ are shown in Table F-1 and Table F-2 respectively.

$$\begin{aligned}
 &H_0 : \mu_{NLR} = \mu_{Boot} \\
 &H_a : \mu_{NLR} \neq \mu_{Boot} \\
 &\text{Test-Statistic: } T = \frac{\bar{Y}_{NLR} - \bar{Y}_{Boot}}{\sqrt{s_{NLR}^2 / N_{NLR} + s_{Boot}^2 / N_{Boot}}} \\
 &\text{where: } \bar{Y}_{NLR} \text{ and } \bar{Y}_{Boot} \text{ are the sample means and } s_{NLR}^2 \text{ and } s_{Boot}^2 \text{ are the variances} \\
 &\text{Significance Level: } \alpha \\
 &\text{Conclusion: If } |T| \leq t(\alpha, \nu), \text{ conclude } H_0, \text{ otherwise conclude } H_a \\
 &\text{where: } \nu = \frac{(s_{NLR}^2 / N_{NLR} + s_{Boot}^2 / N_{Boot})^2}{(s_{NLR}^2 / N_{NLR})^2 / (N_{NLR} - 1) + (s_{Boot}^2 / N_{Boot})^2 / (N_{Boot} - 1)}
 \end{aligned}$$

Figure F-1 T-test for Comparing the Means

Table F-1 T-tests Results for the Averages of |CP-95|

	NLR		Boot		T-stat	dof	T-critical $\alpha=0.05$	T-critical $\alpha=0.1$	Conclude $\alpha=0.05$	Conclude $\alpha=0.1$
	Mean	SD	Mean	SD						
Case A	0.76	0.61	3.29	3.57	-2.71	15	1.75	1.34	H _A	H _A
Case B	0.65	0.00	1.67	2.12	-1.85	14	1.76	1.35	H _A	H _A
Case C	4.98	0.19	3.80	1.84	2.49	15	1.75	1.34	H _A	H _A
Case D	8.27	1.59	4.18	3.77	3.87	19	1.73	1.33	H _A	H _A

Table F-2 T-tests Results for the Averages of |CP-90|

	NLR		Boot		T-stat	dof	T-critical $\alpha=0.05$	T-critical $\alpha=0.1$	Conclude $\alpha=0.05$	Conclude $\alpha=0.1$
	Mean	SD	Mean	SD						
Case A	7.87	1.43	6.91	8.48	0.43	15	1.75	1.34	H ₀	H ₀
Case B	2.17	1.80	2.35	3.06	-0.19	23	1.71	1.32	H ₀	H ₀
Case C	3.38	0.28	7.09	2.60	-5.50	15	1.75	1.34	H _A	H _A
Case D	8.14	0.50	5.12	4.97	2.35	15	1.75	1.34	H _A	H _A