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Application of Artificial Neural Network in the Prediction of Water Pollution for Sustainable Development

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Abstract

In this paper, a Multilayer Feedforward Neural Network model with Bayesian regularization (Levenberg-Marquardt) is developed as a means of predicting water points quality parameters in Nigeria. The use of Bayesian regularized technique reduces the potential of overfitting and overtraining, thereby improving the prediction quality of the model. The MFNN model, uses six input variables identified as key high-risk parameters influencing Total Dissolved Solids (TDS) and these are: Total Coliform (TTC), Cadmium (Cd), Nitrate (NO3-), Fluoride (F), Arsenic (As), and Lead (Pb) concentrations. The output variable TDS was selected as the predicted variable, serving as a general indicator of inorganic water pollution. The complete dataset (n=225) was randomly partitioned into training (70%, n=158), validation (15%, n=34), and testing (15%, n=33) sets. All input variables were normalized to [0,1] range using min-max scaling. The training set was used for weight optimization, the validation set for monitoring overfitting and determining early stopping, and the test set for the final, unbiased evaluation of model performance. All input variables were normalized prior to training. MFNN training with the dataset, shows mean square error (MSE) decreases as a function of the number of epochs. At convergence, the MSE error is 0.000401, and a high correlation (R=0.97) between predicted and observed TDS, demonstrating its potential for predicting water quality parameters above regulatory limits. The model was able to predict the TDS values to be 985.00 which is above the Nigeria Standard for Drinking Water Quality Maximum Permissive Level of 500.

Keywords

Water quality prediction; Neural network; Bayesian regularization; Heavy metal

1. Background

In pursuance of sustainable development, pollution control in groundwater systems via the modeling of qualitative parameters of water is one of the primary factors that warrant a special focus. Water pollution occurs when the quality of water in a body of water is negatively affected. This may be due to addition of large amount of contaminants to the water body. In developing countries such as Nigeria, high pollution levels are found in the groundwater. There is an urgent need for intervention strategies.

In fulfillment of sustainable development, pollution control in groundwater systems through the modeling of qualitative parameters of water is one of the key factors that warrant a special focus. Water is indeed a precious natural resource that exists on our planet and all forms of life need it. Water pollution occurs when the quality of water in a body of water is negatively affected. This may be due to addition of large amounts of contaminants to the water body. In developing countries such as Nigeria, high pollution levels are found in the groundwater system [1,2]. There is an urgent need for intervention approaches. This modeling work is a contribution to these strategies.

Largely, predictive models can be divided into statistical and physically process-based approaches. Statistical approaches are relationships between historical data sets, whereas physically based approaches model the underlying processes directly, [3]. Models developed by statistical techniques are data-driven and computationally very fast and require fewer input parameters than process-based models. Artificial neural network, ANN, is closely related to statistical models. This type of data-driven techniques most suited to forecasting applications, [4,5].

This paper utilized ANN in modeling water quality. The water quality variables interactions are dynamic and complex processes. These interactions are hidden in their measurement data. The ANN model can reveal these hidden relationships in the historical data. The model facilitates the prediction of water quality. The steps followed in the development of ANN models include the choice of performance criteria, division and pre-processing of the available data. Other steps are choosing the model inputs and output variables and network architecture, optimization of the connection weights usually termed training, and model validation [15].

This work will show the accuracy and robustness of an ANN using Bayesian regularization algorithm to predict heavy metal in Nigeria groundwater system. The multi-layered feedforward neural network (MFNN) with Bayesian regularization method [17] minimise overfitting. The model improves the generalization of the neural network model.

The water quality parameters were measured at various locations and states covering the six regions of Nigeria. The models could be used as a prediction tool. This complements the process-based model and field-monitoring programme in the region [3]. The results of the ANN prediction and forecast model for the groundwater in each region of the country are discussed in this paper.

2. Statement of the Problem

Water is undoubtedly the most precious natural resource that exists on our planet. Pollution of water occurs when the quality of water in a body of water is adversely affected due to addition of large amounts of contaminants, [7,8]. Pollution control in groundwater systems through the modeling of qualitative and quantitative parameters of water warrants is a research focus. In water quality modeling, correlations and interactions between water quality variables are investigated. This is to see whether a model governing observed patterns exists. This will allow the predictability of these variables. The identification of such models will serve as a useful mechanism for ecologists and environmentalists, [9], as an example.

3. Methods

3.1 Artificial neural network

Artificial neural network is a mathematical model involving a group of interconnected artificial neurons. The model tries to simulate the neural structure of the human brain. Artificial neural networks are trained against input and output data. This training process is also called a learning process. The training process is used to determine the neural network parameters for the model. A neural network can be described as a multilayer perceptron (MLP) with generalised back propagation optimization algorithm [10]. The MLP can model complex non-linear relations between inputs and outputs. A MLP is composed of an input layer, hidden layer or layers and an output layer. Independent processing units, called neurons, connect the layers. The number of neurons in the input and output layers is determined by the number of input and output variables respectively. The number of hidden layer or layers depends on the level of complexity appropriate for the modelling problem. The number of neurons in the hidden layer or layers is determined throughout the training process.

An example of a neural network with one hidden layer is depicted in Figure 1. Data flow only in one direction through the network, from input x to output y. This type of network is called a multilayer feed forward neural network, MFNN [15] The mapping of the inputs to the output is expressed in a MLP network written as

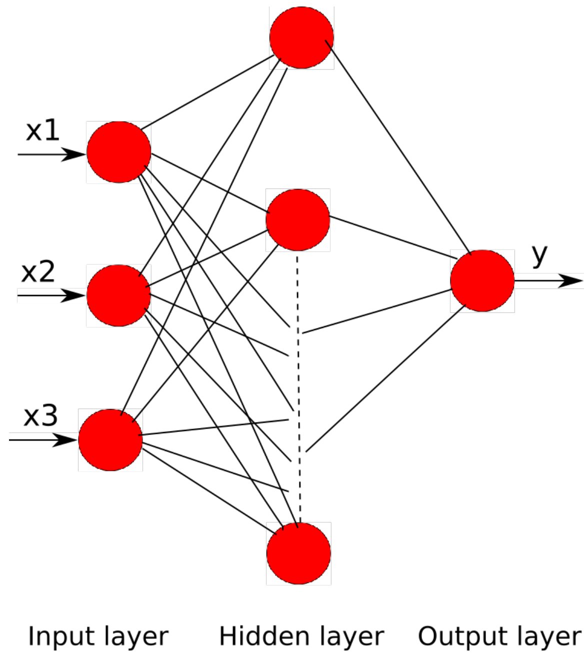

Figure 1. Schematic illustration of neural network architecture.

$$f(x;w;\omega)=g_2\left(\sum_{j=0}^{N} w_j g_1\left(\sum_{i=0}^{k}\omega_{ji}x_i\right)\right) \tag{1}$$

where $g_1(\cdot)$ and $g_2(\cdot)$ are transfer functions or activation functions. w and ω are network weight parameters. The numbers *N and k* of the network parameters in Equation (1) are unknown and they are determined from optimization [11]. The transfer functions $g_1(\cdot)$ and $g_2(\cdot)$mathematically defines the non-linear relationship between inputs and output of a neuron. Several continuous functions that can be used as transfer functions [10]. An example of an activation function typically used in the hidden layer is the sigmoid activation function, defined as

$$g(x)=\frac{1}{1+e^{x}} \tag{2}$$

where, x is the input to a neuron. The sigmoid function, Equation (2), in combination with a linear transfer function in the output layer can approximate any nonlinear function provided a sufficient number of hidden layer units are available [10].

An ANN makes use of an optimization algorithm to determine how good the error on the training input – output data set is minimised. It also determines the number of iteration steps, [11]. However, overfitting, [12,13], defined as the effect of generalization error resulting from the overly complicated model in an optimization process may occur. This is the case as the model may entirely rely on the training samples and thus inadequately model new inputs that are not part of the training set. Bayesian regularization is an optimal method that addresses overfitting and thus improves generalization of the model, [14].

3.2 The water quality data set

The measurement data were obtained in all the 6 geopolitical zones of Nigeria. The country has a large difference in access to quality drinking water sources. The regions are North-West, North-Central, North-East, South-West, South-East and South-South. The country and its regions are as seen in Figure 2. In measuring the water quality variables throughout the regions in the country, different water reservoirs were considered in the measurement. These groundwater reservoirs considered and numbers of measurement water points are shown in Table 1. The data were obtained during the year 2016. Several water quality parameters were measured. These comprise of the six high-risk parameters. They are of Coliform bacteria (TTC), Cadmium Cd, Nitrates NO^-_3, Fluorides Fl^-, Arsenic As, and Lead Pb. The nuisance parameters are of Odour, Taste, Temperature, Colour, pH, EC, TDS, Turbidity, Chlorides Cl-, Sulfates SO^-_4, Nitrites NO^-_3, Iron Fe, Manganese Mn and Sodium Na The largest numbers of water samples were collected from borehole. The borehole's depths were around 100 meters.

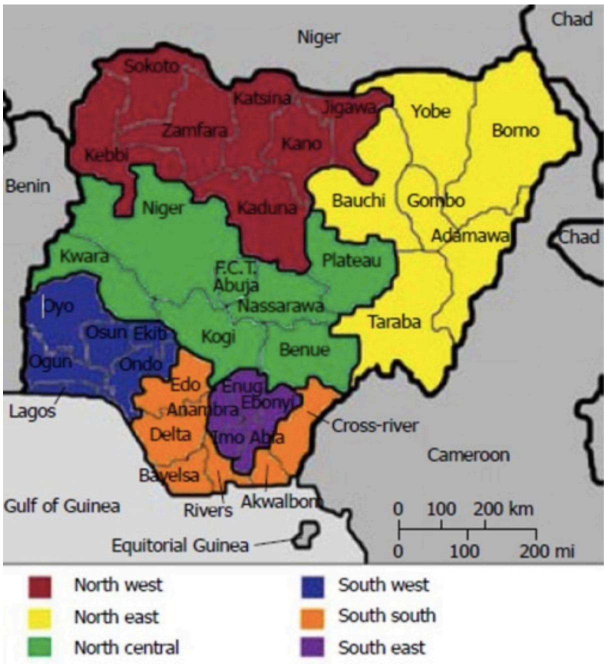

Figure 2. Map of Nigeria showing the 6 geo-political zones.

Table 1. Water reservoir measurement points

Water sources	Acronym	Number of sampling site
Borehole	BH	213
Motorized Borehole	MBH	3
Protected Dug well	PDW	8
Rainwater Harvesting	RWH	1

3.3 Modeling and simulation

The MFNN structure for modelling and prediction of the heavy metal (i.e. TDS) in the groundwater system in Nigeria is depicted in Figure 3.

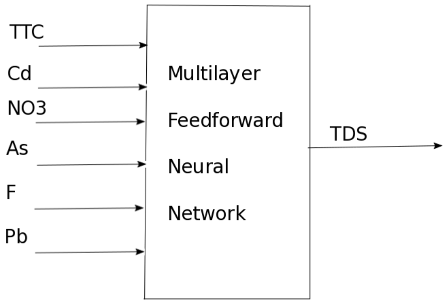

Figure 3. Schematic diagram of the MFNN water quality model.

The MFNN model, depicted in Figure 3, uses six input variables identified as key high-risk parameters influencing TDS: Total Coliform (TTC), Cadmium (Cd), Nitrate (NO3-), Fluoride (F), Arsenic (As), and Lead (Pb) concentrations. The output variable is Total Dissolved Solids (TDS)

In functional form with TDS as dependent variable, the model in Figure 3 is given by

$$TDS = f\left(TTC, Cd, NO_3^-, As, F^-, Pb\right) \tag{3}$$

In Equation (4) and (5), we have the matrix form of the water pollution ANN model with the independent variables in Equation (3) as input variables.

$$\tan sig\left(\begin{bmatrix} \omega 1_{11} & \omega 1_{12} & \omega 1_{16} \\ \omega 1_{21} & \omega 1_{22} & \omega 1_{26} \\ \cdots & \cdots & \cdots \\ \omega 1_{s1} & \omega_{s2} & \omega 1_{s6} \end{bmatrix} \begin{bmatrix} TTC \\ Cd \\ NO_3^3 \\ As \\ F^- \\ Pb \end{bmatrix} + \begin{bmatrix} b1_1 \\ b1_2 \\ \cdots \\ b1_s \end{bmatrix}\right) = \begin{bmatrix} a_1 \\ a_2 \\ \cdots \\ a_s \end{bmatrix} \tag{4}$$

and

$$TDS = \begin{bmatrix} \omega 2_1 & \omega 2_2 & \cdots & \omega 2_s \end{bmatrix} . \begin{bmatrix} a_1 \\ a_2 \\ \cdots \\ a_s \end{bmatrix} + b2 \tag{5}$$

In Equation (3) and (4), s refers to the number of neurons in a hidden layer. The model weights and bias parameters $\omega 1, \omega 2, b1$ *and* b result from the NN training experiments. a is the hidden layer output value.

Following the Kolmogorov theory [15] we are using a $6-13-1$ MFNN in Figure 3. The network input layer consists of 6 neutron nodes, the single hidden layer contains 13 nodes and the output layer has only one node. The activation function for the nodes in the hidden layer is a tangent sigmoid transfer function (TANSIG), while the output layer uses the linear transfer function (PURELIN). Using tangent sigmoid transfer function in the hidden layer nodes means the nodes return values will fall between $[-1,1]$. The neural network package in the MATLAB software [16] was used to develop and execute the model. To address overfitting and improving generalization, the ANN method with Bayesian regularization model functions were used. The MFNN Bayesian regularization model functions and ANN data are shown in Table 2.

Table 2. MFNN functions and training data

Neural network	Standard backpropagation multilayer feedforward
Network configuration	6:13:1
Training algorithm	Bayesian regularization in combination with Levenberg-Marquardt training (TRAINBR)
Transfer functions	Tan-sigmoid transfer function (TANSIG) and linear transfer function (PURELIN)
Initialization	Automatic
Learning rate	0.01
Epoch	10000

The complete dataset (n=225) was randomly partitioned into training (70%, n=158), validation (15%, n=34), and testing (15%, n=33) sets. All input variables were normalized to [0,1] range using min-max scaling. *The training set was used for weight optimization, the validation set for monitoring overfitting and determining early stopping, and the test set for the final, unbiased evaluation of model performance. All input variables were normalized prior to training.*

Table 3. Composition of the dataset used for training the MFNN water quality model

State in Nigeria	Region in Nigeria	Total number in the dataset
Bauchi	North East	80
Benue	North Central	42
Ekiti	South West	19
Enugu	South East	11
Jigawa	North West	20
Plateau	North Central	53

4. Results

The concentration range of the seven water quality input variables in the model domain is given in Table 4. An example of Benue state distribution of the high-risk water pollution parameters across its local councils is shown in Figure 4.

Figure 5 show the mean square error (MSE) curve after the MFNN training with the dataset. The regression analysis, in terms of the target and network's output is shown in Figure 6. The R value is 0.970.

The resulting ANN model parameters in Equation (4) and (5) are given in Equation (6), (7), and (10). In Figure 7, the predictive result of the MFNN model is shown.

Table 4. Seven water quality variables used in the study

Variable Acronym	Unit	**NSDWQMPL	Minimum	Maximum	Mean	Standard deviation
TTC	/100ml	0.00	0.00	320.00	5.58	24.57
Cd	mg/l	0.03	0.00	0.06	0.00	0.01
NO_3^-	mg/l	50	0.00	89.22	8.68	13.04
As	mg/l	0.01	0.00	0.28	0.00	0.02
F^-	mg/l	1.5	0.00	1.52	0.54	0.44
Pb	mg/l	0.00	0.00	0.02	0.00	0.00
TDS	mg/l	500	5.00	985.00	139.74	122.24

**NSDWQMPL is the Nigerian Standard for Drinking Water Quality Maximum Permissible Levels-2007,

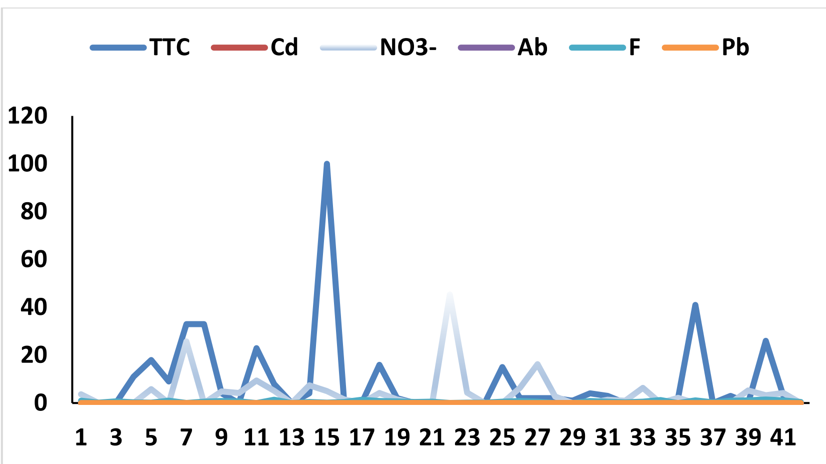

Figure 4. High-risk water points pollution parameters throughout all the 41 Benue State local councils.

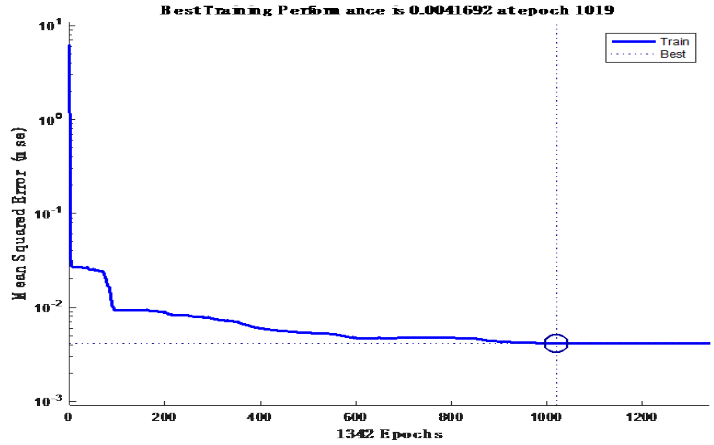

Figure 5. Training curve for the MFNN.

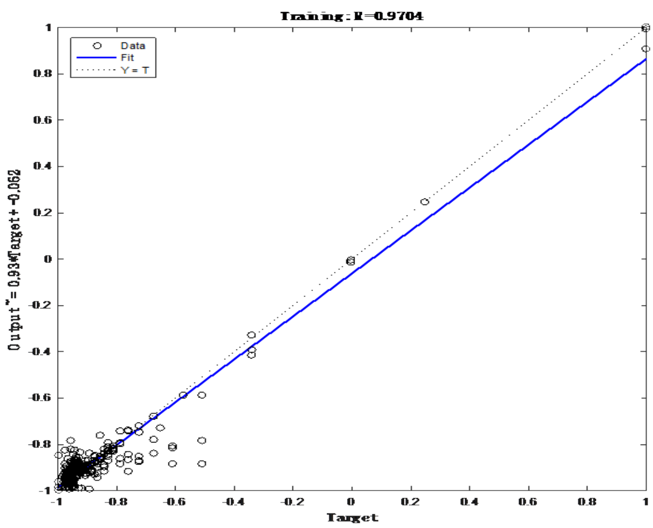

Figure 6. Linear regression analysis for the trained MFNN.

$$\begin{bmatrix} \omega l_{11} & \omega l_{12} & \omega l_{16} \\ \omega l_{21} & \omega l_{22} & \omega l_{26} \\ - & - & - \\ \omega l_{s1} & \omega_{s2} & \omega l_{s6} \end{bmatrix} = \begin{bmatrix} -3.5993859e\text{-}01 & -8.8771208e\text{-}02 & 1.1874462e\text{+}00 & -2.0497991e\text{-}01 & -1.3819485e\text{+}00 & -3.3265750e\text{-}01 \\ 4.1327155e\text{-}02 & 9.0101710e\text{-}03 & 8.1716358e\text{-}01 & -4.5128415e\text{-}02 & 4.2634674e\text{-}01 & 1.6993453e\text{-}02 \\ 8.5114698e\text{-}03 & 1.0959995e\text{-}01 & 4.2159449e\text{-}02 & 4.2547893e\text{-}02 & 6.1084774e\text{-}02 & 3.8855990e\text{-}02 \\ 4.3255642e\text{-}01 & -7.5493746e\text{-}01 & -3.8412918e\text{-}01 & 4.4864101e\text{-}01 & 2.3922802e\text{+}00 & 1.5945125e\text{+}00 \\ 8.1758538e\text{-}02 & -5.1781462e\text{-}01 & -3.9338494e\text{-}01 & 3.0497623e\text{-}03 & -5.3298071e\text{-}01 & -2.6922601e\text{-}02 \\ 3.1648403e\text{-}01 & -8.3315690e\text{-}02 & -1.9622096e\text{-}01 & 3.1263006e\text{-}01 & 2.1007787e\text{-}01 & -9.5179546e\text{-}01 \\ -8.1870929e\text{-}03 & -8.1179267e\text{-}02 & -3.9288289e\text{-}02 & -3.3416012e\text{-}02 & -4.7440019e\text{-}02 & -3.6449649e\text{-}02 \\ 2.1031976e\text{-}01 & -3.2008422e\text{-}01 & -9.3148174e\text{-}01 & -2.1919537e\text{-}02 & 7.5361075e\text{-}01 & -1.7019919e\text{+}00 \\ -2.4175696e\text{-}01 & -4.8898414e\text{-}01 & 6.8496030e\text{-}01 & -4.0829899e\text{-}01 & 4.2612532e\text{-}01 & -1.2867235e\text{-}01 \\ 1.9536533e\text{-}01 & -3.5814602e\text{-}01 & -9.1798461e\text{-}03 & -7.6424336e\text{-}02 & 1.5010990e\text{+}00 & -2.8695839e\text{-}01 \\ 8.3902442e\text{-}02 & 9.9831686e\text{-}01 & -1.5774712e\text{+}00 & -4.4606410e\text{-}01 & 4.8627552e\text{-}01 & 1.4841940e\text{+}00 \\ 4.8984301e\text{-}02 & 5.1665542e\text{-}02 & 2.0397803e\text{-}01 & 4.2316801e\text{-}02 & -1.5684922e\text{-}01 & 6.0466417e\text{-}01 \\ 1.5542637e\text{-}01 & 5.6766376e\text{-}01 & -2.4413684e\text{+}00 & 5.1442572e\text{-}01 & 1.7325692e\text{+}00 & 1.8143240e\text{+}00 \end{bmatrix} \quad (6)$$

and

$$\begin{bmatrix} \omega 2_1 & \omega 2_2 & \ldots & \omega 2_s \end{bmatrix} = \begin{bmatrix} 1.2763085e\text{-}01 \\ 3.2511925e{+}00 \\ 2.1399909e{+}00 \\ -2.5537925e{+}00 \\ -3.3660067e{+}00 \\ 1.3054187e\text{-}01 \\ -4.5526913e{+}00 \\ -1.3186358e{+}00 \\ -4.4153456e\text{-}01 \\ -2.6378615e{+}00 \\ 1.1751923e{+}00 \\ -2.4684719e\text{-}03 \\ 1.0398060e{+}00 \\ 7.6196188e\text{-}02 \end{bmatrix}; \begin{bmatrix} b1_1 \\ b1_2 \\ \ldots \\ b1_s \end{bmatrix} = \begin{bmatrix} 1.2763085e\text{-}01 \\ 3.2511925e{+}00 \\ 2.1399909e{+}00 \\ -2.5537925e{+}00 \\ -3.3660067e{+}00 \\ 1.3054187e\text{-}01 \\ -4.5526913e{+}00 \\ -1.3186358e{+}00 \\ -4.4153456e\text{-}01 \\ -2.6378615e{+}00 \\ 1.1751923e{+}00 \\ -2.4684719e\text{-}03 \\ 1.0398060e{+}00 \end{bmatrix} \quad (7)$$

$$b2 = 7.6196188e\text{-}02 \quad (10)$$

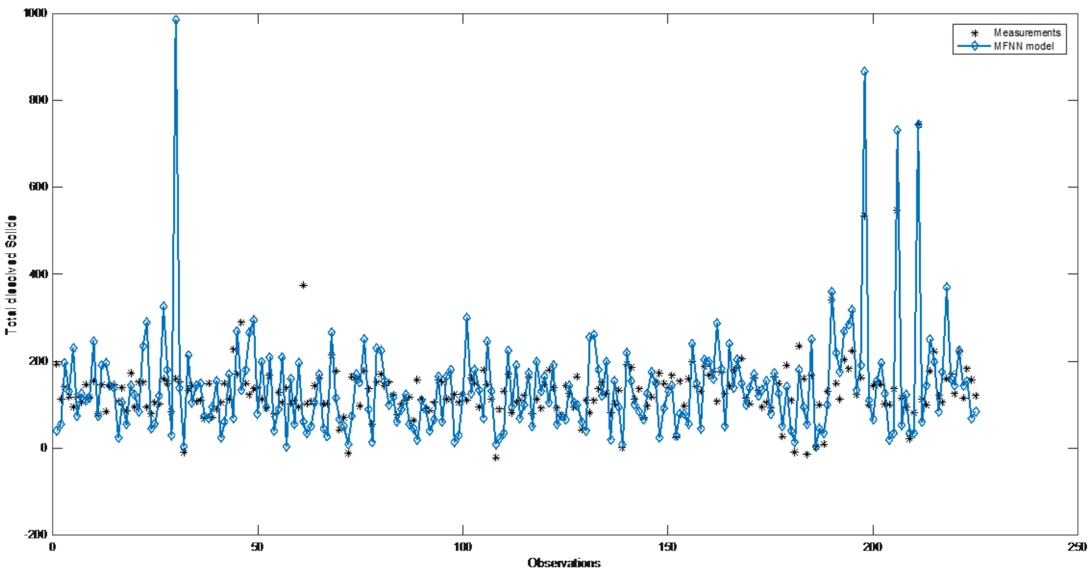

Figure 7. Predictive result of the MFNN model.

5. Discussion

From the example of Benue state distribution of the high-risk water pollution parameters across its local councils as shown in Figure 4. The high-risk parameters are mostly above the NSDWQ maximum permissive levels especially for TTC and Nitrate concentrations

Following the MFNN training with the dataset, the result shows MSE decreases as a function of the number of epochs. At convergence, the MSE error is 0.000401, which is not far to the ideal value of zero. The regression analysis, in terms of the target and network's output exhibit good correlation and they are close on to each other with the angle of passing of the output line 450. This illustrates that the network has been trained properly with no occurrence of overfitting.

From the result in Figure 7, the model is in good agreement with the observed measurements. ANN are effectively used as a groundwater quality prediction model for TDS assessment, [17]. The model was able to predict the TDS values that were above the Nigeria Standard for Drinking Water Quality Maximum Permissive Level of 500

6. Conclusions

This paper described the implementation of an ANN to model and predict pollutants in the groundwater system in Nigeria. The input level for the neural network model consists of 6 variables; TTC, Cadmium, Fluoride, Nitrate, Lead and Arsenic concentrations. The output variable is the Total Dissolved Solids. The measurement data used in training the neural network was obtained in 2016. They consist of high risk and nuisance water pollution parameters.

Resultant models obtained are positively encouraging with high performance accuracy. From this work, the following conclusion can be drawn:

i. Using ANN with Bayesian regularization affords us the opportunity of combining nonlinear functions in parallel for the modelling of the heavy metal in the groundwater system.

ii. The reduced and definite parameters obtained by training the neural network make the interpretation of the MFNN model of Equations (4) and (5) possible.

iii. The model was able to predict water points with TDS above the Nigeria Standard for Drinking Water Quality Maximum Permissive Level.

iiii. The model can be improved as more experimental measurement becomes available.

List of abbreviations

MFNN: Multilayer Feedforward Neural Network model
ANN: Artificial Neural Network
NSDWQMPL: the Nigerian Standard for Drinking Water Quality Maximum Permissible Levels-2007
Coliform bacteria (TTC),

Declarations

Ethics approval and consent to participate

The authors declare that the work is ethically approved and consent to participate.

Consent for publication

The authors declare that the work has a consent for publication.

Availability of data and materials

The datasets supporting the results are included within the article.

Competing interests

The authors declare that they have no competing interests.

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5. Water Aids, Nigeria
6. Commission for Science and Technology in the South (COMSATS)

Authors' contributions

All authors have contributed significantly to the conception and design of the study, the interpretation of data, and the drafting and revision of the manuscript. All authors read and approved the final manuscript.

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4. Water Aids, UK
5. Water Aids, Nigeria

Commission for Science and Technology in the South (COMSATS)

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