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Application of soft computing in water treatment plant and water distribution network

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Analysis of traditional water distribution network (WDN) is more time-consuming and less effective to predict the problem related to water supply systems such as water quality, coagulant dose, and residual chlorine in developing countries. In the present paper water quality neural network, coagulation dose neural network, and residual neural network model were implemented. The performance of the Cascade Feed Forward Neural Network (CFFNN) and Feedforward neural network (FFNN) was excellent for the prediction of water quality parameters and residual chlorine respectively during the training and testing period. CFFNN water quality model (27-30-27) with $R = 0.989$ produced an excellent prediction of outlet water quality parameters. In coagulant dose modelling, CFFNN (2-40-1) yielded a good prediction with $R = 0.947$ for a broad range of turbidities as compared to other models. Similarly in residual chlorine modelling, FFNN (2-25-1) delivered the best prediction with $R = 0.988$ as compared to other models.

Keywords: Artificial neural network (ANN); chlorine dose; coagulant dose; water distribution network (WDN); water treatment plant; water quality

1. Introduction

In the twenty-first century, the application of soft computing techniques for the deriving relationship between hydraulic conditions and temporal variation in Water Treatment Plant (WTP) and WDN is essential to overcome the traditional process. In developing countries, most of the WTP is manually operated, resulting in underdosing or over-dosing of water treatment chemicals. The outlet water quality of WTP relies on raw water quality and water treatment unit processes. The main challenge in the water treatment process is the presence of severe fluctuations in the raw water quality caused by daily and seasonal changes in weather conditions, variations in water dam level and demands by consumers, heavy rainfall/ floods, industrial effluents, and agro-allied activities (Bello et al. 2014). Similarly, complex physical and chemical processes involved in the water treatment process exhibit non-linear behaviour which is difficult to describe by linear mathematical models (Hanbay et al. 2008; Nassir et al. 2012; Zhang et al. 2013; Wadkar et al. 2021). Hence, modelling a WTP is a challenging task due to the complexity of the treatment processes. Similarly, climate change may adversely affect the quality of raw water sources and consequently design and operation of drinking WTP (Krishnaiah et al. 2004; Najafzadeh and Saberi-movahed 2018). To capture this impact, probability-based techniques were used to characterize the uncertainties inherent in the prediction of future climate impact on source water and associated effects on potential mitigation cost in future water treatment operations (Zhiwei Li and Clark 2014; Kote and Wadkar 2019). Needs to implement a sensor in the water supply system to acquire the essential water quality (Aisopou et al. 2012). The cost-effective way of accomplishing this task was to perform a quick and effective condition assessment and then decide whether a more detailed assessment was required (Sarker and Zayed 2009). Previous WTP optimization models were based on nonlinear programming and dynamic programming, however, nonlinear programming is quite complex, time-consuming, and does not guarantee the global optimum solution (Chandwani et al. 2016). The artificial Neural Network (ANN) technique can be used for modelling such WTP processes (Abba and Elkiran 2017; Bekkari and Zeddouri 2019; Djeddou et al. 2019). It can be used for better prediction of the process performance owing to its high accuracy, adequate and promising applications in engineering. (Erickson et al. 2017). Some advanced soft computing models were developed such as adaptive neural fuzzy inference system (ANFIS) and genetic programming (GP) to predict and simulate water quality parameters viz., sodium, potassium, magnesium, sulphates, chloride, pH, electrical conductivity, and total dissolved

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solids. Hamed et al. (2004) developed an ANN model to predict the performance of a wastewater treatment plant (WWTP) based on past information of BOD and SS. Chlorine compounds are widely used in water distribution systems to prevent waterborne diseases (Gibbs et al. 2006). Maintaining a sustainable level of residual chlorine in domestic tap water is essential to ensure the quality of drinking water (Lee et al. 2004). The control-oriented model for chlorine concentration in WDN under unsteady periodic conditions is effective Constans et al. (2003). The reliable assessment for the reservoir where flow pattern and chlorine concentration distributions are closely related to the flow conditions (Zhang and Lee 2011). Chlorine is suspected of stagnating for more extended periods at the flow-recirculation regions, which is supported by the mean age distributions of chlorine (McCoy et al. 2012). The single-input single-output time series neural network model for the prediction of residual chlorine in WDN was effective. Input parameters viz., temperature, electrical conductivity, pH, turbidity, pressure, and water flow rates used for modelling. The model revealed with R between 0.656 and 0.974, while MAE levels between 0.008 and 0.028. Cuesta and Tau (2014) developed FFNN models to predict chlorine concentration at selected nodes of the water supply in Kohoutovice, Czech Republic. Turbidity, pH, initial chlorine, flow, and residual chlorine in three nodes of WDN were used as the dataset for the development of the model (Bowden et al. 2006). The range of 'R' for all points varied from 0.899 to 0.99 for training, 0.403 to 0.915 for testing, and 0.539 to 0.939 for validation Ayvaz and Kentel (2015) established a hybrid Genetic algorithm–linear programing (GA-LP) model for adequate maintaining chlorine residuals within the network to minimize chlorine dose, and developed fuzzy decision-making framework (DMF) useful tool to incorporate the case-specific limitations into the decision process. Kim and Kim (2014) and Kim and Parnichkun (2017) explored a linear regression model by using Reynolds number and the decay coefficients of the chlorine. Also, developed a relationship between hydraulic conditions and the temporal variation in chlorine concentration. A GA was used to calibrate the parameters of the various models and hydraulics with the highest correlation = 0.98. Asnaashari et al. (2014) forecasted water main failure by MLR model with the help of eight independent variables namely pipe, length, diameter, age, break category, soil type, pipe material, year of cement mortar lining, and cathodic protection. Developed MLR model predicted failure rate of pipeline with $R^2 = 0.75$. Wu and Lo (2010) presented two ANN models for free ammonia and chlorine at Goomalling pump station in the network. The total chlorine and free ammonia first order back-propagation ANN models (8-16-1) model performed well with validation Nash-Sutcliffe efficiencies of 0.84 and 0.620, respectively and validation RMSE = 0.132, and MAE = 0. 080. Hebati et al. (2017) developed relationships between microbial indicator organisms, dissolved organic matter (DOM), and trace elements in a biologically stable drinking water distribution system. Fluorescence and absorbance spectroscopy was used for DOM identification in the water body. Medina et al. (2017) described is develop a sampling design (SD) method for localization and quantification of pressure sensors in WDS, aiming for leak detection. Four criteria for SD were used such as maximization of total leak sensitivity and sensitivity consistency, and minimization of information redundancy and sensors number simultaneously. The SD method proposed here could be applied to any WDS and assist advances for data-driven detection of leaks, and even for intelligent systems development for WDS. Amali et al. (2018) adopted dynamic programming and graph theory approaches to optimize chlorine injections at various points of the pipe distribution network for intermediate dechlorination. In comparison with specific hydraulic conditions, this approach provided quick data on the distribution of chlorine in the network, and decreased interventions (sampling, removal, etc.). Librantz et al. (2018) stimulated physical and operational characteristics of WTP using MATLAB. To improve stability, a proportional-integral control was included. In comparison with the technique presently used, the findings of the simulation have shown enhanced stability of residual chlorine, which would decrease chlorine consumption in the process of water treatment. Reilly et al. (2018) reviewed the history of ANNs and their applications and shortcomings in the drinking water sector. From the papers reviewed, it was found that ANNs might be useful modelling tools due to their successful application in areas such as pipes/infrastructure, membrane filtration, coagulation dose, disinfection residuals, water quality, etc. The most popular ANNs applied were FFNN, especially MLPs. It was also noted that over the past decade (2006–2016), ANNs have been increasingly applied in the drinking water sector (Santos et al. 2019). Literature review on the prediction of various parameters related to WDN with FFNN, wavelet packet decomposition, entropy, and neural network, LM algorithm, GA with MCS are sighted (Najafzadeh and Zeinolabedini 2018, 2019; Muharemi et al. 2019; Loc et al. 2020). It is found that common influencing parameters such as pipe material, temperature, pressure, ammonia level, and turbidity for predicting the concentration of residual chlorine in WDNs (Saha et al. 2017; Saberi-Movahed et al. 2020). It is also observed that categorization of study area based on commercial and residential activities affect the concentration of residual chlorine in WDN. In the present paper development of efficient ANN models for prediction of water quality parameters and coagulant dose in WTP and prediction residual chlorine in WDN.

Table 1. Standard statistics of outlet water quality parameters of the WTP.

Water quality parameter	Standard statistics			
	Mean ($\bar{x}$)	Standard deviation (σ)	Skewness ($\gamma 1$)	Kurtosis ($\gamma 2$)
pH	7.604	0.199	− 3.048	9.095
Total Hardness (mg/L)	72.62	28.795	1.096	1.355
Turbidity (mg/L)	1.8	0.471	0.310	0.528
Ca (mg/L)	16.286	6.725	1.601	3.162
Cl^- (mg/L)	22.455	8.875	1.546	3.043
Alkalinity (mg/L)	103.026	31.775	0.641	0.070
K (mg/L)	0.878	0.391	0.032	− 0.312
TDS (mg/L)	73.118	27.214	1.218	0.589
Conductivity	147.273	53.398	1.234	0.687
DO (mg/L)	7.102	1.521	1.000	1.077
Colour (TCU)	0.548	1.214	3.938	14.345
Fe (mg/L)	0.134	0.087	0.790	− 0.658
Cr (mg/L)	0.022	0.050	3.315	9.144
Al (mg/L)	0.041	0.068	3.305	9.133
Mn (mg/L)	0.049	0.019	− 0.180	− 0.524
F^- (mg/L)	0.350	0.228	0.409	− 1.255
Cu (mg/L)	0.015	0.009	2.340	5.265
Nitrate (mg/L)	1.538	0.417	0.125	3.766
BOD (mg/L)	1.432	0.456	− 0.695	− 0.020
TSS (mg/L)	0.103	0.489	5.152	25.739
Phosphate (mg/L)	0.722	0.522	1.172	2.147
Ni (mg/L)	0.022	0.017	1.071	− 0.230
Co (mg/L)	0.025	0.015	1.691	2.726
Detergent (mg/L)	0.025	0.020	0.342	− 1.351
Mo (mg/L)	0.027	0.017	0.327	− 1.060
B (mg/L)	0.228	0.111	1.609	2.083
MPN	0	0	–	–

1.1. Material and analysis of water quality parameters

Dataset of water quality parameters is collected over a period of 4 years (1 January 2012–31 December 2015) with 5643 data points for prediction of water quality parameters at a WTP. The water quality parameters for inlet and outlet water of WTP includes pH, total hardness, turbidity, Ca, Cl^-, alkalinity, K, TDS, conductivity, DO, colour, Fe, Cr, Al, Mn, F^-, Cu, nitrate, BOD, TSS, phosphate, Ni, Co, detergent, Mo, B, and MPN. The standard statistics of outlet water quality parameters of WTP listed above are given in Table 1. It is observed that the mean value of Al, Ni and detergent is higher than standard drinking water quality parameters as per IS 10500: 2012. It is also seen that pH, Mn, and BOD are negatively skewed, whereas remaining all other water quality parameters are positively skewed.

From Table 1, it is seen that the observed Cu has the lowest σ and conductivity has the highest σ. Similarly, $\gamma 1$ of K near to zero which implies data is perfectly symmetrical whereas pH, total hardness, Ca, Cl^-, TDS, conductivity, colour, Cr, Al, Cu, TSS, phosphate, Ni, Co, and B shows high skewness indicating that the data is asymmetrical. Turbidity, Mn, F^-, Nitrate, detergent, and Mo exhibit low skewness indicating that the data is approximately symmetric. Kurtosis of Nitrate, pH, colour, Cr, Al, Cu, and TSS has the leptokurtic distribution of data with a long and fat tail, higher and sharper central peak. Likewise, kurtosis of turbidity, hardness, alkalinity, K, TDS, conductivity, DO, Fe, Mn, F^-, BOD, Ni, Co, detergent, Mo, and B has the platykurtic distribution of data with short and thin tail and lower and broader central peak. Finally, only Cl^- has a normal distribution of data indicating mesokurtic distribution where data is closer to mean as compared to leptokurtic and platykurtic distributions. It is found that parameters viz. K, Fe, Mn, BOD, F^-, Ni, detergent, and Mo have negative $\gamma 2$, which means that distribution is flatter than a normal distribution curve.

2. Methodology

The training algorithms used in this study are namely, BR, LM, resilient back-propagation (RP), BFGS Quasi-Newton (BFG), one step secant (OSS), conjugate gradient back-propagation (CGB), conjugate gradient back-propagation with Fletcher-Powell (GCF), variable learning rate gradient descent (VLRGD), gradient descent (GD), and gradient descent with momentum (GDM) are used for the development of FFNN and CFNN models. The fastest training function is generally LM, and it is the default training function for FFNN. The BFGS Quasi-Newton training algorithm is also quite fast. Both are less effective for

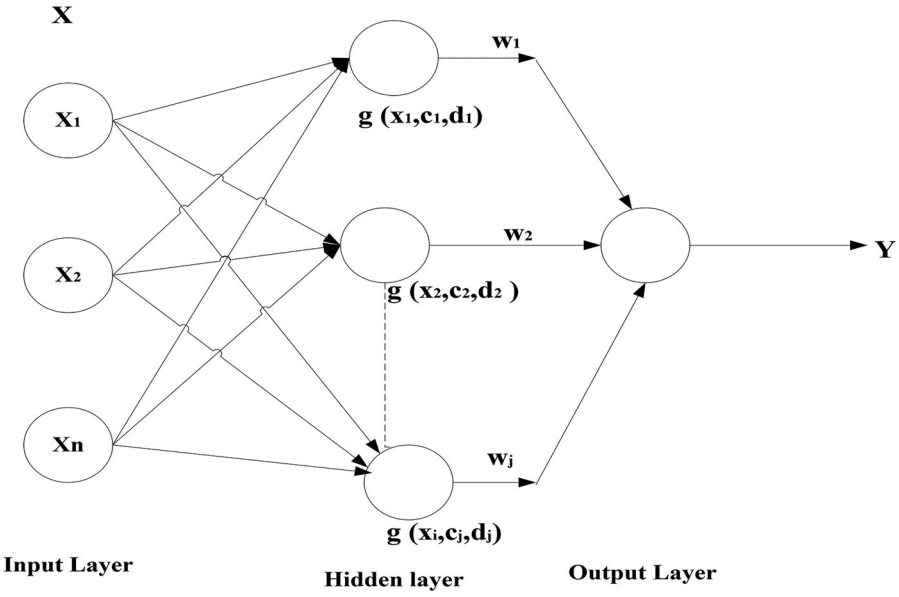

Figure 1. A typical radial basis function neural network.

a big network with thousands of weights because they require more memory and more calculation time. Also, LM training algorithms perform better on function fitting i.e. non-linear regression problems than on pattern recognition problems. Back-propagation is sometimes used to refer specifically to the gradient descent algorithm when applied to ANN training. This terminology is not used here because the gradient and Jacobian matrix processes are applied to all training algorithms mentioned above by calculating retrospectively through the networks. Instead of using the word back-propagation alone, the name of the particular optimization algorithm can be used clearly. Also, the network is sometimes called a back-propagation network. However, the back-propagation technique that is used to compute gradients and Jacobians matrix in a multilayer network can also be applied to many different network architectures.

2.1. ANN modelling

The potential of the neural network is explored in predicting water quality, coagulant dose, chlorine dose, and residual chlorine with different neural networks to achieve the best performing model (Heddam et al. 2011a, 2011b; Haghiri et al. 2018). ANN methodology adopted in the present study includes four neural network models namely; water quality neural network (WQNN) model, coagulant dose neural network (CDNN) model, and residual chlorine neural network (RCNN) model. ANN model is developed using MATLAB 2015 software with defined codes. ANN model development process includes mainly; (1) Data collection and division, (2) Model design, (3) Model training and (4) Model validation. ANN model consists of mainly three layers namely input layer with input data, a hidden layer with hidden nodes, and an output layer with output data. ANN adapts the weights of their hidden neurons based on the input and output data. Therefore, the inclusion of defective data in the training set will alter the mean errors, which are propagated back for weight optimization and resulting in inaccurate predictions.

All the networks are trained multiple times in order to produce the lowest error statistics. The best model is then selected based on performance criteria and representing graphically observed and predicted series (Guan-De and Shang-Lien 2008). The predictions of all ANN models are evaluated for the different ANN configurations with one hidden layer. Several runs are performed for each network structure to prevent the wrong selection of initial weights. All the trained neural networks are validated using the validation data set. The model with the least validation error is selected and further tested using test data set for computing the final network error. Best models from each category are validated with the latest dataset whereas the RCNN model is validated with available residual chlorine in zone 1-Indrayani Nagar and zone 2-Sant Tukaram Nagar from PCMC, Maharashtra, India (Figure 1).

2.2. Water quality neural network model

Inlet and outlet water quality parameters such as pH, total hardness, Ca, Cl^-, alkalinity, K, TDS, conductivity, DO, colour, Fe, Cr, Al, Mn, F^-, Cu, nitrate, BOD, TSS, phosphate, Ni, Co, detergent, Mo, B, and MPN are identified for development of water quality neural network (WQNN) model. WQNN model established with listed 27 inlet water quality parameters in input layer whereas output layer predicts 27 outlet water quality parameters of WTP as shown in Figure 2. The data is divided into three sets namely

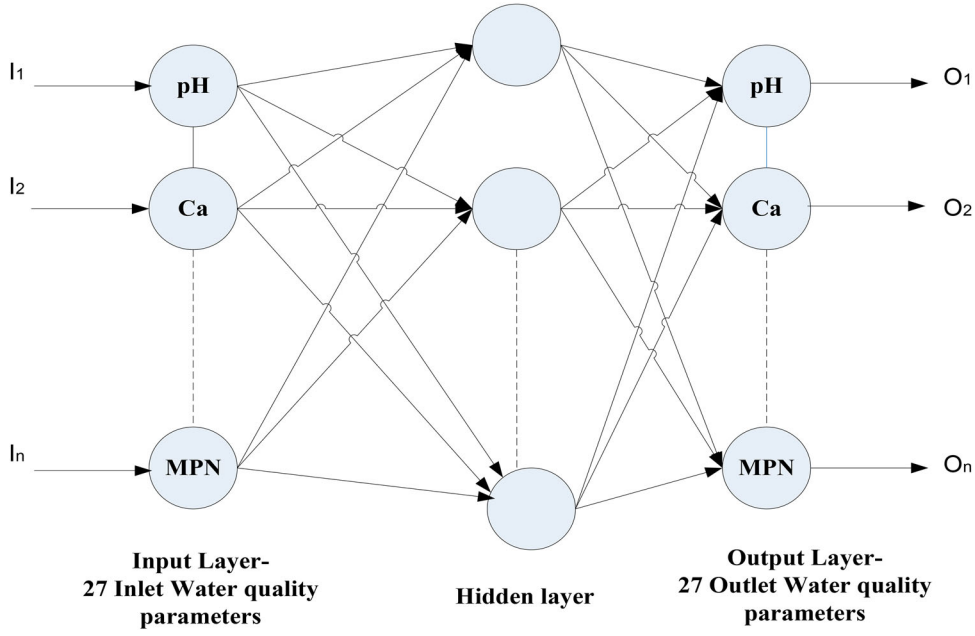

Figure 2. Water quality neural network model.

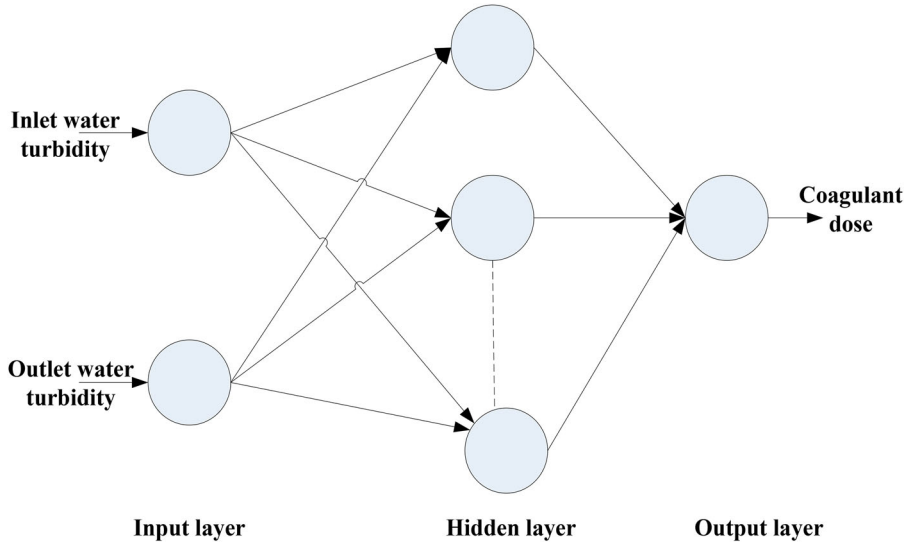

Figure 3. Coagulant dose neural network model.

training, testing, and validation. It is divided into 75% for training, 15% for testing, and 15% for validate. Preliminary investigation of the performance of FFNN and CFNN using various training algorithms such as BR, LM, RP, BFG, OSS, CGB, CGF, VLRGD, GD, and GDM is carried out. During training, the best performing training function is selected for further model development. Various models with different combinations of input vectors are tested in order to design a network that displays acceptable performance in a reasonable amount of time. The performance of the network is evaluated for the above-mentioned training algorithms by increasing the number of neurons in the hidden layer and the number of epochs. The best combination of the training algorithm, the number of neurons in the hidden layer, and the number of epochs for the highest R are determined. All the trained neural networks are validated using the validation data set. The trained neural network with the least validation error is selected as the model for evaluation of WTP and further tested using test data set for computing the final network error.

2.3. Coagulant dose neural network model

Input parameters such as inlet and outlet water turbidity and output parameter as coagulant dose are identified

for the coagulant dose neural network (CDNN) model (Kennedy et al. 2015; Jayaweera and Aziz 2018). The CDNN model is established with inlet and outlet water turbidity in the input layer whereas the output layer predicts coagulant dose as shown in Figure 3. Daily data of input and output parameters spanning four years namely year 2014 and year 2015 are obtained from the plant laboratory. The database of input and output parameters required for the ANN modelling consists of 11688 data points spanning eight data points per day. The data interval is three hours starting from 7 AM current day to 7 AM of next day. Preliminary investigation using various training algorithms such as BR, LM, RP, BFG, OSS, CGB, CGF, VLRGD, GD, and GDM to FFNN and CFNN is carried out. During training, the best performing training function is selected for model development. The best combination of training algorithm, the number of neurons in the hidden layer, and the number of epochs for the highest R are determined. The trained neural network with the least validation error is selected as the model for coagulant dose and further tested using test data set for computing the final network error (Liu et al. 2018; Bobadilla et al. 2019). Lastly, GUI for the prediction of coagulant is developed using the best performing model.

The performance of these ANN models is quantified by using standard statistics viz. $\bar{x}$, σ, $\aleph 1$, $\aleph 2$, and error statistics viz. R, MSE, and MAE. Further best performing ANN model is selected for highest R, lowest MSE, and MAE values. Also, mapping of predicted series with observed series is checked for standard statistics, time series plots, and scatter plots.

ANN models are developed using RBFNN, FFNN, CFNN, and GRNN networks by the trial-and-error method by modifying input variables, hidden nodes, training algorithms, SF, and epochs for improving the performance of models. During the development of ANN models, training and testing data are split into 80:20 respectively. Diversified training algorithms such as BR, LM, RP, BFG, OSS, CGB, CGF, VLRGD, GD, and GDM are used for the development of FFNN and CFNN models, whereas RBFNN and GRNN models are tried for SF ranging from 0.1 to 15. The performance of these ANN models is quantified by using standard statistics viz. $\bar{x}$, σ, $\aleph 1$, $\aleph 2$ and error statistics viz. R, MSE, and MAE. Further best performing ANN model is selected for highest R, lowest MSE, and MAE values. Also, mapping of predicted series with observed series is checked for standard statistics, time series plots, and scatter plots.

3. Results and discussion

3.1. Input parameters and training algorithm identification

Routine examination of outlet water quality of WTP mainly includes pH, turbidity, hardness, alkalinity, and MPN. However, as per the document of the eleventh five-year plan of India (2007–2012), many peoples were affected with excess nitrate, phosphate, B, Ni, Fe, F^-, salinity, and arsenic. Thus, there is a need to consider as many parameters as possible water quality parameters for modelling. Input and output viz., as pH, total hardness, turbidity, Ca, Cl^-, alkalinity, K, TDS, conductivity, DO, colour, Fe, Cr, Al, Mn, F^-, Cu, nitrate, BOD, TSS, phosphate, Ni, Co, detergent, Mo, B and MPN for inlet and outlet water of WTP are used for ANN modelling. The database of inlet and outlet water quality parameters required for the ANN modelling over a period of four consisting of 5643 data points is collected from WTP. The various ANN models were developed for the prediction of water quality parameters, coagulant dose, and chlorine dose at the WTP and residual chlorine in WDN of PCMC, Nigdi, Pune. Each model is trained several times until the best performance is achieved. Best performance is recorded by varying numbers of hidden layers, hidden nodes, and epochs during the training of FFNN and CFNN networks. In RBFNN and GRNN models, SF plays a vital role in establishing a good ANN correlation model with high prediction accuracy and stability. In this study, RBFNN and GRNN models are trained by the varying value of SF from 0.1 to 15. The number of FFNN and CFNN are developed by using various training algorithms such as BR, LM, RP, BFGS, BFG, OSS, CGF, CGB, VLRGD, GDM, and GD. A graph of the coefficient of correlation versus various training algorithms used for modelling is shown in Figure 4. It is observed that LM and BR training algorithms are better as compared to other training algorithms. The LM and BR training algorithms are, therefore, adopted for training of FFNN and CFNN networks for the prediction of outlet water quality of the WTP.

3.2. Cascade feed forward neural network water quality model using Levenberg Marquardt training algorithm

CFNN water quality model using LM training algorithm (CFNNWQ1) is created with the input layer, hidden layer, and output layer in MATLAB software.

The LM algorithm performs a combined training process with the steepest descent algorithm and the Gauss–Newton algorithm. The steepest descent algorithm produces a quadratic approximation, whereas the Gauss–Newton algorithm considerably accelerates convergence. The number of models is developed by varying the number of hidden nodes and epochs by the trial-and-error method. The R and MSE values obtained are then plotted against the number of hidden nodes shown in Figure 5.

During network training, hidden nodes are increased from 7 to 57. The average, minimum and maximum value of $R = 0.970$, $R = 0.929$, and $R = 0.986$ are obtained respectively for various combinations of hidden node and

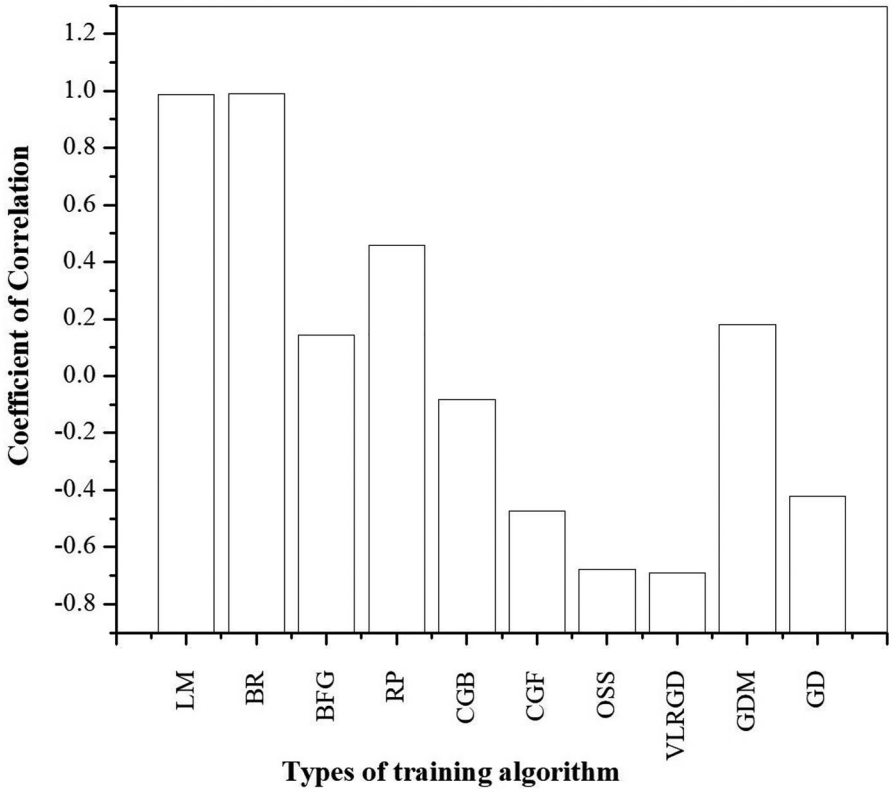

Figure 4. Performance of various types of training algorithm.

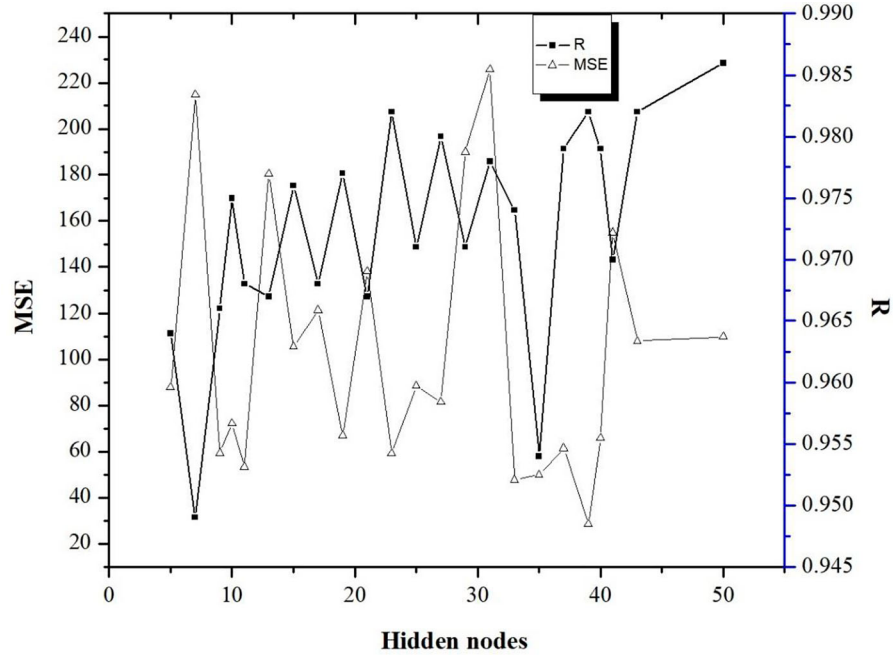

Figure 5. Performance of CFNNWQ1 models during training period.

epoch. Similarly, average, minimum and maximum values of MSE = 142.39, MSE = 22.24, and MSE = 961.85 are obtained. The value of the smallest *R* and the largest MSE for hidden node = 57 are noted. It is observed that hidden nodes are increased from 7 to 57 during the training of the network, where *R* and MSE values are changed. However,

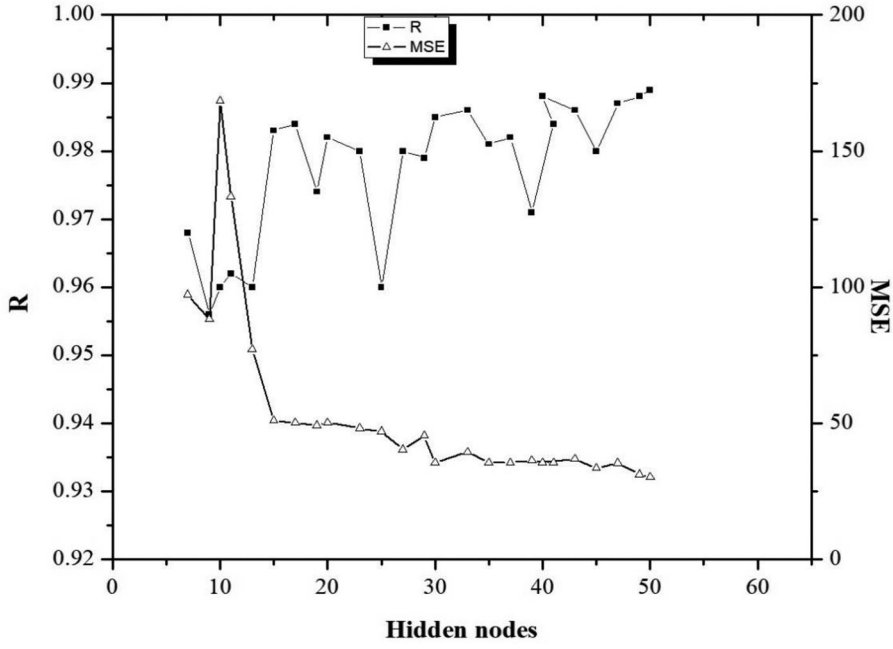

Figure 6. Performance of CFNNWQ2 models during training period.

it does not find any linear relationship between the hidden nodes with 'R'. The lowest 'R' and highest MSE obtained against hidden node = 57. It is found that the CFNNWQ2 (27-40-27) model tracks very well for training ($R = 0.985$) and testing ($R = 0.986$). In this case, the network response is satisfactory, and validation can be used for entering new inputs.

3.3. *Cascade feed forward neural network water quality model using Bayesian regularization training algorithm*

CFNN water quality model using BR training algorithm (CFNNWQ2) is created with the input layer, one hidden layer, and output layer in MATLAB software. For issues of approximation of functioning, BR can achieve

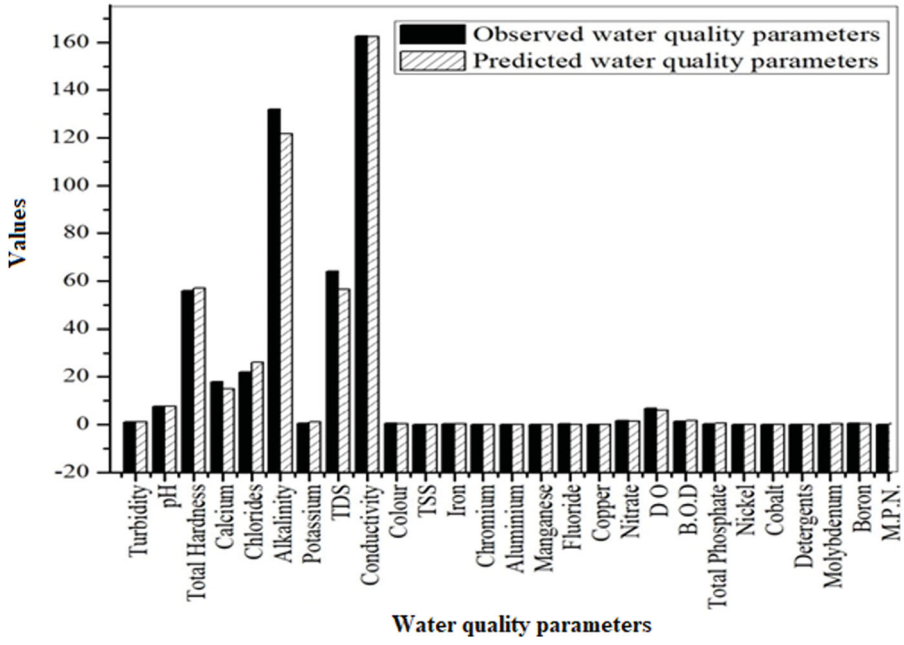

Figure 7. Prediction by CFNNWQ2 (27-30-27) model during testing period.

a lower median squared error than other training algorithms. The Bayesian neural network structure builds on the probabilistic understanding of network parameters. In other words, the Bayesian method implies a probability distribution of network weights, contrary to traditional network formation where an ideal weight set is selected to minimize an error function. Consequently, the network predictions are also a distribution of probability. Training algorithm 'BR' can train any network as long as its weight, net-input and transfer functions have derivative functions. The *R* and MSE values obtained are then plotted against the number of hidden nodes shown in Figure 6. During network training, hidden nodes are increased from 5 to 50. The average, minimum and maximum values of $R = 0.978$, $R = 0.982$, and $R = 0.989$ are obtained respectively for various combinations of hidden nodes and epochs. Similarly, average, minimum and maximum values of MSE = 53.89, MSE = 30.15, and MSE = 168.46 are obtained.

CFNNWQ2 (27-30-27) model tracks the targets very well for training ($R = 0.989$), and testing ($R = 0.9891$). The performance of CFNN is best as compared to FFNN

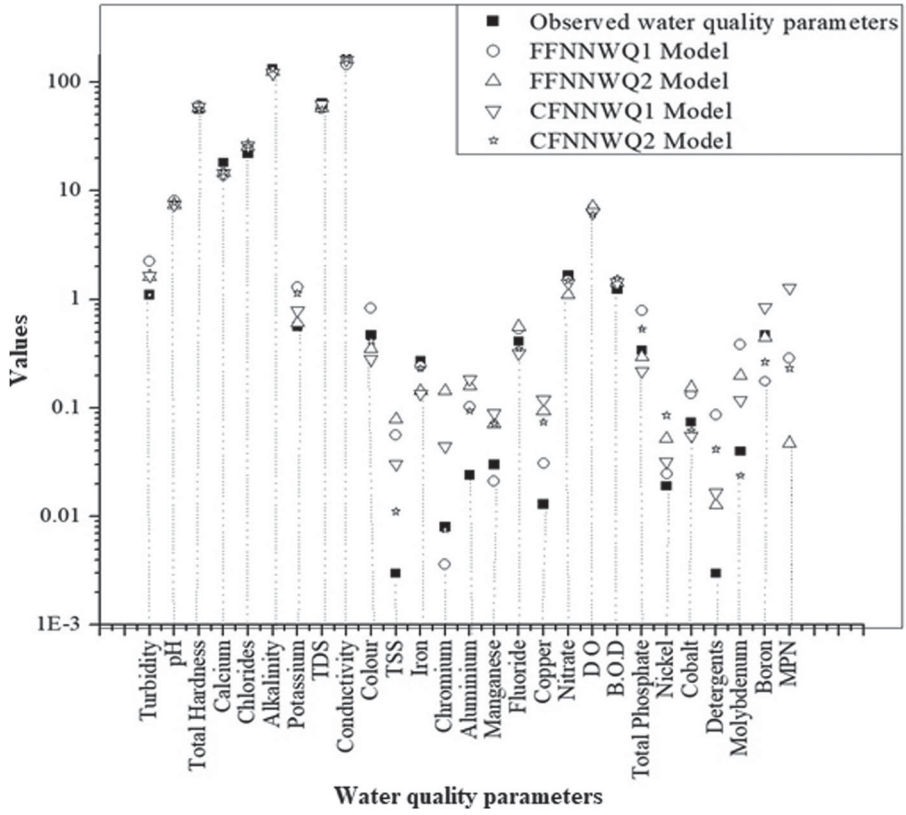

Figure 8. Prediction of water quality parameters by various types of ANN models.

Table 2. Prediction of selected water quality parameters by the various best ANN models.

Water quality parameters	Observed values	FFNNWQ1 (27-50-27) model	FFNNWQ2 (27-30-27) model	CFNNWQ1 (27-40-27) model	CFNNWQ2 (27-30-27) model
Turbidity	1.1	2.226	1.625	1.648	1.089
pH	7.65	8.055	7.469	7.446	7.723
Hardness	56	59.854	58.245	59.756	57.102
Ca	18.043	13.755	14.654	14.577	14.926
Cl^-	22	25.744	25.671	26.214	26.045
Alkalinity	132	125.584	125.704	121.324	121.548
TDS	64	57.475	58.271	62.872	56.512
Conductivity	162.6	143.403	161.822	160.037	162.315
Fe	0.27	0.242	0.143	0.136	0.234
DO	6.7	6.456	7.196	6.358	6.062
MPN	0.000	0.287	0.048	1.274	0.231

because the CFNN input layer has a weighted connection with hidden as well as the output layer. Also, the BR training algorithm delivers a decisive benchmark for finishing the training step and counters overtraining of the network. This potential of the BR training algorithm marks it a more adaptive and convergent network for prediction. The validation results of outlet water quality parameters are presented in Figure 7 by plotting the observed and predicted water quality parameters. It is observed that predicted water quality parameters viz., total

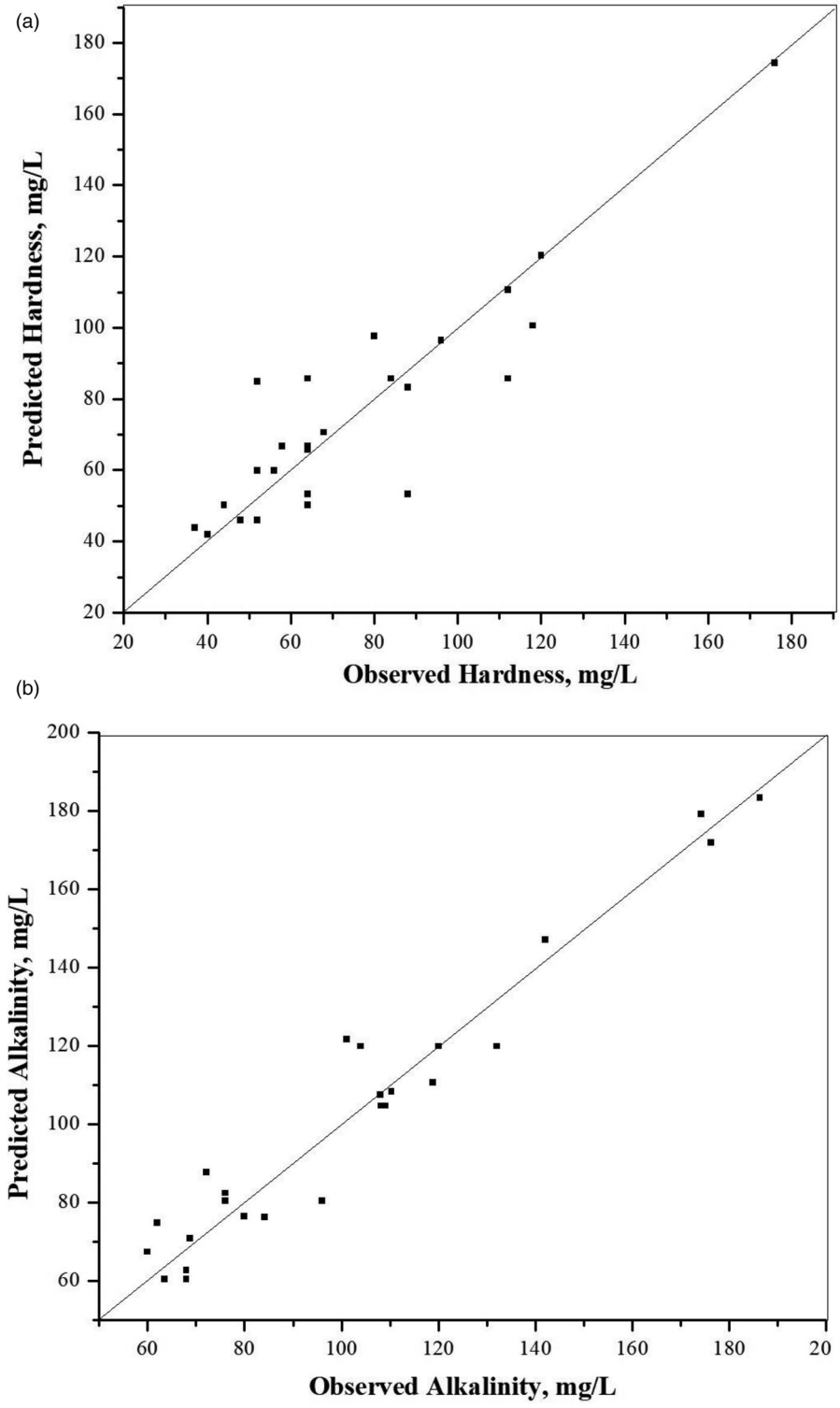

Figure 9. Scatter plot of: (a) Hardness (b) Alkalinity under best fit category during training and testing period.

hardness, Ca, alkalinity, conductivity, TDS, Cl − differ from observed water quality parameters. The performance summary of the resulting error statistics of the best model in each category proves that the CFNNWQ2 (27-30-27) model performed excellent during the training and testing period.

Figure 8 shows a prediction of water quality parameters by various types of ANN model, where predicted water quality parameters namely TSS, aluminium, alkalinity, detergent, and copper, molybdenum are more diverge from observed water quality parameters. The water quality parameters namely pH, hardness, calcium, chloride,

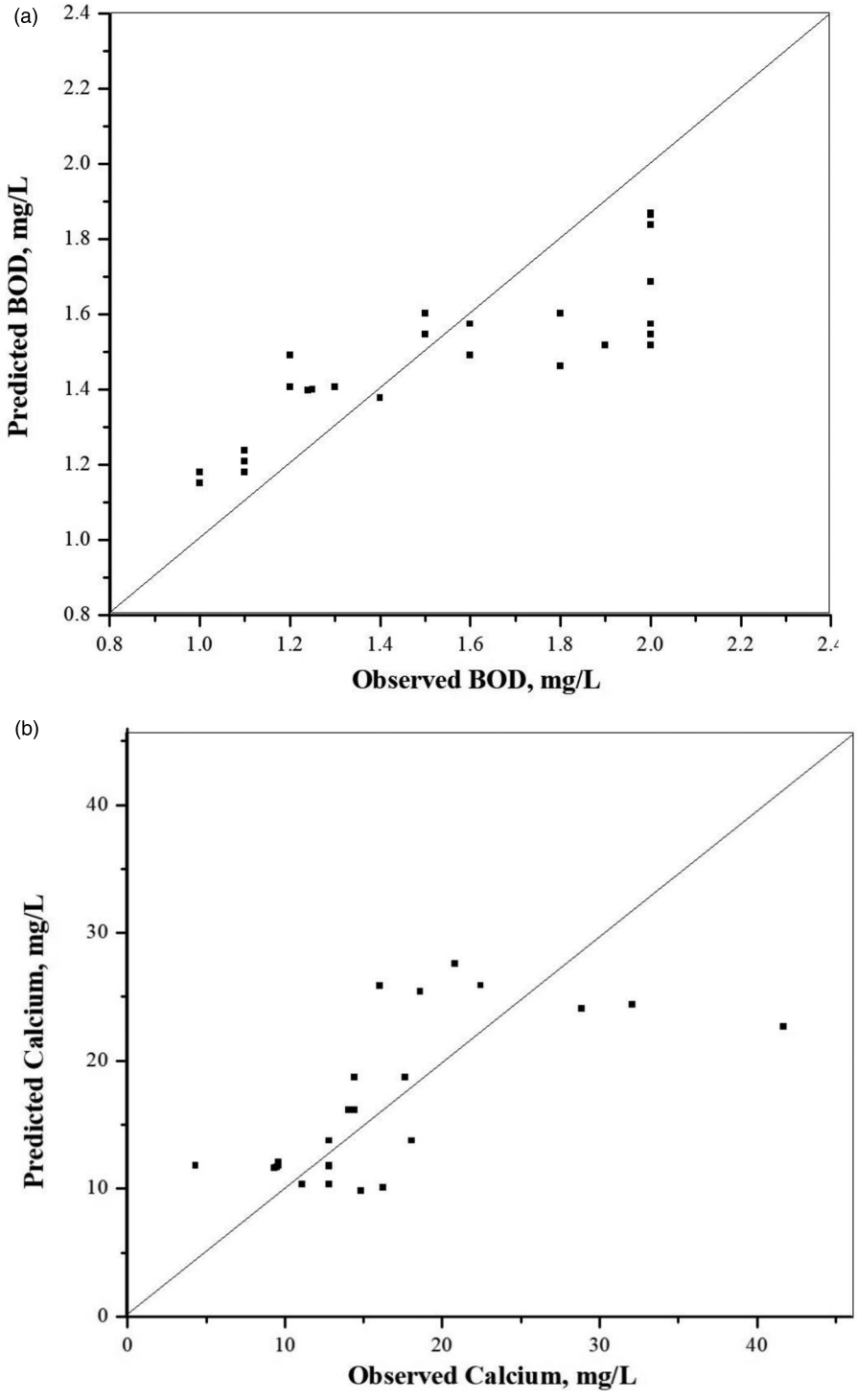

Figure 10. Scatter plot of: (a) BOD (b) Calcium under good fit category during training.

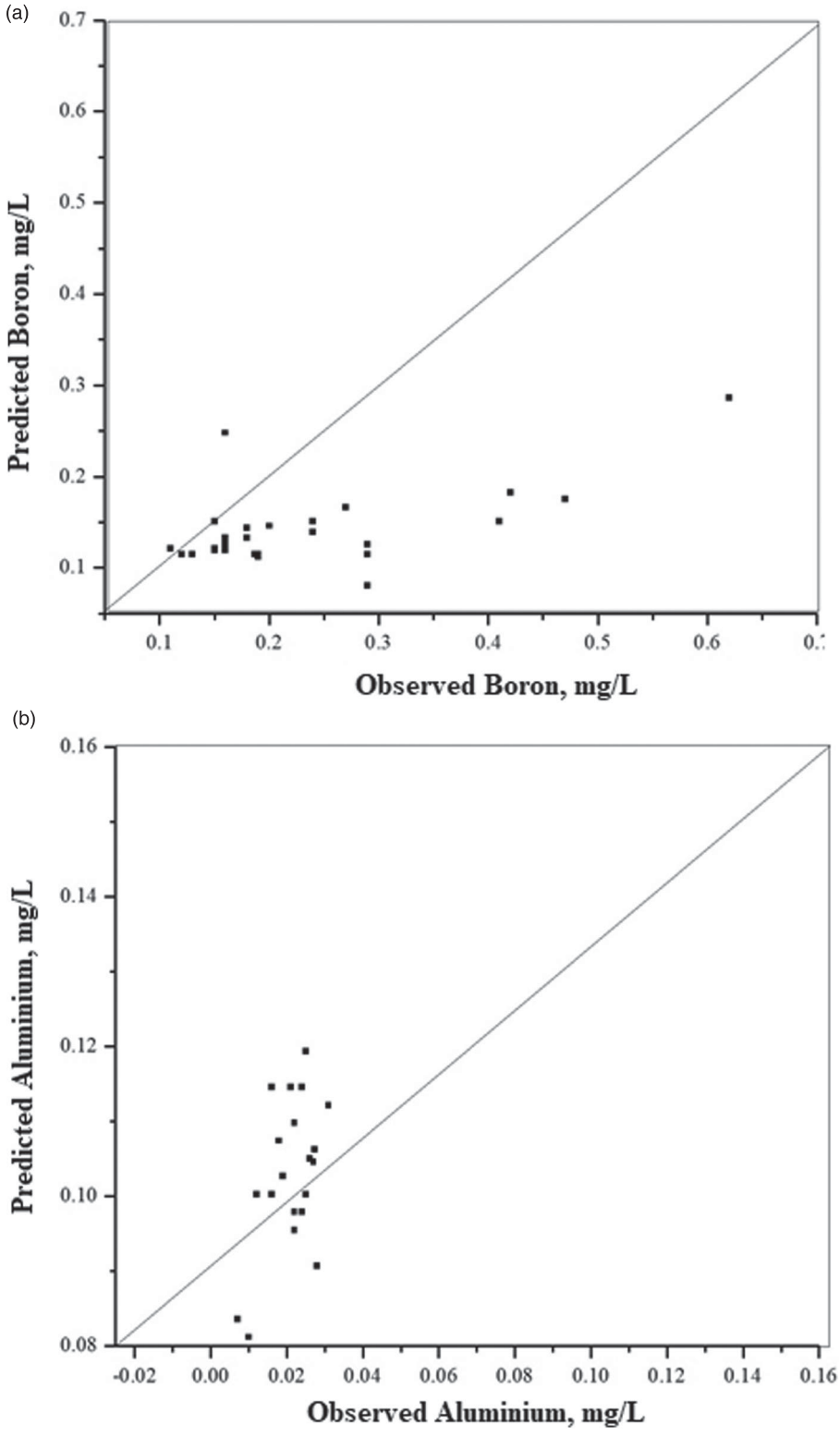

Figure 11. Scatter plot of: (a) Boron (b) Aluminium under poor fit category during training and testing period.

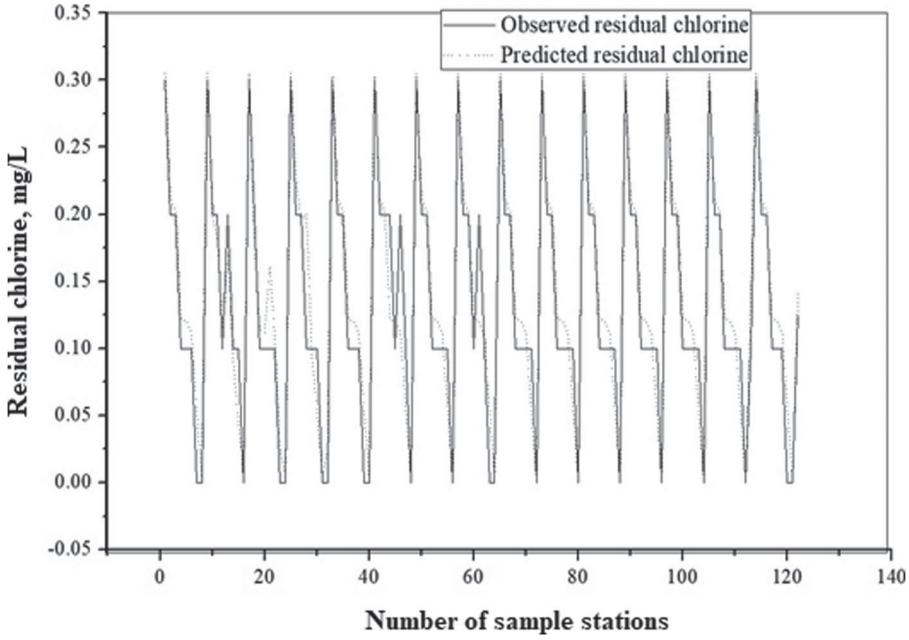

Figure 12. Prediction of residual chlorine at sample station by FFNN (2-25-1) LM model.

alkalinity, TDS, conductivity, fluoride, nitrate, DO, BOD, are closely near to observed water quality parameters. Similarly, other water quality parameters namely potassium, colour, iron, manganese, total phosphate, nickel, cobalt are averagely near to observed water quality parameters. The prediction of high priority water quality parameters namely nitrate, phosphate, boron, nickel, iron, fluoride, and chromium are considered carefully as small change creates an adverse effect on human health.

Table 2 shows the prediction of selected water quality parameters by the various best ANN models. The CFFNNWQ2 model had the best prediction proficiency of turbidity (98.99%), pH (99.06%), hardness (98.03%), Ca (82.73%), chlorides (81.62%), Alkalinity (92.08%), TDS (88.30%), conductivity (99.82%), Fe (86.28%), DO (90.48%) and MPN (100%). Overall, ANN prediction of outlet water quality parameters viz., pH, turbidity, alkalinity, conductivity, DO, hardness, TDS, Ca, MPN, Fe, and Cl^{-} was good as compared to actual values. Furthermore, the prediction of other outlet water quality parameters was less satisfactory due to two possibilities (i) large variation in values (ii) very small fraction numbers.

The scatter plot of the CFNNWQ2 model of water quality parameters is divided into three categories mainly best, good and poor fit. Sample scatter plot of hardness and alkalinity under best-fit category is shown in Figure 9(a, b). The observed and predicted values of alkalinity have $\sigma = 32.07$ and 31.33 during the training and testing period, respectively. Similarly, the $\bar{x}$ of observed and predicted alkalinity are very close to each other with a value of 103.35 and 103.25 mg/L respectively. It is seen that observed and predicted alkalinity showed $\gamma 1 = 0.637$ and $\gamma 1 = 0.788$ respectively. The value of $\gamma 1$ indicates that the data is approximately symmetric. Likewise, observed and predicted values of hardness have $\sigma = 28.93$ and 27.34 during the training and testing period, respectively. Similarly, the $\bar{x}$ of observed and predicted hardness are very close to each other with a value of 72.72 and 72.19 mg/L respectively. It is seen that observed and predicted hardness showed $\gamma 1 = 1.10$ and $\gamma 1 = 1.12$ respectively. The value of $\gamma 1$ indicates that the data is approximately symmetric which is one of its properties of best fit.

The sample scatters plot of BOD and calcium under the good fit category is shown in Figure 10(a, b). The observed and predicted value of BOD has $\sigma = 0.34$ and 0.15 during the training and testing period, respectively. Similarly, the $\bar{x}$ of observed and predicted BOD are very close to each other with a value of 1.50 and 1.43 mg/L respectively. It is seen that observed and predicted BOD showed $\gamma 1 = 0.0637$ and $\gamma 1 = -0.28$ respectively. The value of $\gamma 1$ indicates that the data had low skewness with less symmetric between observed and predicted BOD data. Likewise observed and predicted values of calcium have $\sigma = 6.78$ and 5.46 during the training and testing period, respectively. Similarly, the $\bar{x}$ of observed and predicted calcium are very close to each other with a value of 16.30 and 16.28 mg/L respectively. It is seen that observed and predicted calcium showed $\gamma 1 = 1.6$ and $\gamma 1 = 0.603$ respectively. The value of $\gamma 1$ indicates that the data is less symmetric between observed and predicted BOD data. Finally, the sample scatters plot of boron and aluminium under the poor fit category is shown in Figure 11(a, b). The observed and predicted values of boron have $\sigma = 0.11$ and 0.03 during the training and testing period, respectively.

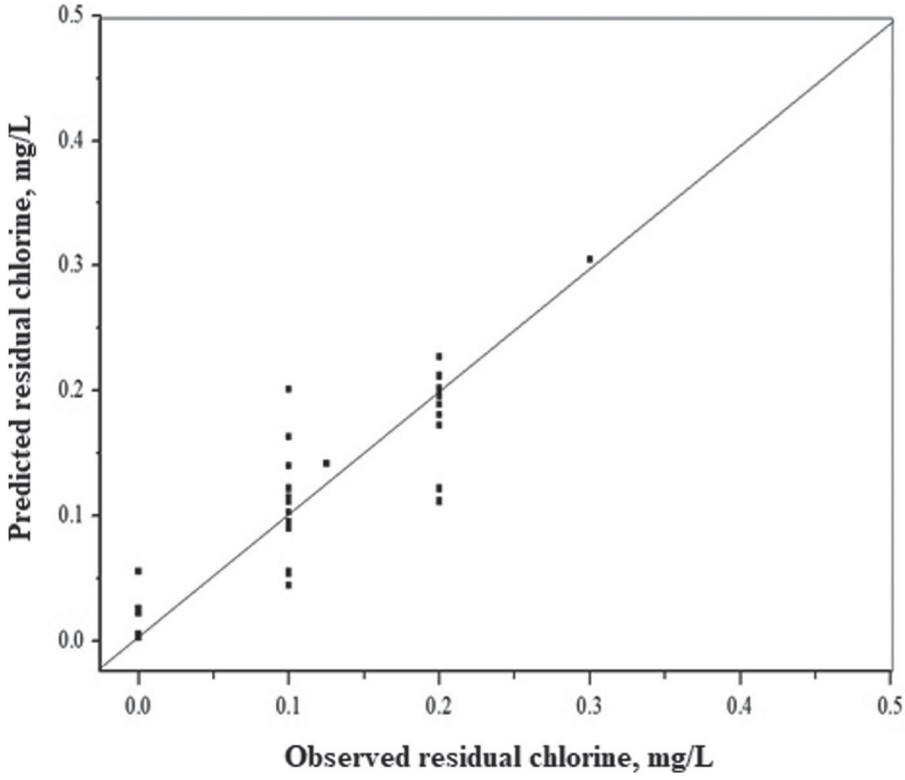

Figure 13. Scatter plot of FFNN (2-25-1) LM model during training and testing period.

Similarly, the $\bar{x}$ of observed and predicted boron are very close to each other with a value of 0.22 and 0.145 mg/L respectively. It is seen that observed and predicted boron showed $\gamma 1 = 1.66$ and $\gamma 1 = 2.09$ respectively. The value of $\gamma 1$ shows high skewness indicating that data is asymmetrical which one of the properties of poor fit.

3.4. *Analysis of residual chlorine neural network models*

In this study, the number of ANN models for the prediction of residual chlorine in WDN are developed. The various ANN and training algorithms are tested in order to develop the best network, which displays acceptable performance in a reasonable amount of time. Each model is trained many times and the best performance is evaluated. The behaviour of ANNs is compared based on various performance indices during training and testing are shown in Table 3. For ANN prediction with FFNN and CFNN, different training algorithms were tried with varying hidden nodes from 15 to 60 to achieve the best-performing network.

It is observed that LM, BR, and BFG training algorithms give good results and the best prediction can be achieved by the FFNN model with LM training function. By comparing performance indices of ANN models, it is found that FFNN (2-25-1) LM model produced excellent results. Similarly, for RBFNN and GRNN models, SF varied and the best results are depicted in Table 3. All ANN models are trained until minimum MSE and maximum R is achieved. Figure 12 shows the prediction of residual chlorine at sample stations and Figure 13 shows a scatter plot of residual chlorine during the training and testing period by FFNN (2-25-1) LM model. In this case, the highest (0.3 mg/L) and lowest (0 mg/l) values are very well predicted whereas a few average (0.2 mg/L) values are still under-predicted. For further evaluation of model performance, standard statistics including $\bar{x}$, σ, $\gamma 1$, and $\gamma 2$ are used shown during the training and testing period. It is observed that during the training period, standard statistics such as σ varied from 0.021 to 0.048, the absolute value of $\gamma 1$ varied from 0.071 to 1.210, and $\gamma 2$ varied from 2.512 to 13.639. Similarly, during the testing period, standard statistics such as σ varied from 0.017 to 0.046, the absolute value of $\gamma 1$ varied from 0.004 to 2.121, and $\gamma 2$ varied from 2.654 to 5.637. However, in the case of RBFNN models, values of σ, $\gamma 1$, and $\gamma 2$ are nearly the same for different values of SF during the training and testing period. Similarly in the case of GRNN models as SF decreases: values of σ are nearly the same, the absolute value of $\gamma 1$ decrease and the value of $\gamma 2$ increases. By comparison of the mean value for ANN models during testing, where it is found that the observed mean value of residual chlorine is near to the mean value of residual chlorine for the FFNN (2-25-1) LM model. Similarly, by the comparison of σ for ANN models

Table 3. Performance of various ANN models during training and testing period.

	Training period			Testing period		
ANN models	*R*	MSE	MAE	*R*	MSE	MAE
FFNN (2-25-1) Bayesian regularization	0.962	0.001	0.016	0.983	0.001	0.015
FFNN (2-25-1) Levenberg-Marquardt	0.967	0.001	0.018	0.988	0.001	0.016
FFNN (1-25-1) BFGS Quasi-Newton	0.961	0.001	0.014	0.971	0.001	0.014
CFNN (2-25-1) Bayesian regularization	0.964	0.001	0.016	0.984	0.001	0.014
CFNN (2-25-1) Levenberg-Marquardt	0.941	0.001	0.024	0.954	0.001	0.024
CFNN (1-25-1) BFGS Quasi-Newton	0.852	0.002	0.038	0.962	0.001	0.027
RBFNN1 SF = 0.5	0.973	0.000	0.009	0.974	0.001	0.013
RBFNN2 SF = 1	0.973	0.000	0.009	0.974	0.001	0.013
RBFNN3 SF = 2	0.973	0.000	0.009	0.975	0.001	0.013
GRNN1 SF = 4	0.886	0.002	0.037	0.937	0.002	0.036
GRNN2 SF = 2	0.913	0.001	0.029	0.952	0.001	0.027
GRNN2 SF = 1	0.918	0.001	0.026	0.947	0.001	0.025
GRNN3 SF = 0.5	0.921	0.001	0.026	0.949	0.001	0.024

during testing, where lowest σ is obtained against FFNN (2-25-1) LM model.

4. Conclusion

Diversified training algorithms such as BR, LM, RP, BFGS, BFG, OSS, CGF, CGB, VLRGD, GDM, and GD are used for the development of ANN models. It is observed that BR training algorithms produced excellent predictions as compared to other training algorithms. The performance of CFNN is best as compared to FFNN because the CFNN input layer had a weighted connection with hidden as well as the output layer. CFNNWQ2 (27-30-27) water quality model with $R = 0.989$ produced an excellent prediction of outlet water quality parameters namely pH, turbidity, alkalinity, conductivity, DO, hardness, TDS, Ca, MPN, Fe, and Cl^- as compared to other water quality parameters. Prediction of outlet water quality parameters namely potassium, colour, iron, manganese, total phosphate, nickel, cobalt is less satisfactory due to two possibilities (i) significant variation in values (ii) minimal fraction numbers. In coagulant dose modelling, CFNNCD2 (2-40-1) yielded a good prediction $R = 0.947$ for a broad range of turbidities as compared to other models. Moreover, in the monsoon season, when turbidity suddenly increases model gave a low prediction of coagulant dose. Prediction of coagulant dose in the monsoon season was less satisfactory due to the probability of past database where coagulant dose was kept constant for a longer duration. For residual chlorine modelling, FFNN (2-25-1) delivered the best prediction with $R = 0.988$ as compared with CFNN, RBFNN, and GRNN models for farthest zones in WDN.

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