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Simulation and Prediction of Groundwater Quality of a Semi-Arid Region Using Fuzzy Inference System and Neural Network Techniques

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ABSTRACT

The groundwater is the main source of domestic and agricultural purposes in the arid and semi-arid regions where the surface water availability is limited. To protect and manage the groundwater system effectively, a thorough knowledge and understanding of groundwater quality and application of computational methods to simulate the complex and nonlinear groundwater system are paramount necessary. Generally, three types of models such as physically based model, conceptual models and Blackbox models are applied to study the interconnected processes in the subsurface media. In this study, Artificial Neural Network (ANN) (3 Models with 1, 2 and 3 outputs) was used to simulate and predict the concentration of groundwater quality parameters and Mamdani Fuzzy Inference System (MFIS) was used to simulate the water quality indices. Classification algorithms of NEUROSHELL and MATLAB were used to predict the class of items in a data set. The model was constructed using already-labelled items of similar data sets. The WQI of 29 samples was determined using weighted average method. Based on MFIS, 10 samples were classified as 'good', four samples as 'poor' and remaining samples as 'very poor'. The simulation model using the classification algorithm of ANN was used to predict the concentration of groundwater quality parameters and it was observed that three ANN models values and the actual data fit well with correlation coefficient varying from 0.93 to 0.99. When the soft computing techniques can be coupled with geospatial and geostatical method to map the spatial and temporal distribution of water quality parameters.

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2588-2872/

1. Introduction

The pollution of groundwater has been increasing over the past due to industrial development. Over exploitation of the groundwater resources also leads to rapid drop in the groundwater level in many areas, which also results in groundwater contamination. The quality of the groundwater changes due to discharge of sewage, agricultural and irrigational activities, physical and chemical parameters influenced by geological formations and type of aquifers through which it passes. To understand the knowledge of the subsurface system, the numerical flow models are generally used which demands a huge amount of temporal and spatial information to depict the subsurface system. So advanced statistical methods involving data mining techniques can be also used to explain the underlying structure of the data obtained to explain hydro chemical processes occurring in the aquifers. Artificial Neural Network (ANN) has been applied to simulate groundwater quality and Geographic Information System (GIS) has been applied to pre-processing and post-processing tool in simulating groundwater quality in Iran, India, Turkey and Ghareh-subasin. In addition to the water quality parameters, land use and land cover pattern, geological factors and groundwater level have been taken for simulation [1–8]. It has been observed that the integration of ANN and GIS has proved the more accurate and efficiency in prediction and simulation of groundwater quality. It has been also proved that ANN results are better reliable than linear regression models [9–11]. Also, optimization -simulation models have been developed by applying ANN, and Particle Swarm Optimization (PSO) models along with wireless network in managing groundwater resources [12–14]. Several authors have studied the influence of hidden neurons in the ANN in prediction and simulation of water quality parameters. It was observed that the number of neurons in the hidden layers has to be identified by trial and error based on the location. The groundwater pollution source and groundwater level prediction have been predicted using feed forward and back propagation algorithms [15–18]. From the results, it was noted that tangent algorithm with momentum-training algorithm gives less error than the sigmoid algorithms with Levenberg-Marquet [19,20]. Several researchers have applied fuzzy membership functions (Mamdani Fuzzy Inference System (MFIS)) and the weights for each groundwater quality parameters according to analytic hierarchy process (AHP) (which depends on pairwise comparison) in classifying the groundwater quality from different well locations [21–24]. Water quality index (WQI) is valuable and unique rating to depict the overall water quality status in a single term that is helpful for the selection of appropriate treatment technique to meet the concerned issues. However, WQI depicts the composite influence of different water quality parameters and communicates water quality information to the public and legislative decision makers. The weighted groundwater quality index based on the spatial and temporal variations of groundwater quality was developed using Fuzzy-AHP. In few papers, the use of geostatistical approach combined with Fuzzy logic approach has been reported to develop zoning map by identifying the spatial distribution of groundwater quality [25–27]. Adaptive Neural-Based Fuzzy Inference System (ANFIS) adopted for estimation and prediction of pollutant level in groundwater systems [28]. Deep learning algorithms and soft computing applications are applied to solve problems in engineering applications, geotechnical engineering, groundwater, sediment transport and meteorological characteristics [29–35].

2. Study Area

Coimbatore district is one of the largest districts of Tamil Nadu which has an aerial extent of 7470 km^2, accounting for 5.74% of the total geographical area of Tamil Nadu (Fig. 1). It consists of 19 blocks and is a part of subbasins of Cauvery such as Bhavani, Noyyal, Amaravathy, Parambikulam, Aliyar and Valparai. About 87% of the total irrigated areas is through dug wells. The annual rainfall over the district varies from 550mm to 900mm. Shallow aquifers exist within 30m in most of the parts of the district expect in the west. Structural hills, Deep Pediments, Valley fill are most of the prominent geomorphic units identified in that area. Six major soil types such as Red Calcareous soil, Black Soil, Red non-calcareous, Alluvial and Coalluvial Soil Brown Soil and Forest Soil, cover the district. The alluvium and colluvium formations in the district are composed of silt, kantar, sand and gravel bed. There exists high level of water level fluctuations due to over exploitation for domestic and agricultural activities. It has been reported by Central Groundwater Department that out of 19 blocks, 15 blocks are either ‘over exploited’ or ‘critical’. So, regarding quality, total hardness, nitrate and fluoride are found to in excess of permissible limits due to industrial pollution, geological formations and agricultural activities. It is also reported that the groundwater quality in many areas of the district do not conform to the standards of drinking water quality. So proper planning is required.

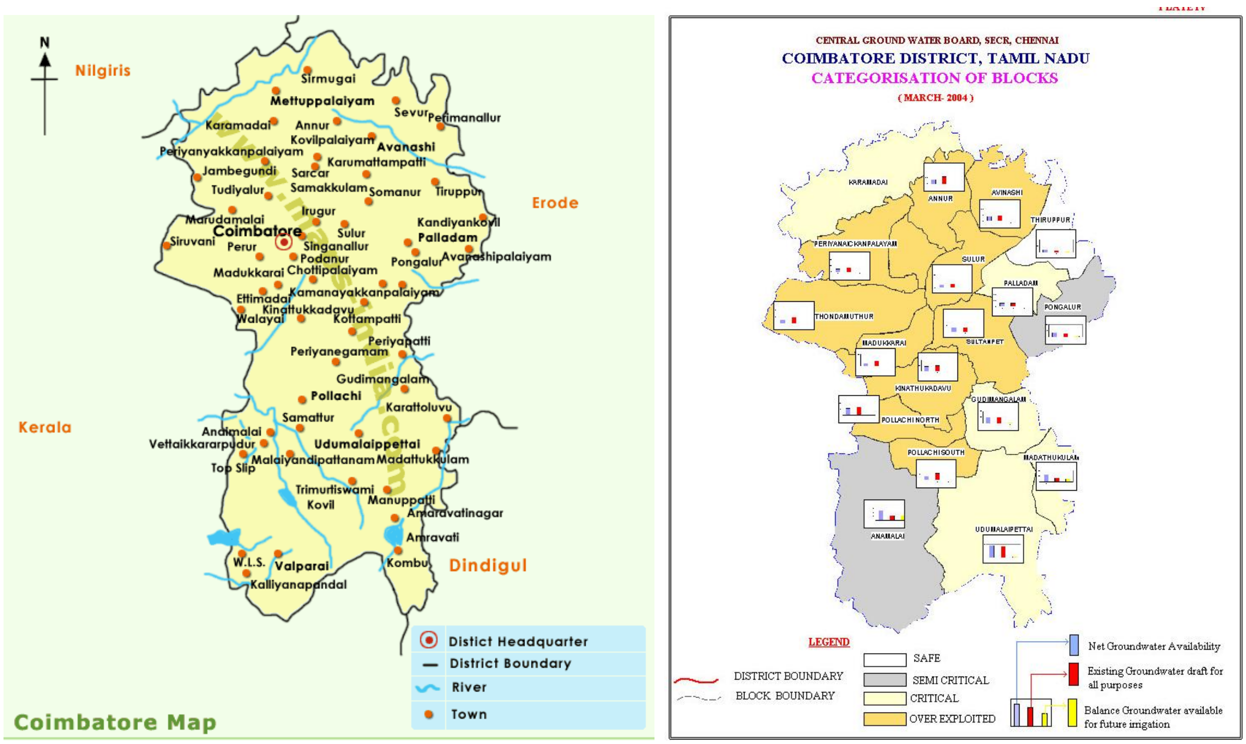

Fig. 1. Study area Coimbatore in Tamil Nadu, India [36].

3. Methodology

In this study, Artificial Neural Network (Three Models with 1, 2 and 3 outputs) was used to simulate and predict the concentration of groundwater quality parameters and Mamdani Fuzzy Inference System was used to simulate the water quality indices. FIS is the key unit of a fuzzy logic system having decision making as its primary work. It uses the "IF…THEN" rules along with connectors "OR" or "AND" for drawing essential decision rules. MFIS system was proposed in 1975 by Ebhasim Mamdani. Basically, it was anticipated to control a steam engine and boiler combination by synthesizing a set of fuzzy rules obtained from people working on the system. A classification algorithms using NEUROSHELL and MATLAB were used to predict the class of items in a data set using a certain model of a classifier. The model was constructed using already-labelled items of similar data sets. This step allows classification techniques to be considered as a supervised machine learning method.

ANN is a computational tool that is designed to simulate the way in which the brain performs a particular task or function of interest. ANNs are made up of highly interconnected processing elements called artificial neurons with weights that constitute a network. The artificial neurons are information-processing units that are used to build our neural networks and are truly primitive in comparison to those found in the brain. Each neuron receives several inputs from neighbouring elements, but only sends one output. The four basic elements of the neuronal model are Synapses or connecting links, an adder, an activation function and bias. Synapses or connecting links are characterised by weights. A signal x_j at input of synapse 'j' connected to a neuron is multiplied by the synaptic weight w_j. An adder is used to sum up all the input signals to the neuron, weighted by the respective synapses of the neuron. An activation function is applied for limiting the amplitude of the output of a neuron. Typically, the normalised amplitude of the output of a neuron is written as the closed unit interval [0,1] or alternatively [-1,1]. The neural network model includes an external bias, denoted by b, which has the effect of increasing or lowering the net input of the activation function. The network consists of three layers namely input layer, output layer and hidden layer in which the information from the outside world is received by the input layer, the simulation results are communicated to the outside world through output layer and the two layers are connected by the hidden layer.

3.1. Feedforward network

Generally, the ANN model consists of three layers and the data is being fed forward from the input layer and is being processed in the hidden layer(s) using activation function. The output from the second layer is sent as input to the third layer and the data is being processed in the forward manner/acyclic type.

3.2. Learning the pattern of the data for classification

The neural network learns the pattern through training algorithm by weight adjustment in each layer. The network learns by training the network in the forward direction from the input layer through summation and processing and the error obtained by comparing the model and target values is back propagated from the output layer. The different steps involved in back propagation algorithm are: 1. Initializing the connection weights of the neural network, 2. Using three activation functions like Threshold function, Piecewise linear function, and Sigmoid function (logistic function) to determine the output from each layer and the final target value from the output layer, 3. Computation of model output and comparing with defined target value to determine the error, and 4. Back propagating the error and calculation of new weight in each layer. Finally, the weights and biases in each layer are updated using delta rule. The gradient descent algorithm is used to identify the global minima in the weight space by seeking a direction for weight change that reduces the value of e(n). The above steps are repeated till the network is trained and global minima in the case of error is obtained. To avoid overfitting and noise, the overall groundwater quality data is divided into training and testing data. The training phase occurs either in batch or online mode. In addition to that either 'supervised learning' or 'unsupervised learning' may be used to train the network.

4. Modelling and simulation

4.1. Neural networks

In this study, 29 water quality samples were collected from 29 wells located in the selected area and 10 water quality physicochemical parameters such as pH, Carbonate (CO_3^{2-}), Bicarbonate (HCO_3^{2-}), Chlorides (Cl^-), Sulfate (SO_4^{2-}), Calcium (Ca^{2+}), Magnesium (Mg^{2+}), Potassium (K^+) and Total dissolved solids (TDS) were analysed using Standard methods [37]. The nine water quality parameters as input and TDS parameter as output were given in Neuroshell ANN function. The statistical parameters were determined as given in Table 1.

Table 1
Statistical parameters of the data.

Variable	pH	DO mg/l	Cl^- mg/l	CO_3- mg/l	HCO_3^- mg/l	SO_4^- mg/l	TH mg/l	Ca hardness mg/l	Mg hardness mg/l	TDS mg/l
	Input	Input	Input	Input	Input	Input	Input	Input	Input	Output
Min.	**6.5**	**0.9**	**222.1**	**0**	**100**	**100**	**200**	**75**	**75**	**603**
Max.	**8**	**6.3**	**2551.3**	**7.5**	**485**	**700**	**2055**	**875**	**1450**	**4623**
Mean	**7**	**4.2**	**923.6**	**3.75**	**350.6**	**296.8**	**704.0**	**325**	**379.1**	**1915**
SD	**0.49**	**1.5**	**674.3**	**1.31**	**106.7**	**161.1**	**485.6**	**223.4**	**304.7**	**1132**

From the data, 60% of data was extracted as training set and 30% as testing the data to find optimum for interrupt model training. After extracting, a standard net architecture was created whether each layer is connected to the previous layer only. The back propagation training architecture using Wardnet was used as training algorithm, which has multiple hidden neurons with different activation function in one layer similar to neuron of human. Before output is given, this architecture receives the output from each neuron and analyses the data. Thus, all input parameters given in this are related to each other, which are similar to water quality parameters of the study area. Next, selecting the optimum point, which is the minimum of average error of test data, sets the end point of the training. The average error of training set always decreases even if the number of iterations cross the optimum point but the average error of test-set increases. If the number of iterations is more than the number of iterations of the optimum point, the model is suitable for training data. The network is trained till minimum average error is reached and statistical parameters such as R-square, r-square, mean square error, mean absolute error, correlation coefficient etc. are determined.

4.2. Fuzzy logic

In this study, fuzzy inference system is applied to classify the water quality index. Fuzzy set is a suitable set for making the decision in complex and unclear system. The membership functions were created for ten water quality parameters based on Bureau of India Standards (BIS) and the criteria of World Health Organization (WHO). Water Quality Index (WQI) may be defined as a rating reflecting the composite influence of different water quality parameters on the overall quality of water. The main objective of computing of water quality index is to turn the complex water quality data into information which is easily understandable and usable. Weighted arithmetic water quality index method classifies the water quality according to the degree of purity by using the most commonly measured water quality variables. In this study, WQI has been classified into five type "Excellent, good, poor, very-poor and unsuitable for drinking" as shown in Table 2. To determine WQI, creation of fuzzy inputs, membership functions and rules are the important steps in FIS. The values of five major water quality parameters are fuzzified based on the normalization. The membership functions are created to identify the degree of membership in each classification. Based on values of BIS and WHO standards, best value is chosen to be an excellent category and the worst value to be the last value of poor category. The fuzzy distribution is used to generate membership-functions for various water quality parameters.

Table 2
The criterion for water quality index.

WQI value	Water quality
0-25	excellent
25-50	good
50-75	poor
75-100	Very poor
>100	Unsuitable for drinking

4.3. Fuzzy distribution

If r_a = Reference value A (angle point A, which is the average of minimum and mean value) and r_b = Reference value B (angle point B, which is the average of mean and maximum value, the widths can be defined as W1 = [min- r_a], W2 = [r_a –r_b], W3 = [r_a- max], where W1 is the width of left triangle in the trapezoid, W2 is the width of the square, W3 is the width of the right triangle in the trapezoid. The height of the distribution is normalized to (0,1). When the fuzzy distribution is used to generate membership-function, it does not have intersection-area as shown in Fig. 2. Fuzzy set has intersection area for each membership function. Table 3 shows the membership function for pH. Similarly, the membership functions are created for other water quality parameters and water quality index as given in Fig. 3 to Fig. 7.

Table 3
Membership functions for water quality parameter pH.

Parameter	Classification	Min1	Max1	Mean1	Min2	Max2	Mean2
pH	Excellent	7.00	8.5	7.75			
	Good	6.88	7.00	6.94	8.5	8.65	8.58
	Poor	6.75	6.88	6.81	8.65	8.8	8.73
	very poor	6.5	6.75	6.63	8.80	9.2	8.99
	unsuitable for drinking	0.00	6.5	3.25	9.20	14	11.6

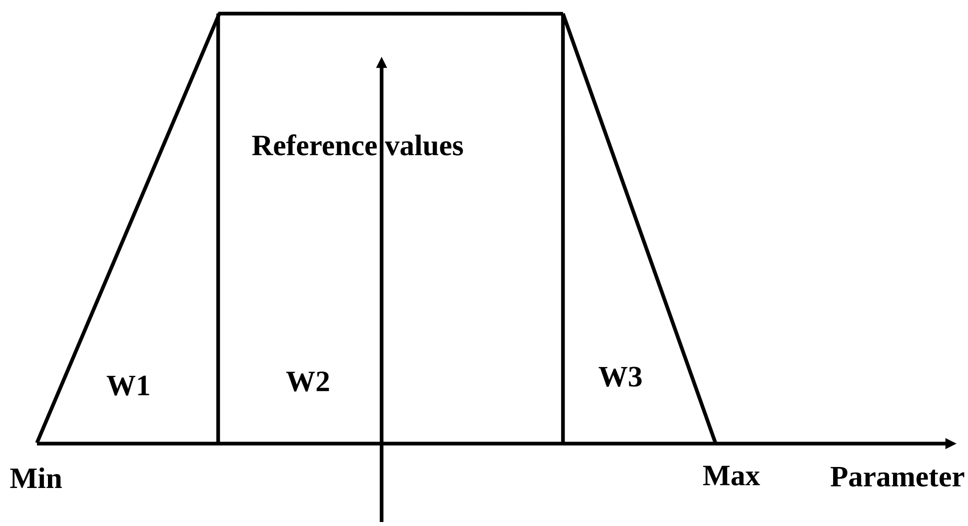

Fig. 2. A trapezoid membership-function.

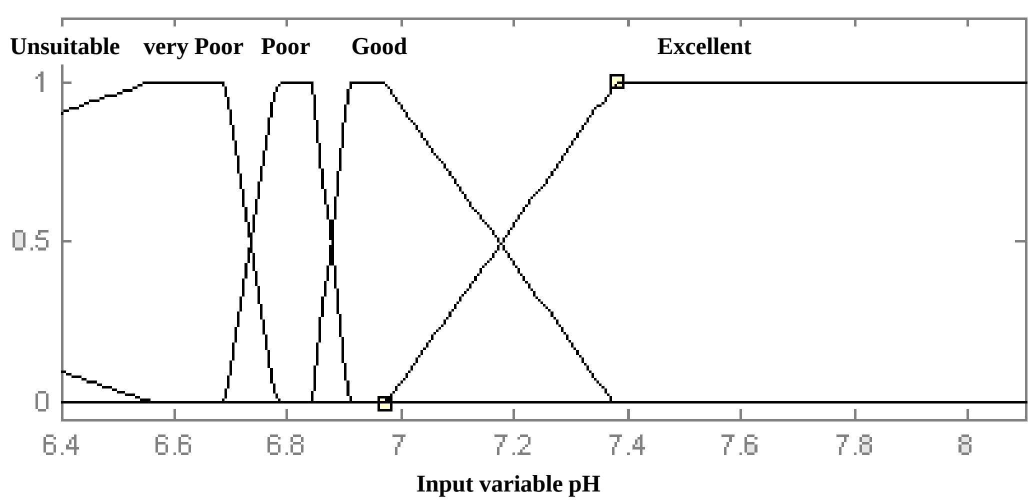

Fig. 3. pH membership-function.

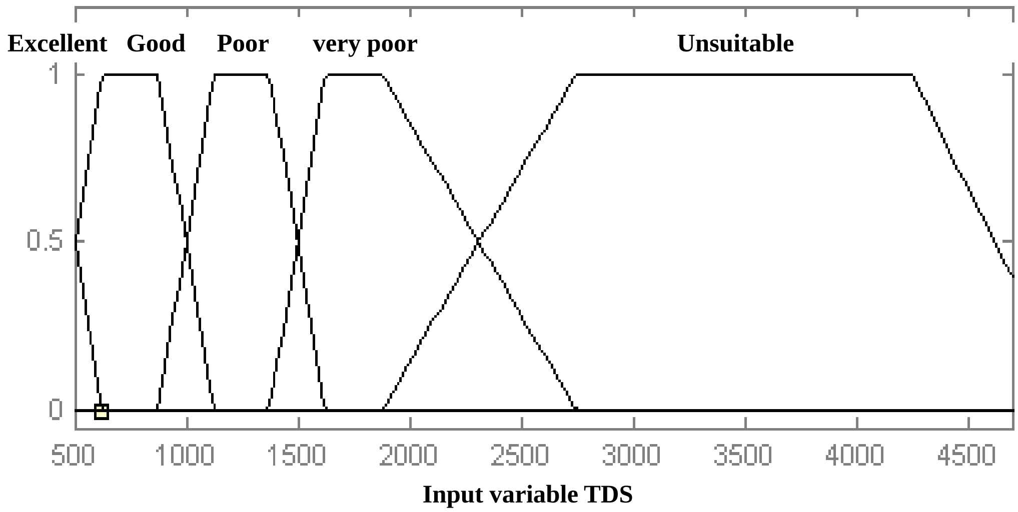

Fig. 4. TDS membership-function.

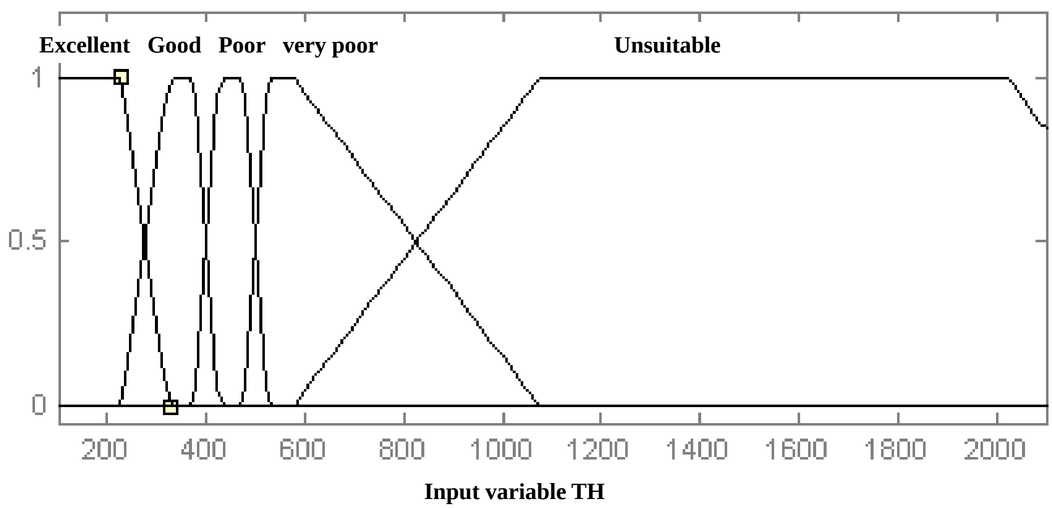

Fig. 5. TH membership-function.

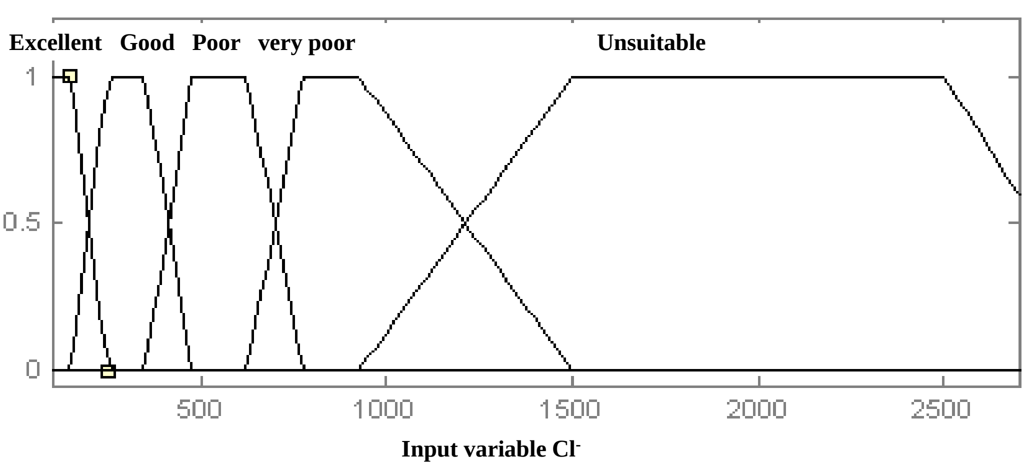

Fig. 6. Cl^- membership-function.

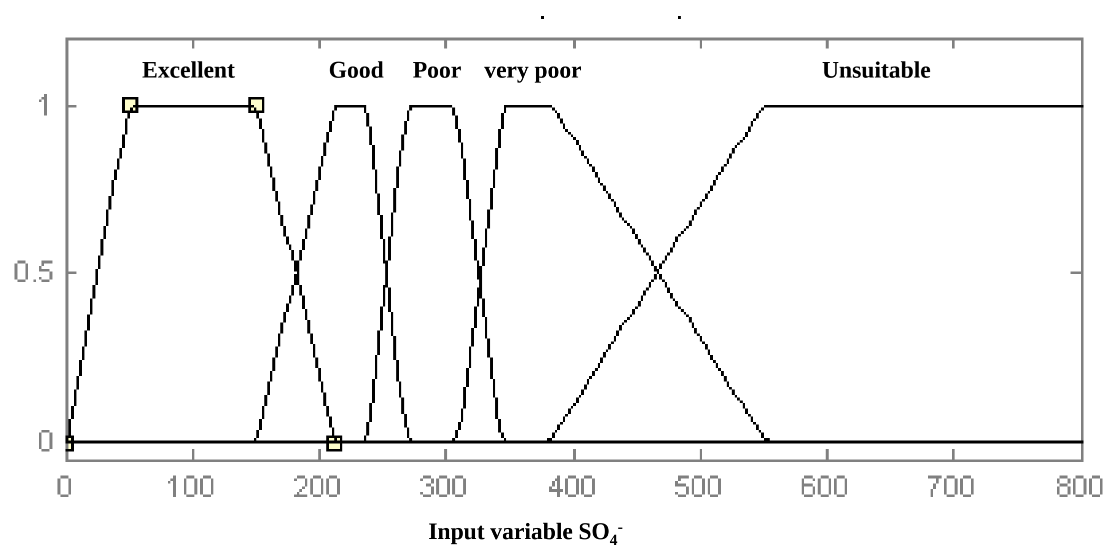

Fig. 7. SO_4^- membership-function.

Once the membership functions are created, the rules are formulated based on min-max method. Since the objective of the work is to classify the irrigation water quality based on WQI value, it is necessary to generate the rules based on five classifications such as unsuitable for drinking, very poor, poor, good and excellent. To formulate rules in efficient manner, it is paramount necessary to have field knowledge on the impact of water quality parameters on irrigation. Different number of rules was generated for five classifications as given below:

- Unsuitable: If the values of two water quality parameters are above the standards, then the water quality is unsuitable for irrigation. So, treatment is to be given before applying for irrigation. For this classification, 7 rules have been written.
- Very Poor: Condition 1: If the values of two quality parameters are very poor, WQI is poor. For these 7 rules are generated; Condition 2: If the values of one parameter is unsuitable for irrigation and other parameter is suitable, WQI is very poor
- Poor: If the values of two water quality parameters are poor, the WQI is poor. For these 7 rules are generated.
- Good: Condition 1: If the values of two water quality parameters are good, WQI is good; Condition 2: If the values of one of the water quality parameters are excellent and other parameter is not excellent, WQI is good. For this, 7 rules are generated.
- Excellent: If both water quality parameters are excellent, WQI is excellent. 7 rules have been generated for this.

Totally 35 rules were generated for 5 classifications of WQI. Finally, defuzzification is done using centroid method to get Water Quality Index value.

5. Result and discussion

5.1. Neural networks

The neural network software Neuroshell 2.0 was used to build and run ANN models with one hidden layer of 10 neurons, sigmoid function with normalized values for one output, two outputs, and three outputs respectively with different momentum factors (0.3, 0.99 and 0.99) and learning rates (0.1, 0.08 and 0.1). When the momentum factor and learning rates were increased, there was no further change in the error. Using the back propagation algorithms, new weights were calculated by updating the weight through error distribution. When the momentum factor was increased to 1, larger values were assigned to new weights. This led to increase in the minimum average error. For one output (TDS–Model A), the best results of training were obtained at momentum factor of 0.3 while the learning rate was 0.1. When the values of momentum factor and learning rate were increased, the computational time required to train the network was reduced. For two outputs (TDS and TH –Model B) and three outputs (pH, TDS and TH –Model C), the minimum average error of 0.0002 was obtained at momentum factors of 0.99, while the optimum learning rates were 0.08 and 0.1 respectively (shown in Fig. 8 to Fig. 10). The performance values of three different ANN models (Table 4) shows that the model B with two outputs (TDS and TH) showed the best prediction results (Fig. 11) compared to other two models A and C.

Table 4
Performance of three different ANN Models.

Statistical Analysis	1 output	2 outputs		3 outputs		
	TDS	TH	TDS	pH	TH	TDS
r squared	0.94	0.98	0.96	0.87	0.96	0.92
Mean absolute error	220.5	44.9	115.5	0.12	75.85	196.8
Correlation coefficient r	0.97	0.99	0.98	0.93	0.98	0.96

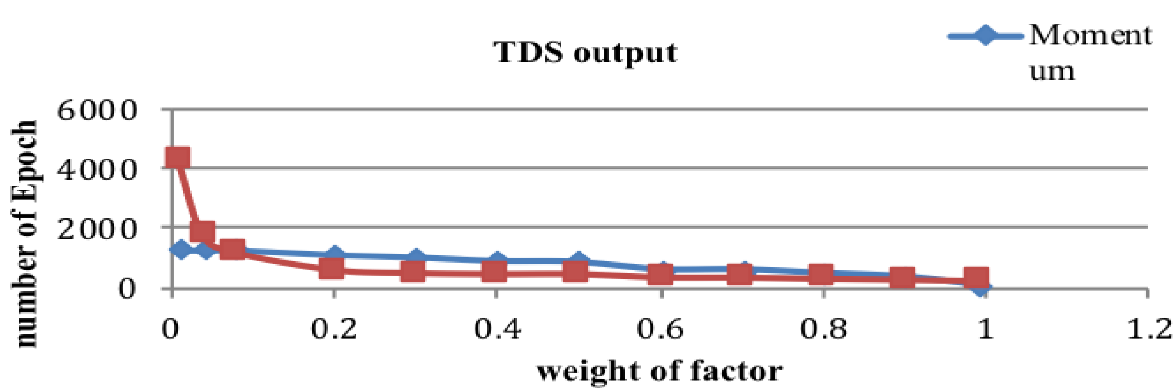

Fig. 8. Comparing of the weight of momentum and learning rate with number of Epoch on 1 output ANN model (Model A).

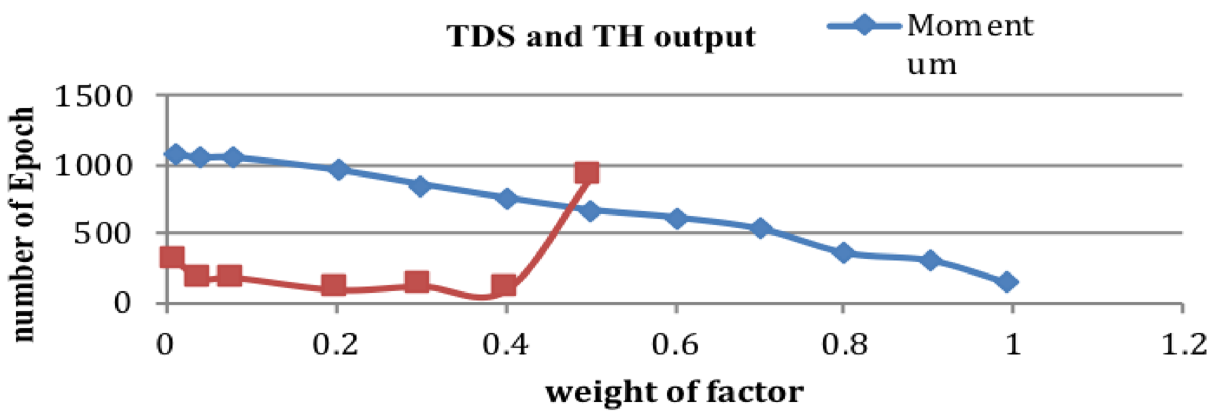

Fig. 9. Comparing of the weight of momentum and learning rate with number of Epoch on 2 outputs ANN model (B).

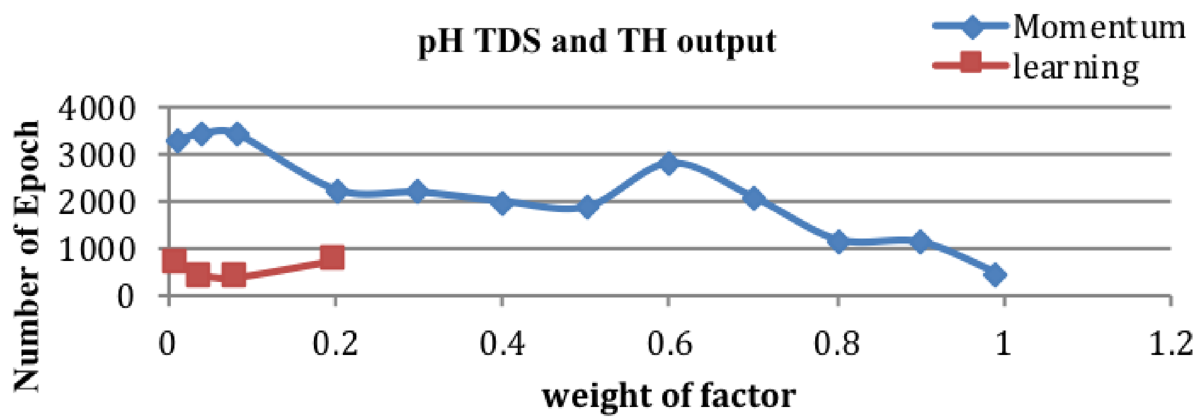

Fig. 10. Comparing of the weight of momentum and learning rate with number of Epoch on 3 outputs ANN model (C).

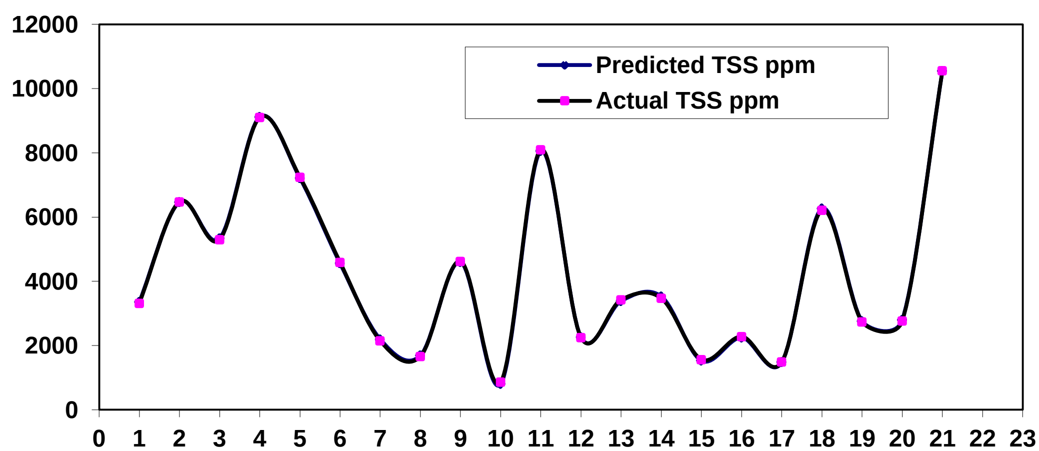

Fig. 11. The comparison between actual values and ANN model (B) results

5.2. Fuzzy logic

Fuzzy inference system (FIS) can be used for decision making when there exists uncertainty in the system. There are two categories based on which the output is obtained. Both are based on the selection of rules. In the first category, if only one rule is active, the FIS will use a mean of membership-function range. In the second category the ranges of all the membership functions (classifications of five water quality parameters) are taken into account for calculating the final output. The maximum value of the activated rule of each category is taken which is multiplied with the weight of the membership function to get the final output. Fig. 12 shows the weight and centroid of membership-function.

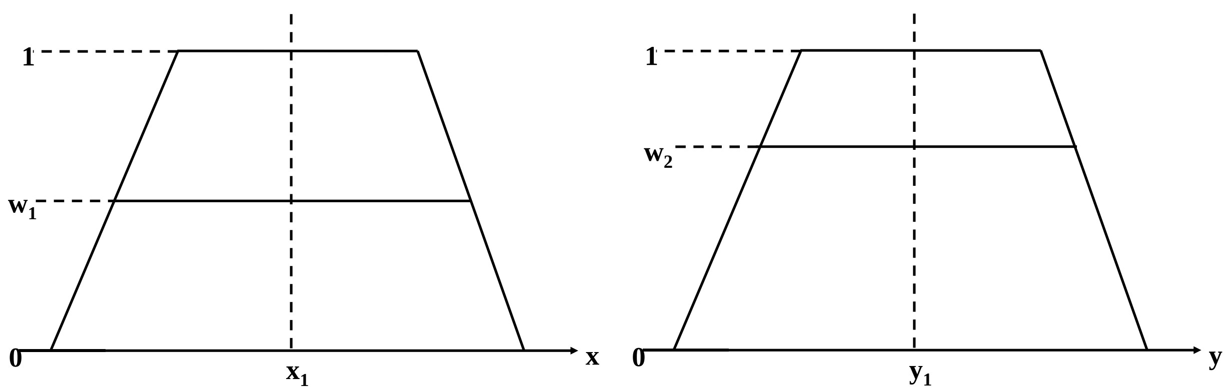

Fig. 12. The weight and centroid of membership-function.

The weight of membership-function starts from 0 to 1. Then fuzzy will calculate the answer by using the formula (1).

$$\frac{w1x1+w2y2}{w1+w2} \tag{1}$$

where x1 and y1 are centroid position of membership-function on x axis. In this study, there should not be any water quality parameter (out of 5) in the range of unsuitable category of membership function for the WQI value to be in good category. For the WQI value to be in the category of poor, maximum of two water quality parameters out of five can be in the range of unsuitable category. Similarly, for very poor classification of WQI, there can be maximum of three water quality parameters under the range of unsuitable category. When minimum number of two water quality parameters is in the range of unsuitable category, the water is unsuitable for irrigation. Comparison between water quality index classified using fuzzy logic and actual WQI is shown in Table 5 and Fig. 13. This shows fuzzy logic classification produced very good WQI classification and it helps in taking decision on the water quality whether it can be used as it is or to be treated well before it is being used for any purpose.

Table 5
Results of fuzzy simulation.

SNo	pH (Input)	TDS (Input)	TH mg/l (Input)	Cl^- mg/l (Input)	SO_4^{2-} (Input)	WQI (Fuzzy Output)	WQI (Actual)	Classification
1	7.5	603	315	222	110	26	27	Good
2	7.3	670	260	237	100	27	22	Good
3	8.0	938	300	395	140	31	38	Good
4	7.9	1072	240	390	130	31	38	Good
5	7.7	1072	490	405	145	37	35	Good
6	7.9	938	325	400	160	32	34	Good
7	8.0	1005	200	400	130	33	31	Good
8	8.0	1072	325	390	110	32	40	Good
9	7.0	1139	315	321	295	49	43	Good
10	7.6	2211	900	1036	150	107	120	unsuitable
11	6.8	2814	770	1352	215	129	121	unsuitable
12	6.7	3685	1370	2551	380	122	127	unsuitable
13	6.7	4623	1950	2398	440	124	121	unsuitable
14	6.6	3417	1225	1767	390	122	121	unsuitable
15	6.9	2412	785	1209	210	94	95	very poor
16	6.8	1541	865	1476	270	105	106	unsuitable
17	6.6	4154	1385	1392	330	124	130	unsuitable
18	6.5	4020	2055	2028	590	136	133	unsuitable
19	6.7	2881	795	1925	420	123	126	unsuitable
20	6.9	1072	440	553	160	51	58	poor
21	6.6	2345	620	1189	410	115	118	unsuitable
22	6.9	1139	295	498	200	48	47	Good
23	6.8	1809	535	829	300	79	76	very poor
24	7.0	1541	600	543	500	86	80	very poor
25	7.3	1273	650	494	420	75	79	poor
26	7.1	1608	768	691	423	94	99	very poor
27	6.9	1675	825	632	700	118	115	unsuitable
28	7.1	1206	500	474	270	55	54	poor
29	7.3	1608	315	592	510	65	57	poor

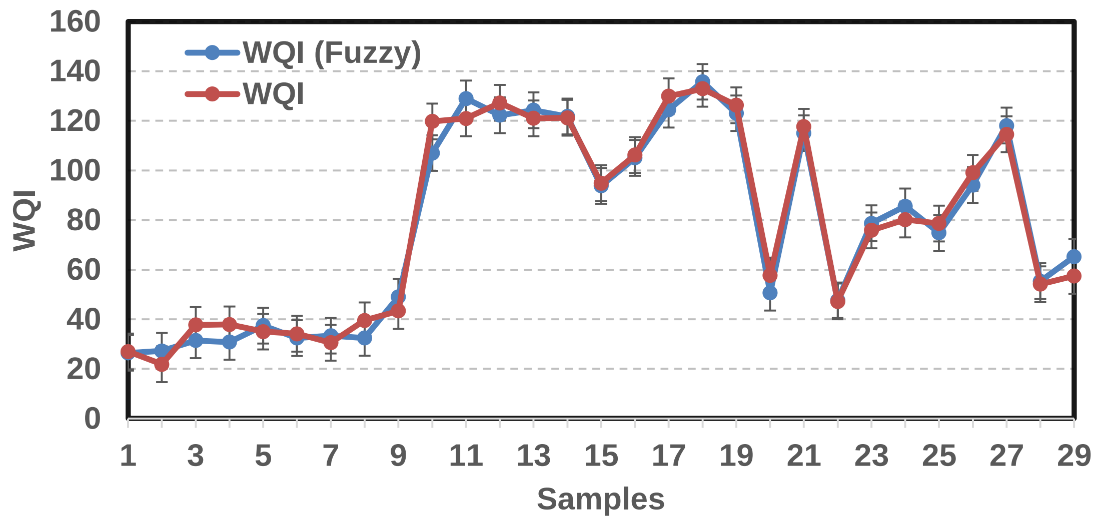

Fig. 13. Comparison of actual WQI to that classified using fuzzy logic inference system.

6. Conclusions

Groundwater quality is an important water resource for irrigation, drinking and agriculture needs. It is important to study and develop new methods and strategies to understand the vulnerability of groundwater to agricultural chemicals and other human activities for its better management. This study is about the simulation and prediction of groundwater quality in the study area with complex pollution sources such as agriculture, domestic and industrial effluent. Based on the variation in the water quality parameters and significance of each parameter (based on the field condition) the membership functions and rules were formulated. The water quality of 29 wells located in the area was classified and predicted using soft computing techniques such as ANN and Fuzzy Logic system using NEUROSHELL and MATLAB tools. The input parameters and membership functions for the Fuzzy Inference System were selected based on the field experience. The calculated WQI of the samples were compared with the simulated values using Fuzzy Inference system. It was observed that, the samples from 20 wells were classified under the category, ‘good’, while the four samples were classifying as ‘poor’ and the remaining samples were not suitable for irrigation. The uniqueness of fuzzy logic technique is centroid of membership-function that can activate several rules in the same time. Further, the simulation and prediction was done using ANN and the results depicted that there is a high correlation between actual and model values with correlation coefficient varying from 0.93 to 0.99. It was concluded that, both simulation and prediction models (Fuzzy Logic and ANN with 2 outputs) which showed high accuracy may be used for classifying the wells located in the area polluted by different complex sources.

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Conflicts of interest

The authors declare no conflict of interest.

Authors contribution statement

Jegathambal, Sundarambal: Conceptualization, Methodology, Investigation; Jegathambal, Anitha, Jansi, Apinun Tungsrimvong, Babithesh Babu: Data collection, Formal analysis; Investigation; Jegathambal, Project administration and Resources; Jegathambal, Sundarambal Software, Validation

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