Chapter 14
Estimation of Groundwater Quality from Surface Water Quality Variables of a Tropical River Basin by Neurogenetic Models

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Abstract According to the hydrological cycle, after rainfall infiltration becomes high and once the soil pores become saturated, surface runoff begins. The infiltrated water is added to the groundwater and depressions and canals are utilized to store or drain out excess water. Because surface water and groundwater have the same source, their quality is related, but the physiochemical properties of the soil layers and geological characteristics of the catchments also influence the quality of water in the surface and ground. Many scientific studies have established that surface water is not as pure and fit for drinking as groundwater. Groundwater is free of turbidity, suspended impurities, and organic and inorganic micropollutants. This reactive nature of water is almost neutral. Although groundwater is affected by dissolved metals (like arsenic, iron, etc.), volatile organic compounds and toxic gases, but the intensity of groundwater pollutants varies with location and surrounding geophysical and ecological structures. In most of the places people use groundwater for drinking without adopting any means of purification. If the source is free of organic and inorganic pollutants and if the metal and gaseous concentrations are low, then the ground/surface water can easily be used for drinking or washing purposes without much threat to human health. But if the surface water contaminates the source through leakage or accidental removal of the impervious layers, then it may contaminate the source, and use of the contaminated groundwater could cause affect public health. The present study attempts to predict the quality of groundwater with the help of surface water quality parameters along with some climatic and geophysical parameters. The study utilized neurogenetic models for

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predicting the quality of groundwater. The results show that predictions of pH and chlorine levels based on the parameters was found to be more accurate and reliable than the prediction of any other quality variables. Thus it can be concluded that if surface water and groundwater are mixed, the pH and turbidity will undergo the most dramatic change among all other quality variables.

Keywords Groundwater quality • Neurogenetic models • Damodar Basin

14.1 Introduction

"Groundwater and surface water are fundamentally interconnected. In fact, it is often difficult to separate the two because they 'feed' each other" (CTIC 2008). The quality of surface water thus impacts the quality of groundwater. Because groundwater from unconfined aquifers are extracted for domestic, agricultural, and industrial purposes, showing the interrelationship between the two in a spatial scale is necessary. Reay et al. (1992) established the impact of groundwater discharge on surface water quality of Chesapeake Bay Inlet. The conclusion supports the notion of interactivity between the two types of water and suggests the inclusion of this relationship in water quality management strategies. The impact of surface and groundwater interactivity on herbicide concentration was measured by Verstraeten et al. (1998), and according to the results, the concentrations of one-half to one-fifth of herbicides decrease in groundwater. Gallagher et al. (2007) investigated the transport of land-applied nutrients and pesticides from unconfined aquifers to the tidal surface waters of Virginia's coastal plain; the study revealed that the levels of nitrogen contaminating the surface water was significant and overall levels of pesticide movement through groundwater, although generally quite low, represented a transport route that is commonly neglected in watershed management. An integrated numerical model was developed to estimate the flow and chemical transport between an integrated surface-subsurface hydrologic system (Van der kwaak 1999). The study concluded that hydrograph separation theory is fundamentally flawed if diffusive modification of tracer concentrations in surface water is prevalent in nature. The aforementioned studies explain the importance of determining the relationship between the main chemical parameters of surface water and groundwater. These studies mainly used field measurements and linear numerical models to estimate that relationship. But linear models were often found to deviate from the actual relationship because of their failure to replicate the temporally or spatially abrupt changes. Also, linear models are unable to separate episodic changes from normal but large changes. In recent years artificial neural networks have been often and successfully applied to the modeling and forecasting of time series. Artificial neural networks offer a relatively quick and flexible means of modeling.

14.1.1 Objective and Scope

This investigation will try to estimate the quality variables of groundwater that has been contaminated by surface water. Each of the quality parameters was examined separately by considering 11 inputs involving climatic, geophysical, and quality parameters of the surface water. Because neurogenetic models can map nonlinearity and the highly complex interrelationship between the input and output variables of the present problem, such models were used to identify the interrelationships between the surface and groundwater quality parameters and other climatic and geophysical properties of the catchment.

The successful development of the model could help engineers to predict the probability of various health hazards if surface water contaminates groundwater. Necessary mitigation measures could be adopted once contamination is detected without having to verify the quality of the groundwater. Thus the compensatory action to recover from the disequilibrium would be fast and control of the situation would be efficient enough to check the spread of the contaminant.

A case study was selected for verification and analysis of the model output where groundwater is often contaminated by surface water. The next section describes the area of investigation and the model development methodology.

14.1.2 Study Area

The Damodar River, which lies between the latitudes 23°30′N and 24°19′N and longitudes 85°31′E and 87°21′E, originates from the Palamu Hills of Chota Nagpur at an elevation of approximately 610 m above mean sea level. It flows in a southeasterly direction, entering the deltaic plains below Raniganj in the Burdwan district of West Bengal, India. Near Burdwan the river abruptly changes course and starts flowing in a southerly direction to join the Hoogli River approximately 48 km below Kolkata. The slope of the river bed during the first 241 km is approximately 1.89 m/km. During the next 161 km the slope is approximately 0.57 m/km and approximately 0.19 m/km over the next 145 km. The river is fed by six streams, of which the principal tributary, Barakar, joins it where the Damodar River emerges from the Palamu Hills. Four main multipurpose reservoirs are located at Tilaiya, Konar, Maithon, and Panchet, and a barrage at Durgapur was commissioned during the period 1953–1959. Another tributary, Khudia, whose catchment is not intercepted by either the Maithon or the Panchet reservoir, joins Damodar near its confluence with Barakar. In the plains, the river splits into several channels and ultimately joins the Roopnarayan and Hoogli rivers. The total length of the river is approximately 541 km, and its total catchment area is 28,015 km^2, of which 10,985 km^2 lies under Panchet (Konar –997 km^2, Tenughat –4,500 km^2, and Panchet 5,488 km^2) and 6,293 km^2 under Maithon (Tilaiya –984 km^2 and Maithon –5,309 km^2). Figure 14.1 shows a schematic diagram of the Damodar River and the location of the Panchet reservoir.

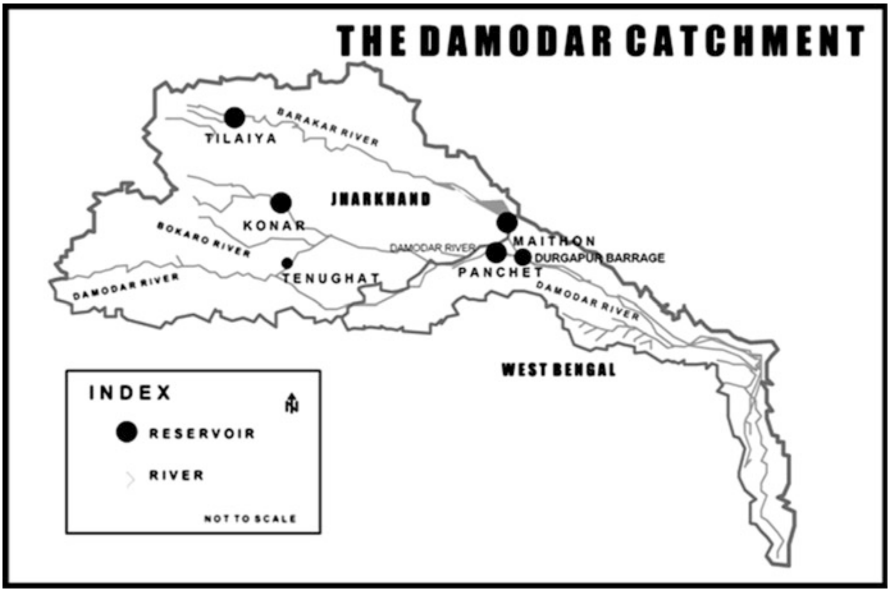

Fig. 14.1 Location of Panchet and Maithon Reservoir in the Damodar Watershed (Majumder et al. 2010)

14.1.3 Brief Methodology

The present study tried to apply the searching capabilities of a neural network and a genetic algorithm to estimate the relationship between surface and groundwater quality of four different locations on the catchments of the Damodar River. The water quality values, as found from field study of surface and groundwater sampling points, along with soil type, surface water discharge, temperature, relative humidity, and rainfall, served as input. Different models were developed to predict the five selected water quality parameters. Even if the same algorithm and training settings were used for all five models, the mean square error (MSE) of the models was different. The reason behind such varied MSEs lies in the degree of the inherent relationship that exists between the values of the output parameter found in surface water and groundwater.

The selection of quality parameters was based on availability of data for both types of water and impact on public health.

14.1.4 Data Description

The average yearly values of maximum temperature (T), maximum and minimum relative humidity (h_{max} *and* h_{min}), discharge (Q), rainfall (P), and concentration of surface water quality parameters like conductivity (cond), turbidity (Turb), chloride (Cl), total hardness (TH), and pH measured from surface water and groundwater at

23 monitoring locations of different areas were considered. Soil type (ST) of the selected locations was also included. The output was quality variables cond*,* Turb*,* Cl*,* TH, *and* pH. One model was developed for each of the output variables. Thus five models were prepared. All the models were trained with three different training algorithms and validated by the three performance metrics MSE, coefficient of relationship (r), and standard deviation (STDDEV).

The selected sites were located in and around Tandwa on the bank of the rivers Garhi, Chandrapura, and Maithon, which were located respectively on the banks of the Barakar River, a tributary of the Damodar River, which are respectively in the upstream and downstream of the Damodar River.

The relationships between surface and groundwater quality parameters as measured from the field locations are compared in Fig. 14.2a–e. The correlation coefficient between surface and groundwater Turb, cond, Cl, TH, and pH of the three study areas according to field survey results was found to be equal to 0.5–0.55, 0.02–0.91, 0.6–0.95, 0.57–0.97, and 0.44–0.62, respectively. The relationship between chloride concentration of surface and groundwater was found to be the most prominent and for conductivity it was found to have deviated significantly as the gap between minimum and maximum correlation was nearly equal to 89%. The gap between the maximum and minimum values was a lowly 35%, but the lowest gap was observed in Turb correlation, which was equal to 5%. pH and TH had a correlation gap percentage (CGP) equal to 18 and 40%, respectively. A large CGP indicates the unpredictability of a parameter with respect to the variable, which in this case is a spatial reference number.

14.2 Methodology

14.2.1 Mathematical Modeling of Neural Networks

Artificial Neural Networks are nowadays widely applied (Gaur et al. 2013; Shiri et al. 2013; Ranjithan et al. 1993; Coulibaly et al. 2001; Kuo et al. 2004; Coppola Jr et al. 2003; Nayak et al. 2006; El Tabach 2007)in various field of science, engineering and management. The present study has utilized the advancements of the neural network modeling to predict the impact of surface water contamination of groundwater quality parameters. Simulating an artificial functional model from the biological neuron has three basic components. First, the synapses of the biological neuron are modeled as weights. The synapse of the biological neuron is the one which interconnects the neural network and gives the strength of the connection. For an artificial neuron, the weight is a number, and represents the synapse.

A negative weight reflects an inhibitory connection, while positive values designate excitatory connections. All inputs are added and modified by the weights. This activity is referred as a linear combination.

Finally, an activation function controls the amplitude of the output. For example, an acceptable range of output is usually between 0 and 1, or it could be −1 and 1. The activation functions are of three types:

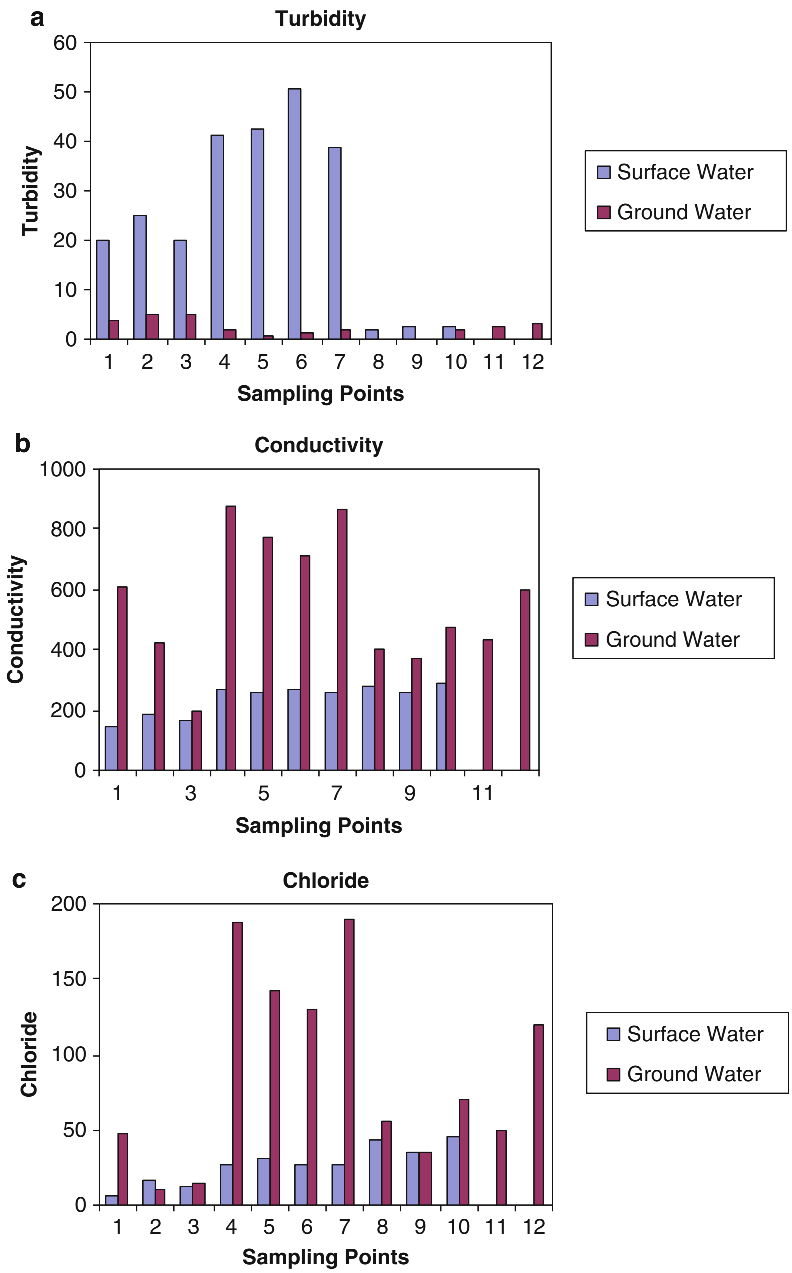

Fig. 14.2 (**a**) Variation in turbidity with respect to sampling points. (**b**) Variation in conductivity with respect to sampling points. (**c**) Variation in chloride with respect to sampling points. (**d**) Variation in total hardness with respect to sampling points. (**e**) Variation in pH with respect to sampling points

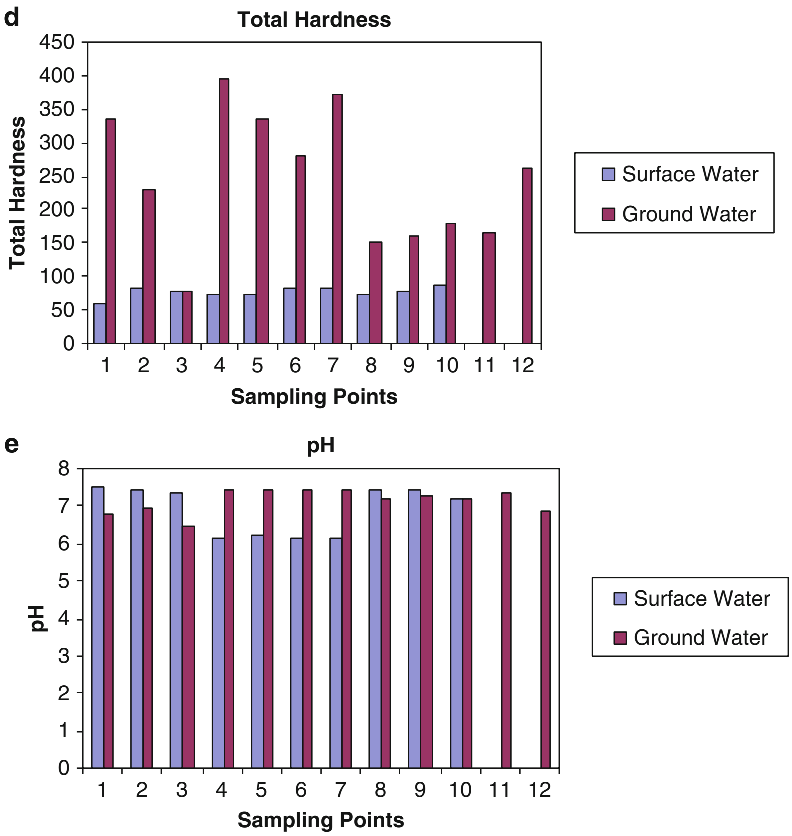

Fig. 14.2 (continued)

The **Threshold Function** takes on a value of 0 if the summed input is less than a certain threshold value (v), and the value 1 if the summed input is greater than or equal to the threshold value.

$$\varphi(v) = \begin{cases} 1 & \text{if } v \geq 0 \\ 0 & \text{if } v < 0 \end{cases}$$

The **Piecewise-Linear function** can also take on the values of 0 or 1, but intermediate values between that depending on the amplification factor in a certain region of linear operation is also possible.

$$\varphi(v) = \begin{cases} 1 & v \geq \frac{1}{2} \\ v & -\frac{1}{2} > v > \frac{1}{2} \\ 0 & v \leq -\frac{1}{2} \end{cases}$$

The **Sigmoid function** can range between 0 and 1, or −1 to 1 range. There are various types of sigmoid function. For example the hyperbolic tangent function can be represented by:

$$\varphi(v) = \tanh\left(\frac{v}{2}\right) = \frac{1-\exp(-v)}{1+\exp(-v)}$$

The Fig. 14.3 describes the basic architecture of an Artificial Neural Networks.

From this model the interval activity of the neuron can be shown to be:

The output of the neuron, y_k, would therefore be the outcome of some activation function on the value of v_k.

$$v_k = \sum_{j=1}^{p} w_{kj} x_j \tag{14.1}$$

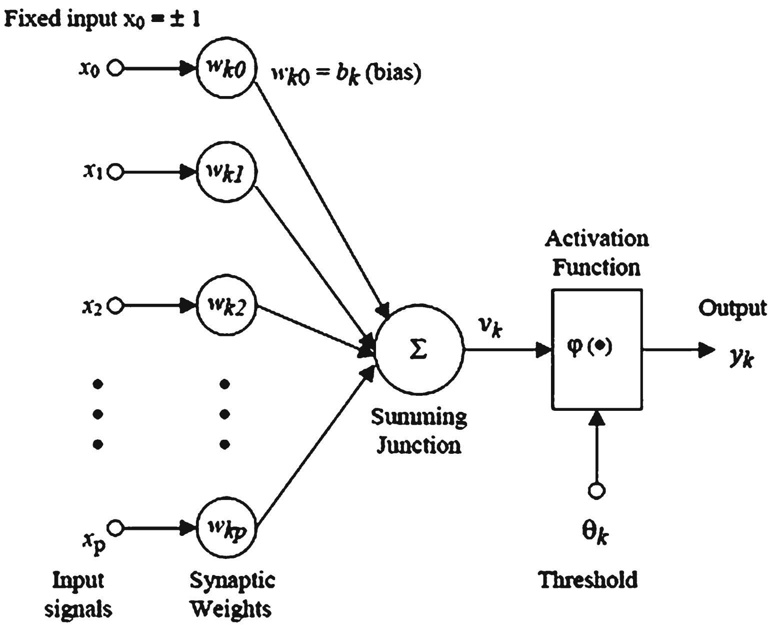

Fig. 14.3

14.2.1.1 Selection of Network Topology

The network topology or number of hidden layers is another parameter which is needed to be determined with the help of trial and error or any other heuristic search algorithms like Genetic Algorithms due to its influence on network accuracy. As many studies (Beniwal et al. 2013; Xin and Zhang 2002; White and Ligomenides 1993; Angeline et al. 1994; Leung et al. 2003; Blanco et al. 2000; Yen and Lu 2000) nowadays are utilizing genetic algorithm for identifying optimal topology of neural networks the present study applied the efficacy of GAs in searching for the optimal solution to estimate the best network topology for the present problem.

After the model topology was selected the network is trained with a set of dataset with known value of the output variables and by applying different training algorithms to identify the optimal weightage (Eq. 14.1) that can result in a neural network model for the present problem which can accurately predict the value of the output variables for unknown situations which are not included in the training dataset.

14.2.1.2 Training Algorithms

In the present study following training algorithms were utilized to find the optimal value of weightage at which the model yields the best results.

Quick Propagation

Quick Propagation algorithm (eg: Constantin et al. 2013) is a batch technique which exploits the advantages of locally adaptive techniques that adjust the magnitude of the steps based on local parameters (for instance, the non-global learning rate). Second, knowledge about the higher-order derivative is used (such as Newton's mathematical methods). In general, this allows a better prediction of the slope of the curve and where the minima lies. (This assumption is satisfactory in most cases.)

Conjugate Gradient Descent

The basic backpropagation algorithm adjusts the weights in the steepest descent direction (negative of the gradient). This is the direction in which the performance function is decreasing most rapidly. It turns out that, although the function decreases most rapidly along the negative of the gradient, this does not necessarily produce the fastest convergence. In the conjugate gradient algorithms a search is performed along conjugate directions, which produces generally faster convergence than steepest descent directions. (e.g., Benli 2013)

Levenberg Merquadart

The Levenberg-Marquardt algorithm was designed to approach second-order training speed without having to compute the Hessian matrix. When the performance function has the form of a sum of squares (as is typical in training feedforward networks), then the Hessian matrix can be approximated as

$$\mathbf{H} = \mathbf{J}^T \mathbf{J}$$

and the gradient can be computed as

$$\mathbf{g} = \mathbf{J}^T \mathbf{e}$$

where **J** is the Jacobian matrix that contains first derivatives of the network errors with respect to the weights and biases, and **e** is a vector of network errors. The Jacobian matrix can be computed through a standard backpropagation technique that is much less complex than computing the Hessian matrix (e.g., Adib and Hadis 2013)

14.2.2 Performance Metrics

Although there are many varieties of metrics to analyze performance of a numerical model Root Mean Square Error; which represent the degree of matching achieved by the model; Correlation Coefficient; represents the magnitude and direction of relationship that exist between the observed and predicted dataset and Covariance; which depicts the deviation of the modeled data from the target dataset; are the three commonly used metrics supported by majority of the scientific community.

14.2.2.1 Root Mean Square Error

The Root Mean Square Error (RMSE) of an estimator $\hat{\theta}$ with respect to the estimated parameter θ is defined as

$$\mathrm{RMSE}(\hat{\theta}) = \sqrt{\mathrm{E}[(\hat{\theta} - \theta)^2]}.$$

The MSE thus assesses the quality of an estimator in terms of its variation and un-biasedness. Note that the MSE is not equivalent to the expected value of the absolute error.

14.2.2.2 Correlation Coefficient

The correlation coefficient (often denoted by Greek rho) is given by the following important equation:

$$Correlation = \rho = \frac{\mathrm{cov}(X, Y)}{\sigma_x \sigma_y}$$

14.2.2.3 Covariance

The covariance between two jointly distributed real-valued random variables x and y with finite second moments is defined as:

$$\sigma(x,y) = \mathrm{E}[(x-\mathrm{E}[x])(y-\mathrm{E}[y])]$$

where E[x] is the expected value of x, also known as the mean of x. By using the linearity property of expectations, this can be simplified to:

$$\sigma(x,y) = \mathrm{E}[xy] - \mathrm{E}[x]\,\mathrm{E}[y]$$

where E[xy] is the correlation between x and y; if this term is zero then the random variables are orthogonal. Covariance represents the independency of two variables with respect to each other. If Covariance is zero then both the variables is dependent on each other.

14.3 Results and Discussion

Table 14.1 show the neural network topology, GA search settings, MSE, STDDEV, and r achieved by the 15 models that were developed to establish the objective of the present study. For each of the water quality parameters, three algorithms, QP, CGD, and LM, were used. MSE, STDDEV, and r helped to select the best performing algorithm among them. The GA was applied to search for the ideal network architecture with the settings shown in Table 14.1. The search was followed by training of the network with the architecture selected. The three algorithms discussed earlier were now applied to train the models to learn the encoded pattern or relationship between the output and input parameters. As the data set was small (23×11), QP, CGD, and LM algorithms were selected. For training purposes, 75% of the data set was used, 15% was used for validation, and the remaining 15% was applied for testing the model performance.

All 15 models were named by adding the type of training algorithm in the prefix and the parameter considered output in the suffix. Hence, the model trained with the QP algorithm to find the chloride concentration was named QP-Cl.

QP-Turb, QP-pH, CGD-Cl, LM-TH, and LM-Cond were selected as the best performing models respectively for predicting Turb, pH, Cl, TH, and Cond. Among the selected models, the best MSE was obtained by QP-pH followed by CGD-Cl, and the worst MSE was found using LM-Cond followed by LM-TH.

As all the models were trained with the same parameters and the number of iterations for all the models was fixed at an equal value, the accuracy of the models may be influenced by the correlation of the input and output quality variables. Thus it can also be concluded that pH and Cl are largely influenced by the surface water quality. In the case of the other variables, it was found that prediction of conductivity and hardness is relatively complex. Conductivity was affected by the dissolved ions whose concentration depends on the chemical impurities present in the water.

Table 14.1 Attributes and Performance Evaluation of Neuro-genetic Models Considered in the study

Model	Neural network architecture	GA search settings (P-G-Pe-CR-MC)	MSE	STDDEV	r
QP-Cl	11-6-1	40-50-5-0.8-0.2	0.32	6.73	0.97
QP-Turb	**11-16-1**	**40-50-5-0.8-0.2**	**0.37**	**1.33**	**0.99**
QP-TH	11-10-1	40-50-5-0.8-0.2	18.60	18.83	0.92
QP-pH	**11-5-1**	**40-50-5-0.8-0.2**	**0.04**	**0.16**	**0.85**
QP-Cond	11-10-1	40-50-5-0.8-0.2	3.55	2.80	0.99
CGD-Cl	**11-3-2-1**	**40-50-5-0.8-0.2**	**0.05**	**6.38**	**0.98**
CGD -Turb	11-2-1-1	40-50-5-0.8-0.2	3.22	2.47	0.94
CGD -TH	11-4-3-1	40-50-5-0.8-0.2	7.25	10.84	0.95
CGD -pH	11-5-1	40-50-5-0.8-0.2	0.01	0.18	0.68
CGD -Cond	11-1-5-1	40-50-5-0.8-0.2	9.38	13.14	0.94
LM-Cl	11-4-6-1	40-50-5-0.8-0.2	4.87	7.08	0.96
LM -Turb	11-2-8-1	40-50-5-0.8-0.2	0.75	1.74	0.97
LM -TH	**11-1-2-1**	**40-50-5-0.8-0.2**	**1.54**	**9.47**	**0.97**
LM -pH	11-2-8-1	40-50-5-0.8-0.2	0.04	0.30	0.22
LM -Cond	**11-2-3-1**	**40-50-5-0.8-0.2**	**3.09**	**10.61**	**0.99**

The effluent from industrial infrastructure and waste water treatment plants contaminates surface water bodies with such impurities. Again, the presence of certain kinds of geophysical properties (presence of stalagmite or sandstone) can increase the conductivity of the groundwater. The geophysical properties of the study area were favorable for increasing the conductivity, and thus the groundwater displayed higher conductivity than surface water where chemical impurities were present at a lower level. This explains the indifferent relationship between the conductivities of surface and groundwater. The hardness was also higher compared with that of the groundwater due to the same geophysical properties of the catchment. Calcium and magnesium ions were present in much higher concentrations than in the surface water. The presence of hardness in the surface water was also due to the presence of sandstone and stalagmites in the region and because most surface water bodies had been created in depressions like mountain caves and funnels that arose as a result of landslides or earthquakes in those regions millions of years ago. But as the seepage of surface water to the aquifer is minimal due to the presence of impervious layers of sandstone or stalagmites, the hardness of the groundwater was unable to influence that of the surface water. Also, the reaction time of hardness and conductivity is higher than that of Cl or pH.

14.4 Conclusion

This study tries to establish the interactivity of surface water and groundwater with the help of 15 neurogenetic simulation models. The accuracy of the estimation was determined as the criteria of the relationship between surface and groundwater values of the quality parameters. According to the simulation results, pH and Cl models had the smallest MSEs and groundwater values, whereas Cond and TH had the lowest MSEs. It was found from the model that although it would be easier to predict the concentration of chlorine and pH in groundwater due to contamination by surface water, it would be difficult to predict the results in the case of hardness and conductivity which is actually a property of the groundwater itself and is no way related to surface water contamination. That is why there is no significant interrelationship between the surface and groundwater hardness and conductivity. Also, the parameters of surface and groundwater quality may not have a direct relationship to each other in the local areas due to the soil texture, soil characteristics, geology, and geohydrology of the area and the depth of the aquifers. But in larger areas there may be some relationship between different parameters of surface and groundwater quality. In this study, very few sampling points were considered compared to the enormous size of the selected catchment. The same model could be developed with more values from increased sampling points; then the relationship given by the model trained with a larger data set could provide a more practical scenario with greater accuracy. But overall, from the values of the performance metrics it can be concluded that with proper attention to the temporal scale, it would be possible to make an accurate representation of the level of degradation and the threat to human health posed by the contamination of groundwater by surface water.

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