Prediction of groundwater quality indices using machine learning algorithms

Hemant Raheja *, Arun Goel and Mahesh Pal
Department of Civil Engineering, NIT Kurukshetra, Haryana 136119, India
*Corresponding author. E-mail: raheja.hemant788@gmail.com

ABSTRACT
The present paper deals with performance evaluation of application of three machine learning algorithms such as Deep neural network (DNN), Gradient boosting machine (GBM) and Extreme gradient boosting (XGBoost) to evaluate the ground water indices over a study area of Haryana state (India). To investigate the applicability of these models, two water quality indices namely Entropy Water Quality Index (EWQI) and Water Quality Index (WQI) are employed in the present study. Analysis of results demonstrated that DNN has exhibited comparatively lower error values and it performed better in the prediction of both indices i.e. EWQI and WQI. The values of Correlation Coefficient (CC = 0.989), Root Mean Square Error (RMSE = 0.037), Nash-Sutcliffe efficiency (NSE = 0.995), Index of agreement (d = 0.999) for EWQI and CC = 0.975, RMSE = 0.055, NSE = 0.991, d = 0.998 for WQI have been obtained. From variable importance of input parameters, the Electrical conductivity (EC) was observed to be most significant and 'pH' was least significant parameter in predictions of EWQI and WQI using these three models. It is envisaged that the results of study can be used to righteously predict EWQI and WQI of groundwater to decide its potability.

Key words: deep neural network (DNN), entropy water quality index (EWQI), extreme gradient boosting (XGBoost), gradient boosting machine (GBM), water quality index (WQI)

HIGHLIGHTS
- Evaluating groundwater quality using WQI and EWQI method.
- Machine learning techniques are used for predicting groundwater quality.
- Prediction performance of DNN, XGBoost, and GBM models are compared.
- Present model optimizes number of parameters to be determined for evaluating water quality.
- DNN based groundwater quality prediction performs much superior than other two models.

1. INTRODUCTION
Water, being one of the most essential resources for mankind is used for different purposes like drinking, irrigation, recreation, navigation, domestic, fisheries, industrial and many more. About 75% of the surface area of the earth is covered by water with a total quantity of about 1,386 M km³ (Kaushik et al. 2004). Out of which 97.5% of the earth's water is in the oceans, which is not appropriate for human utilization or consumption without proper treatments. Only 2.5% is available as a freshwater. Out of this, about 24.4 M km³ is locked in polar ice caps and only 10.6 M km³ is available as fresh water in reservoirs, rivers, lakes, streams, and groundwater. Groundwater is one of the basic source, which is used for several purposes throughout the world such as for irrigation, drinking and industrial use. The groundwater quality is dependent on environmental conditions and geological features. The groundwater contamination is a major problem, which poses serious threats to human health and environmental quality worldwide (Mohamed et al. 2015). It may be due to various human activities such as industrial, agricultural, and other related activities which lead to leaching of organic matter, pesticides, and nitrates deep into the aquifer (Su et al. 2019). Further groundwater quality is usually determined by the concentration of physical, chemical, and biological parameters (Kumari & Rai 2020). Panghal et al. (2021) reported that approximate 82% area of Tosham block Haryana having poor and very poor water quality for drinking purposes and 18% of area was unsuitable for drinking. It is also observed by Kumari & Rai (2020) that 45.31% area of southern Haryana has got poor and very poor water quality for drinking purposes in the May month of
year 2014. Hence, it is necessary to know the chemical composition of groundwater in order to determine its suitability for drinking purposes.

Many researchers have evaluated the potability of ground water based on major parameters i.e. pH, Electrical Conductivity (EC), Total Hardness (TH), Calcium (Ca^{2+}), Magnesium (Mg^{2+}), Sodium (Na^+), Potassium (K^+), Sulphate (SO_4^{2-}), Chloride (Cl^-), Bicarbonate (HCO_3^-), Nitrate (NO_3^-), and Fluoride (F^-) as mentioned by (Vasanthavigar et al. 2010; Zahedi 2017; Kumari & Rai 2020; Maghrabi et al. 2021). However, Measurement of all these parameters in groundwater is often poses difficulty as it is quite expensive and tedious task (Kumar et al. 2016). Hence, for reducing the effective cost and the subjectivity for evaluating water quality is a great challenge. Keeping in view of the typical issues related to easy determination of water quality, several water quality indices has been derived in past based on various water quality parameters and are available in the literature. Therefore, the researchers have mentioned index-based methods for evaluating water quality for drinking purposes i.e. water quality index (WQI) by Adimalla et al. (2020b); Tyagi et al. (2020); Wang et al. (2020), Entropy water quality index method (EWQI) by Kumar & Augustine (2021), Canadian WQI by Dao et al. (2020), US National Sanitation Foundation WQI by Lumb et al. (2011) etc. However, the EWQI is considered as an effective method to provide exact and comprehensive information about the overall quality of water for drinking purposes and has been used in recent studies takenup by Adimalla et al. (2020b) and Wang et al. (2020).

Various machine learning approaches have been used extensively to predict the groundwater quality for drinking purpose due to their improved performances in comparison to statistical methods over last three decades (Haghiabi et al. 2018; Aldhyani et al. 2020; Lu & Ma 2020; Nayan et al. 2021). Due to easy availability of water quality data from different sources in India, machine learning approaches are being successfully applied. With the advancement of new machine learning tools like Deep Neural Network and XGBoost, these new approaches are being used to analyze and, further, to predict the water quality in comparison to already reported work using other conventional machine learning models. Granata et al. (2017) purposed two models namely Support Vector Regression (SVR) and Regression Trees (RT) for predicting waste water quality. Najafzadeh et al. (2019) suggested a model to forecast the water quality index of Karoun River in Iran by pairing gene expression programming (GEP), evolutionary polynomial regression (EPR), and model tree (MT). Another study conducted by Najafzadeh & Ghaemi (2019) in predicting biochemical oxygen demand (BOD) and chemical oxygen demand (COD) of Karoun River in Iran using machine learning models. Najafzadeh et al. (2021) have used four different machine learning models such as Polynomial Regression (EPR), M5 Model Tree (MT), Gene-Expression Programming (GEP), and Multivariate Adaptive Regression Spline (MARS). These four models have helped in predicting the water quality index of Karoun River in Iran. Najafzadeh & Niazmardi (2021) have attempted to predict the water quality of the Karoun River with eleven water quality indicators using a Support Vector Regression (SVR) model using different kernels.

Traditional groundwater quality modelling approaches use either time series analysis or statistical methods. These approaches work by assuming some relationship between the dependent and independent variables as well. Mostly require data to be satisfying some statistical characteristics (e.g. normal distribution etc.), hence, found to achieve inferior results during prediction. On the other hand, Artificial Intelligence (AI) based models do not require any assumptions about data as well as relationship between dependent and independent variables. Exhaustive literature review suggests that AI based predictive models are found to perform better than the statistical methods also. Meyers et al. (2017) have proposed three different models such as ANN, SVM, and RF for evaluating the water quality in United Kingdom (UK). Nayan et al. (2021) have used the GBM model to predict the water quality of the Bangladesh river for irrigation purposes for the time period of 2013–2019. El Bilali et al. (2020) determined the groundwater quality for drinking purposes by using ANN models. Di et al. (2019) had applied machine learning models to predict water quality in the Yangtze River in China. These studies suggest that ANN, SVM, GBM works well in predicting water quality and hence can effectively be used for water quality modelling with the available datasets. Recently, new machine learning models like Extreme gradient boosting (XGBoost) and Deep Neural Network (DNN) have been applied in water engineering applications (Najah Ahmed et al. 2019; El Bilali et al. 2021; Ibrahim Ahmed Osman et al. 2021). DNN has emerged as a powerful tool for various applications in civil engineering as studied by (Wu et al. 2018; Dick et al. 2019; Kumar & Abraham 2019; Pal 2019). It seems from literature review that limited number of studies are available on the use of DNN, XGBoost and GBM algorithms in water resource engineering specially predicting water quality
for drinking purposes using two indices such as EWQI and WQI over Haryana state in India. This study is aimed to compare the performance of these three machine learning models on basis of performance parameters such as Correlation Coefficient (CC), Root Mean Square Error (RMSE), Nash-Sutcliffe efficiency (NSE) and Index of agreement (d) on 392 data set from Haryana state for 12 hydrochemical parameters. Two indices EWQI and WQI were manually calculated for the data set and compared with the predicted values obtained by applying DNN, XGBoost and GBM algorithms. Further most significant parameters affecting the groundwater quality were also determined from the same data set by using three algorithms. At the end uncertainty and reliability analyses was also carried out. The outcomes of the article are expected to provide scientific information about quality of groundwater which will be further useful in management and sustainable development of groundwater resource in Haryana state.

2. MATERIALS AND METHODOLOGY

2.1. Machine learning models

2.1.1. Gradient boosting machine (GBM)

Boosting algorithms have been originally introduced by the machine learning community as stated by Freund (1995). The Gradient boosting machine learning brings together weak learners in a different way to develop a strong learner. As each weak learner is added, a new model is fitted to provide a more accurate estimate of the response variable. The new weak learners are maximally correlated with the negative gradient of the loss function, associated with the whole ensemble. The main aim of the GBM is to create a stronger prediction model by merging a group of relatively weak prediction models. The model forecasts values for the structure \( \hat{y} = F(x) \) by limiting the mean squared error as given in Equation (1).

\[
\frac{1}{n} \sum_{i} (\hat{y}_i - y_i)^2
\]

where, \( y_i \) = actual value, \( \hat{y}_i \) = predicted value, \( i \) = equities over some test data of size, \( n \) = number of samples in \( y \).

2.1.2. Extreme gradient boosting (XGBoost)

The XGBoost algorithm has recently been used for classification/regression problems (Chen & Guestrin 2016) and is based on gradient boosting algorithm (Friedman 2002). The XGBoost algorithm has been implemented in various engineering applications, e.g., shear strength (Zhang et al. 2021), streamflow (Hadi et al. 2019; Yu et al. 2020). Two major changes in the design of the XGBoost over the gradient boosted decision tree includes (1) using a regularization term in its objective function allowing it to be less prone to overfitting in comparison to gradient boosted decision tree and (2) using Taylor expansion on the objective function compared to gradient boosted decision tree which uses first derivative in optimization, thus allowing XGBoost to define the loss function more accurately. The objective function of XGBoost that need to be minimized is defined by Equations (2) and (3) and given below:

\[
\text{obj}(\theta) = \sum_{i=1}^{n} L(y_i, \hat{y}_i^{(t)}) + \sum_{i=1}^{T} \Omega(D_i)
\]

where

\[
\Omega(f) = \gamma T + \frac{1}{2\lambda} \sum_{i=1}^{T} w_i^2
\]

where, \( \hat{y}_i^{(t)} \) is the predicted value of target variable \( y_i \) at the \( t \)th round, \( L \) is loss function, \( T \) is number of leaves in the tree, \( w_i \) is score of \( j \)th leaf and lambda (\( \lambda \)) is the regularization parameter (Chen & Guestrin 2016).

Further, \( D_i \) denotes an independent tree with \( \gamma \) as the penalty coefficient and \( 1/2\lambda \sum_{j=1}^{T} w_i^2 \) is L2 norm of leaf score. After \( t \) iterations, the function of the model is the \((t-1)^{th}\) iteration prediction function plus a new decision
tree. Thus, the Equation (2) is updated as Equation (4) and mentioned below

\[ \text{Obj}^j = \sum_{i=1}^{n} L(y_i, \hat{y}_i^{(t-1)}) + D_t(x_i) + \Omega(D_t) \]  \hspace{1cm} (4)

The importance of each feature is calculated based on their prediction performance. Each feature is replaced by the noise and prediction takes place for the particular instance. The higher the value of prediction indicates greater score of each feature. Thus, it assesses all features by the individual scores which become important during training and the feature with higher score plays major role in making the key decision with boosted trees.

2.1.3. Deep neural network (DNN)

The processing node is basic component of a back-propagation neural network (BPNN). Each processing node of BPNN performs two functions and behave as a biological neuron. Initially it sums up the input values and this sum of input is then passed through the activation function to create the output. The activation function, \( f \) can be used as any differential function. In BPNN, all processing nodes arranged into layers which fully interconnected to the next layer. There is no connection of nodes of the same layer. A BPNN, typically, consists of an input layer that serves as a distribution structure of data that is inputted into the network and is not used for any form of processing. After this layer, one or more processing layers are known as hidden layers. The output layer is final processing layer. A neural network having two or more hidden layers with a huge number of nodes and using mathematical modeling is mostly known as a DNN (Pal 2019).

All the interconnections between each node have an associated weight. When a value is passed from the input layer, down these interconnections, these values are multiplied by the associated weight and summed to derive the net input \( n_j \) to the unit as shown below in Equation (5)

\[ = \sum_i W_{ji} O_i \]  \hspace{1cm} (5)

where, \( W_{ji} \) denotes the weight of the interconnection to unit \( j \) from unit \( i \) (called input) and \( O_i \) denotes the output of unit \( i \). The net input obtained by the above equation is then transformed by the activation function to produce an output \( (O_j) \) for unit \( j \).

Activation functions introduce non-linearity in the neural network to learn more complex features present in the data. Traditional activation functions: sigmoid and hyperbolic tangent with a BPNN are found to be affected by saturation and sensitivity to changes around their mid-point (Goodfellow et al. 2016). The rectified linear activation function (RELU); (Nair & Hinton 2010) is a piecewise linear function and considered to be a milestone in the design of a deep neural network. RELU activation function output the input value itself if it is positive, otherwise the output would be zero and easy to train. The use of RELU is found to achieve better performance than other activation functions with DNN. The RELU function is defined in Equation (6) as below:

\[ f(n_j) = \max(0, n_j) \]  \hspace{1cm} (6)

Initializing BPNN weights is an important factor that affects the functioning of the neural network. The initial weights should be selected before the start of network training and should be in a reasonable range. Random weight initialization, which is normally used with a standard BPNN to find an optimal set of weights using a stochastic gradient descent approach. Xavier weight initialization was proposed as the weight initialization technique for DNN because of the poor performance of random weight initialization with a standard gradient descent-based optimization approach. This approach assigns the weights from a Gaussian distribution with zero mean and some finite variance, thus allowing the variance of the outputs of a layer to be equal to the variance of its inputs.

During training phase of BPNN, network weights are continuously updated and adjusted using learning rate as one of the user-defined parameters. The value of learning rate is generally selected randomly, based on the experiences and the earlier reported works. Gradient descent algorithms were generally used to update the network weights with the help of a learning rate in a BPNN. The introduction of adaptive learning rate methods allowed adjusting the learning rate adaptively throughout the training process of a DNN. In order to update the weights of
a DNN, an adaptive moment estimation based optimization algorithm was proposed (Kingma & Ba 2015) and found to perform well. Use of Adam requires several user-defined parameters during training but studies suggest that the default values as suggested by (Kingma & Ba 2015) works well with most of the datasets.

Similar to BPNN, optimal values of several user-defined parameters need to be obtained during training of deep neural network. These parameters include activation function, optimization algorithm, number and type of hidden layers, number of nodes in hidden layer, hidden and dropout layers, updaters (i.e., learning rate optimization algorithm), weight initialization method, batch size (i.e., number of training samples used in one iteration) and the number of epochs. One epoch is defined as when an entire training dataset has passed once through the neural network both in forward and backward direction.

2.2. Study area and data

Haryana state is a landlocked state in the north-west part of India as shown in Figure 1. The latitude of Haryana state extends between 27°39′ and 30°35′N and longitudes between 74°27′ and 77°36′E. The total geographical area of Haryana state is 44,212 Km². The normal average annual rainfall is about 617 mm which is receive primarily through southwestern monsoon. The climate of the state is arid to semi-arid with very hot in summer temperature approximate 45 °C.

The dataset used in this study was downloaded from India Water Resources Information System (IWRIS; https://indiawris.gov.in). Dataset collected from national groundwater monitoring stations distributed Figure 1(b) over 20 districts of Haryana state during year 2016 which was used to predict the groundwater quality for drinking purposes given in Table 1. Total 392 samples were collected and analyzed for 12 important hydrochemical parameters so as to access the groundwater quality. This dataset was randomly divided in such a way that 294 (75%) samples are used for the training, whereas the remaining 98 (25%) were used for testing the models. To calculate the groundwater quality, two different water quality indices Entropy water quality index (EWQI) and Water quality index (WQI) were calculated using 12 parameters. In order to reduce the effect of large variation in input and output values, normalization of different input and output parameters was also performed.

2.3. Entropy water quality index (EWQI)

EWQI has been frequently used to estimate the water quality for domestic/drinking, agricultural purpose etc. in the past and have been applied to determined water quality by (Shannon 1948). The steps involved in the calculation EWQI are as under follow.

In first instance, normalization is carried out on initial matrix ‘X’. After this, the standard matrix as (7) & (8) is stated as

\[
X = \begin{bmatrix}
  x_{11} & x_{1n} \\
  x_{m1} & x_{nm}
\end{bmatrix}
\]

(7)

\[
Y = \begin{bmatrix}
  y_{11} & y_{1n} \\
  y_{m1} & y_{nm}
\end{bmatrix}
\]

(8)
In Equations (7) and (8) \( m \) and \( n \) are the number of ground water samples and parameter for a sample respectively.

Then the value of \( y_{ij} \) is obtained by the Equation (9)

\[
y_{ij} = \frac{x_{ij} - (x_{ij})_{\text{min}}}{(x_{ij})_{\text{max}} - (x_{ij})_{\text{min}}}\tag{9}
\]

where, \( x_{ij} \) is the \( j \)th evaluation index of the \( i \)th groundwater sample.

After calculating the standardized value, the ratio of index value of the \( j \) index using \( i \) sample is calculated by Equation (10)

\[
P_{ij} = \frac{y_{ij}}{\sum_{i=1}^{m} y_{ij}}\tag{10}
\]

Next step is to calculate entropy weight \( w_j \) and information entropy \( e_j \) by Equations (11) and (12) as

\[
e_j = -\frac{1}{\ln m} \sum_{i=1}^{m} y_{ij} \ln y_{ij}\tag{11}
\]

\[
w_j = \frac{1 - e_j}{\sum_{j=1}^{n} (1 - e_j)}\tag{12}
\]

To calculate EWQI, a quality rating scale \( q_j \) for each parameter is assigned where \( q_j \) is obtained from the following Equation (13)

\[
q_j = \frac{c_j}{s_j} \times 100\tag{13}
\]

where, \( c_j \) represents the concentration of the parameter (mg/l), and \( s_j \) denotes the water standards of groundwater for each drinking parameter according to Bureau of Indian standards (BIS). The EWQI can then be calculated by the following Equation (14)

\[
EWQI = \sum_{j=1}^{n} w_j q_j\tag{14}
\]
The results of EWQI obtained from above equation are listed in Table 2 (Aouiti et al. 2021). Out of 392 groundwater samples, only 14.80% of groundwater samples are unsuitable for drinking, while 32.40% of samples have good quality and only 17.60% samples exhibited excellent quality of groundwater for drinking purposes.

### Table 2 | EWQI scale, water type, and % of samples in the study area (Wang et al. 2017)

<table>
<thead>
<tr>
<th>Sr. No.</th>
<th>EWQI scale</th>
<th>Quality of groundwater</th>
<th>Number of samples</th>
<th>% of samples</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>&lt;50</td>
<td>Excellent</td>
<td>69</td>
<td>17.60</td>
</tr>
<tr>
<td>2</td>
<td>50–100</td>
<td>Good</td>
<td>127</td>
<td>32.40</td>
</tr>
<tr>
<td>3</td>
<td>100–200</td>
<td>Poor</td>
<td>101</td>
<td>25.76</td>
</tr>
<tr>
<td>4</td>
<td>200–300</td>
<td>Very Poor</td>
<td>37</td>
<td>9.44</td>
</tr>
<tr>
<td>5</td>
<td>&gt;300</td>
<td>Not suitable for drinking</td>
<td>58</td>
<td>14.80</td>
</tr>
</tbody>
</table>

### 2.4. Water quality index (WQI)

The WQI method has been commonly used to assess the drinking water quality in various geological topographies (Aly et al. 2015; Chung et al. 2015; Adimalla & Qian 2019; Adimalla et al. 2020a; Gaikwad et al. 2020). The following steps are includes for calculation of WQI according to Horton (1965):

1. In first instance, ‘assigning weight’: twelve parameters are weighted according to its relative importance. The weight 5 is assigned to the most significant parameters and 1 is for the least significant. is obtained The relative weight ($W_i$) is obtained from Equation (15) and has been shown in Table 3.

$$W_i = \frac{w_i}{\sum_{i=0}^{n} w_i}$$  

where, $w_i$ is the weight of each parameter and $n$ is the number of parameters.

### Table 3 | Relative weight of hydrochemical parameters

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Weight ($w_i$)</th>
<th>Relative weight ($W_i$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>pH</td>
<td>4</td>
<td>0.091</td>
</tr>
<tr>
<td>EC</td>
<td>4</td>
<td>0.091</td>
</tr>
<tr>
<td>TH</td>
<td>4</td>
<td>0.091</td>
</tr>
<tr>
<td>Ca$^{2+}$</td>
<td>3</td>
<td>0.068</td>
</tr>
<tr>
<td>Mg$^{2+}$</td>
<td>3</td>
<td>0.068</td>
</tr>
<tr>
<td>Na$^+$</td>
<td>4</td>
<td>0.091</td>
</tr>
<tr>
<td>K$^+$</td>
<td>1</td>
<td>0.023</td>
</tr>
<tr>
<td>HCO$_3^-$</td>
<td>1</td>
<td>0.023</td>
</tr>
<tr>
<td>Cl$^-$</td>
<td>5</td>
<td>0.11</td>
</tr>
<tr>
<td>SO$_4^{2-}$</td>
<td>5</td>
<td>0.11</td>
</tr>
<tr>
<td>NO$_3^-$</td>
<td>5</td>
<td>0.11</td>
</tr>
<tr>
<td>F$^-$</td>
<td>5</td>
<td>0.11</td>
</tr>
</tbody>
</table>

2. In second instance, ‘quality rating ($q_i$) scale calculation’ firstly water sample concentration is multiplied by 100 and then dividing the results by its limits given by the BIS (2015) in Equation (16).

$$q_i = \frac{C_i}{S_i} \times 100$$  

where, $C_i$ is the concentration of chemicals in the water sample in (mg/l), and $S_i$ is the drinking water standard for each chemical parameter BIS (2015).
3. In third instance, ‘calculation of water quality index (WQI)’, firstly $S_{i}$ (water quality index of the $i^{th}$ parameter) value is calculated by Equation (17) and WQI equals sum of all the value of $S_{i}$ of each parameters as by Equation (18).

$$S_{i} = \frac{W_{i}}{C_{2i}}$$  \hspace{1cm} (17)

$$WQI = \sum_{j=1}^{n} S_{i}$$  \hspace{1cm} (18)

Wang et al. (2017) described the WQI into five categories as listed in Table 4, it can be noted from Table 4 that 16.58% sample exhibited the excellent water quality, 29.34% good water quality and 13.26% of water samples falls under unsuitable for drinking purpose.

**Table 4 | WQI scale, water type and % of water samples in the study area (Aouiti et al. 2021)**

<table>
<thead>
<tr>
<th>Sr. No.</th>
<th>WQI scale</th>
<th>Quality of groundwater</th>
<th>Number of samples</th>
<th>% of samples</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>&lt;50</td>
<td>Excellent</td>
<td>65</td>
<td>16.58</td>
</tr>
<tr>
<td>2</td>
<td>50–100</td>
<td>Good</td>
<td>115</td>
<td>29.34</td>
</tr>
<tr>
<td>3</td>
<td>100–200</td>
<td>Poor</td>
<td>119</td>
<td>30.36</td>
</tr>
<tr>
<td>4</td>
<td>200–300</td>
<td>Very Poor</td>
<td>41</td>
<td>10.46</td>
</tr>
<tr>
<td>5</td>
<td>&gt;300</td>
<td>Not suitable for drinking</td>
<td>52</td>
<td>13.26</td>
</tr>
</tbody>
</table>

The values of EWQI and WQI obtained for predicting the groundwater quality are shown in Tables 2 and 4. The perusal of Tables 2 and 4 show that 50% of the samples falls under 0–100 for EWQI, while 45.92% of the samples falls under 0–100 in WQI. The comparison of EWQI and WQI shows that most of the sample of EWQI are more effective than WQI. As compared with past studies under taken by Kumari & Rai (2020) and Panghal et al. (2021), the results obtained in this study are superior thereby, suggesting the importance of application of three machine learning models successfully.

### 3. PARAMETER OPTIMIZATION OF DIFFERENT MACHINE LEARNING ALGORITHMS

The use of algorithms XGBoost, DNN and GBM needs setting of several user-defined parameters. For all three algorithms used in present study, H2o Auto-ML software (H2O.ai. 2020) was applied. To obtain the optimal value of various hyper parameters of different algorithms, Auto-ML uses with 5 -fold cross validation and grid search method were used. During training phase, the DNN produces a ranked list of different input variables using Geodon’s method (Gedeon 1997) whereas GBM and XGBoost use a gain value to rank various input attribute as discussed in (Xu et al. 2014; Chen & Guestrin 2016). The optimal values of various parameters obtained in predicting EQWI and WQI are provided in Table 5.

**Table 5 | Optimal value of user-defined parameters DNN, XGBoost and GBM**

<table>
<thead>
<tr>
<th>Name of Algorithm</th>
<th>User-defined parameters for EWQI</th>
<th>User-defined parameters for WQI</th>
</tr>
</thead>
<tbody>
<tr>
<td>DNN</td>
<td>One Hidden layer with 200 nodes, Epochs = 4211 Activation Rectifier with Dropout = 0.2, initial weight distribution = Uniform Adaptive, Batch size = 1, distribution = gaussian</td>
<td>One Hidden layer with 50 nodes, Epochs = 8380 Activation Rectifier with Dropout = 0.2, initial weight distribution = Uniform Adaptive, Batch size = 1, distribution = gaussian</td>
</tr>
<tr>
<td>XGBoost</td>
<td>Distribution = gaussian, booster = gbtree, ntree = 54, maxbins = 256, max depth = 5, $\text{eta} = 0.3$ and $\lambda$ = 0.01</td>
<td>Distribution = gaussian, booster = gbtree, ntree = 43, maxbins = 256, max depth = 20, $\text{eta} = 0.3$ and $\lambda$ = 0.1</td>
</tr>
<tr>
<td>GBM</td>
<td>Distribution = gaussian, ntree = 72, nbins = 20, max depth = 9</td>
<td>Distribution = gaussian, ntree = 75, nbins = 20, max depth = 10</td>
</tr>
</tbody>
</table>
3.1. Performance indices

The performance of these three algorithms (DNN, XGBoost and GBM) used in this study is predicted after the desired training and testing phases are completed. The calculated output values are estimated using the following measures of goodness-of-fit: Correlation Coefficient (CC), Root Mean Square Error (RMSE), Nash–Sutcliffe efficiency (NSE) and Index of agreement (d). The CC range is varied from −1 to 1. If the CC value is approaching to 1 and the RMSE value is approaching to 0 then the accuracy of model is high. If the CC value is approaching to 0 and the RMSE value is approaching to 1 then the accuracy of model is low. Nash & Sutcliffe (1970) initially proposed Nash–Sutcliffe efficiency (NSE) and commonly used statistic index. The range of NSE is varied from 0 to +1 and It is also called efficiency index ($E_\eta$). Willmott (1981) first used the Index of agreement (d) which varied between 0 and 1. The values of CC, RMSE, NSE, and d are computed by using from the Equations (19)–(22) as given below:

$$\text{CC} = \frac{\sum_{i=1}^{N} (X_0i - \bar{X}_0)(X_pi - \bar{X}_p)}{\sqrt{\sum_{i=1}^{N} (X_0i - \bar{X}_0)^2} \sum_{i=1}^{N} (X_pi - \bar{X}_p)^2}$$  \hspace{1cm} (19)

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{N} (X_pi - X_0i)^2}{N}}$$  \hspace{1cm} (20)

$$\text{NSE} = 1 - \left[ \frac{\sum_{i=1}^{N} (X_p - X_o)^2}{\sum_{i=1}^{N} (X_o - \bar{X}_o)^2} \right]$$  \hspace{1cm} (21)

$$d = 1 - \left[ \frac{\sum_{i=1}^{N} (X_p - X_o)^2}{\sum_{i=1}^{N} |X_p - X_o| + |X_o - \bar{X}_o|^2} \right]$$  \hspace{1cm} (22)

where $X_0$, $X_p$ and $\bar{X}_o$ are the observed and predicted and mean of observed values respectively.

3.2. Uncertainty and reliability analysis

Saberi-Movahed et al. (2020) carried out the uncertainty ($U_{95}$) and reliability analysis, for evaluating the overall consistency of the model used in predictions for longitudinal dispersion coefficients in water pipelines. The main purpose of uncertainty analysis is to adjust the expected range within which the true value of the experimental result lies and is obtained from the Equation (23) and the reliability analysis is determined by using Equations (24) and (25) which are given below:

$$U_{95} = \left( \frac{1.96}{N} \right) \sqrt{\frac{\sum_{i=1}^{N} (X_0i - \bar{X}_0)^2}{N} + \frac{\sum_{i=1}^{N} (X_0i - X_pi)^2}{N}}$$  \hspace{1cm} (23)

$$\text{Reliability} = \left( \frac{100\%}{N} \right) \sum_{i=0}^{N} K_i$$  \hspace{1cm} (24)

$$\text{RAE} = \left| \frac{X_o - X_p}{X_o} \right|$$  \hspace{1cm} (25)

For obtaining the $K_i$ value, first relative average error is determined from Equation (25) and next, if the value of $\text{RAE} \leq \Delta$ then $K_i = 1$, otherwise $K_i = 0$.

Where, $\Delta$ is the threshold value of water quality parameter and as per Chinese standards the optimum value of $\Delta$ is 0.2 or 20%. $K_i$ is determined as number of times the value of $\text{RAE} \leq \Delta$. The same equations have been applied in determining the water quality of data set for estimating EWQI and WQI.
4. ANALYSIS OF RESULTS AND DISCUSSION

Table 6 provides results obtained in terms of CC, RMSE, NSE and d values with both training and test datasets for predicting the groundwater quality using EQWI and WQI. A comparison of these values suggests the slightly improved performance of EWQI by optimized DNN (CC = 0.989, RMSE = 0.037, NSE = 0.995 and d = 0.999) in comparison to XGBoost (CC = 0.976, RMSE = 0.056, NSE = 0.994 and d = 0.999) and GBM (CC = 0.959, RMSE = 0.074, NSE = 0.992 and d = 0.998). However, the performance of WQI using DNN (CC = 0.975, RMSE = 0.055, NSE = 0.991 and d = 0.998) in comparison to XGBoost (CC = 0.944, RMSE = 0.082, NSE = 0.986 and d = 0.998) and GBM (CC = 0.968, RMSE = 0.062, NSE = 0.980 and d = 0.998). The overall results also suggest slightly improved performance by GBM in comparison to XGBoost while using WQI as a groundwater quality index whereas XGBoost achieves better results with EWQI.

Table 6 | Modeling performance for EWQI and WQI with a training and test dataset

<table>
<thead>
<tr>
<th>Index</th>
<th>Modeling approach</th>
<th>CC Training</th>
<th>Testing</th>
<th>RMSE Training</th>
<th>Testing</th>
<th>NSE Training</th>
<th>Testing</th>
<th>d Training</th>
<th>Testing</th>
</tr>
</thead>
<tbody>
<tr>
<td>EWQI</td>
<td>DNN</td>
<td>0.998</td>
<td>0.989</td>
<td>0.012</td>
<td>0.037</td>
<td>0.989</td>
<td>0.995</td>
<td>0.997</td>
<td>0.999</td>
</tr>
<tr>
<td></td>
<td>XGBoost</td>
<td>0.998</td>
<td>0.976</td>
<td>0.016</td>
<td>0.056</td>
<td>0.935</td>
<td>0.994</td>
<td>0.982</td>
<td>0.999</td>
</tr>
<tr>
<td></td>
<td>GBM</td>
<td>0.998</td>
<td>0.959</td>
<td>0.015</td>
<td>0.074</td>
<td>0.922</td>
<td>0.992</td>
<td>0.978</td>
<td>0.998</td>
</tr>
<tr>
<td>WQI</td>
<td>DNN</td>
<td>0.999</td>
<td>0.975</td>
<td>0.018</td>
<td>0.055</td>
<td>0.965</td>
<td>0.991</td>
<td>0.999</td>
<td>0.998</td>
</tr>
<tr>
<td></td>
<td>XGBoost</td>
<td>0.996</td>
<td>0.944</td>
<td>0.048</td>
<td>0.082</td>
<td>0.943</td>
<td>0.986</td>
<td>0.982</td>
<td>0.998</td>
</tr>
<tr>
<td></td>
<td>GBM</td>
<td>0.996</td>
<td>0.968</td>
<td>0.020</td>
<td>0.062</td>
<td>0.949</td>
<td>0.980</td>
<td>0.986</td>
<td>0.998</td>
</tr>
</tbody>
</table>

Table 7 shows the performance results obtained in terms of uncertainty (U₉₅) and reliability analysis for predicting the groundwater quality using EWQI and WQI in both training and testing stages. From this table, it is evident that the performance of EWQI using DNN achieved lowest value of U₉₅ (21.60) when compared with XGBoost (U₉₅ = 22.31) and GBM (U₉₅ = 22.17) in training stage. While in testing stage, the value of U₉₅ of EWQI optimized by DNN is more accurate (U₉₅ = 19.78) in comparison to XGBoost (U₉₅ = 20.91) and GBM (U₉₅ = 20.22). Additionally, prediction of EWQI using DNN is more reliable (98.59) in comparison to XGBoost (96.46) and GBM (97.17) in training stage. While in testing stage, the performance of EWQI using DNN have higher level of reliability (98.16) when compared with XGBoost (97.08) and GBM (97.16). To conclude, in terms of uncertainty (U₉₅) and reliability, DNN performs better than other two models for training as well as testing. Same trend has been observed for estimation of WQI in terms of uncertainty and reliability under training and testing category. However, when two indices EWQI and WQI are compared, the prediction of EWQI is superior than WQI in three algorithms used in this article.

Table 7 | Performance results for the uncertainty and reliability analysis of DNN, XGBoost and GBM algorithms

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>EWQI</th>
<th>WQI</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Uncertainty (U₉₅)</td>
<td>Reliability (%)</td>
</tr>
<tr>
<td>Training</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DNN</td>
<td>21.60</td>
<td>98.59</td>
</tr>
<tr>
<td>XGBoost</td>
<td>22.31</td>
<td>96.46</td>
</tr>
<tr>
<td>GBM</td>
<td>22.17</td>
<td>97.17</td>
</tr>
<tr>
<td>Testing</td>
<td></td>
<td></td>
</tr>
<tr>
<td>DNN</td>
<td>19.78</td>
<td>98.16</td>
</tr>
<tr>
<td>XGBoost</td>
<td>20.91</td>
<td>97.08</td>
</tr>
<tr>
<td>GBM</td>
<td>20.22</td>
<td>97.16</td>
</tr>
</tbody>
</table>

Further, Figures 2 and 3 provide plots between predicted and actual values of EWQI and WQI using DNN, XGBoost, and GBM respectively. It can be observed from Figure 2 that generally, most of the predicted values...
for EWQI as groundwater quality index falls near the line of perfect agreement (i.e. a line at 45°). Four more lines in the range of ±25% and ±10% error between the actual and predicted value of EWQI and WQI are also plotted in the graphs. Figure 2(a) shows that most of the value predicted by DNN of EWQI were well ±10% error line from the line of perfect agreement. It can be inferred from Figure 2(b) that some predicted values by XGBoost of EWQI are lying away from ±25% error line also. Figure 2(c) shows that some predicted values by GBM are lying away from ±10% error line and ±25% error line. Figure 3(a) demonstrate that most of the value predicted of WQI by DNN were well ±10% error line from the line of perfect agreement. Comparison of Figures 2(a)–2(c) and 3(a)–3(c) also suggests that the predicted EWQI and WQI values by DNN are in good agreement with the actual EWQI and WQI respectively, suggesting its improved performance in comparison to both XGBoost and GBM in the present study.

In this study the relative importance of each hydrochemical parameter has been compared with each algorithm, so that the variability in the dependent variable can be explained by the independent variables.
Figure 4(a)–4(f) depicts the relative importance of different independent chemical variables calculated by using DNN, XGBoost and GBM algorithms. Figure 4(a)–4(c) represents the relative importance of variables for modeling EWQI and Figure 4(d)–4(f) represents the relative importance of variables for modeling WQI. From the Figure 4(a)–4(f), it can be observed that the EC is most significant variable having highest relative importance to predict the EWQI and the WQI by using three algorithms DNN, XGBoost and GBM. The pH having lowest relative importance in prediction of EWQI (DNN = 0.2212, XGBoost = 0.0013 and GBM = 0.0008) and WQI (DNN = 0.1476, XGBoost = 0.04781 and GBM = 0.0016). The most interesting fact is that Mg attains moderate relative importance for the prediction of EWQI (DNN = 0.4239 and GBM = 0.0033) and WQI (DNN = 0.3645 and GBM = 0.0314) but XGBoost shows a higher relative importance in WQI (0.5545) and lower relative importance in EWQI (0.0021) of this variable. Similarly, for TH has moderate relative importance for the prediction of EWQI (DNN = 0.4145 and GBM = 0.0032) and WQI (DNN = 0.3534 and GBM = 0.0213) but XGBoost shows a higher relative importance in WQI (0.873) and lower relative importance in EWQI (0.0481) of this variable. However, the perusal of Figure 4(a)–4(f) shows that there is no definite trend of variable importance of hydrochemical parameters in estimating EWQI and WQI using three algorithms i.e. DNN, XGBoost and GBM on this data set.
5. CONCLUSIONS

In the present work, a study has been taken up to assess the performance of DNN, XGBoost, and GBM algorithms for predicting the groundwater quality based on two indices i.e. EWQI and WQI. The comparison of three techniques has been made on the basis of four goodness-of-fit indices, namely: CC, RMSE, NSE and $d$. The conclusions drawn from this work are as given below:

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**Figure 4** | Relative importance of input variables from DNN, XGBoost and GBM algorithms.
1. Three different machine learning models were used to predict EWQI, i.e. DNN, XGBoost, GBM. Out of the three algorithms it is observed that DNN algorithm is performing best in terms of training as well as testing dataset. For testing dataset performance indices have following values: (CC = 0.989, RMSE = 0.037, NSE = 0.995 and d = 0.999) and for training (CC = 0.998, RMSE = 0.012, NSE = 0.989 and d = 0.997).

2. Also, in terms of predictions of WQI, DNN performed the best in terms of training and testing dataset. For testing dataset performance indices have following values: (CC = 0.975, RMSE = 0.055, NSE = 0.991 and d = 0.998) and for training (CC = 0.999, RMSE = 0.018, NSE = 0.965 and d = 0.990).

3. After comparison of all the three algorithms, it is found that DNN based modeling is performing slightly better than XGBoost and GBM in estimating both EWQI and WQI in training as well as testing data set.

4. After observing the values of various relative importance of variables as given by the three models the variable ‘EC’ was given most significance in predicting the dependent variable. However, the parameter ‘pH’ has been considered as least significant parameter in prediction using three machine learning models in the present study.

5. The uncertainty (U95) and reliability analysis of the data set also revealed that the DNN performs better than other two algorithms (XGBoost and GBM) for training as well as testing in prediction of EWQI and WQI.

6. The promising results observed in the study suggest that DNN can be used to predict various other bio-chemical and physio-chemical properties of groundwater consumed for drinking purpose.

7. The findings of this study can be extended further by examining the performance of DNN model as compared to other machine learning models, considering different possible hydrochemical input parameters.

8. Furthermore, this study aims to be a mere suggestion to the research community about the application of machine learning models in prediction of ground water quality indices, as it is much needed for economical weaker regions, where not much equipment and resources are available.

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CONFLICT OF INTEREST

Authors claim there exists no warfare of interest in any form concerning the work done within the present manuscript.

DATA AVAILABILITY STATEMENT

Data cannot be made publicly available; readers should contact the corresponding author for details.

REFERENCES


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