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Prediction and Assessment of Minerals Contamination in Groundwater: Analytical Tools Approach

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Abstract: Accumulation of minerals in groundwater over years degrades the water quality and thus affects the surrounding ecosystem if left untreated. Rapid urbanization and industrialization paves way for serious harm to the natural resources; particularly for the water bodies. One such study area is chosen for this analytical investigation to predict the consecutive concentration of important minerals for the next five years with some prediction tools. Artificial Neural Network, Support Vector Machine, and, Deep Learning methods are adopted for prediction analysis. The results of MSE, RMSE, and MAPE in each mentioned method were compared and concluded which performed better for the collected data of mineral concentration. Among these tools, SVM showed better results with less error and efficient accuracy (MSE-64.31, RMSE-8.07, and MAPE-3.92) though the other two techniques gave slight accuracy. The annual rainfall values are highly correlated with the mineral values in which the decreasing trend shows the mineral values when rainfall is higher and vice versa. These predicted values aids in creating awareness among the local residents as well as preventing the further pollution of the groundwater by the accumulation of minerals.

Keywords: Minerals, Neural network, Support vector machine, Deep learning, Water Quality

Groundwater being the major source of water often gets degraded by the acute dumping of solid as well as liquid wastes into it. These wastes turn out to be the major pollutant of the groundwater making it undrinkable. There are more than 4000 minerals so far identified upon the earth's crust. Among which few are very common ones; particularly the different forms of silicate mineral comprise more than 90 percent of the total minerals on the earth's crust. Mineral pollution has become more common in water which predominantly causes health risks in humans as well as other living species. This pollution also affects the environment (Ukah et al 2019) and the ecosystem (Belkhiri et al 2018). Identification of mineral types effectuates the physicochemical properties which impact groundwater quality (Goswami et al 2020). Groundwater quality and assessment of human health risk in Bangladesh were reported to be acidic to, alkaline. The findings also depicted exceeding limits of iron and manganese which is then sighted for safe and sustainable groundwater management (Bodrud-Doza et al 2020). Drinking water of good quality is very important for human life, particularly in developing countries with large populations (Ayedun et al 2015). Wetland areas are mostly affected by pollution of the minerals in the surrounded water bodies (Pandiyan et al 2020) often by rapid industrialization and urbanization leading the poor water quality (Cao et al 2019). Multivariate statistical analysis and hydro geochemical analysis has been integrated to determine the groundwater quality in which the source of contamination water intrusion from the nearby tailings pond is studied (Huang et al 2015). Fluoride enrichment in groundwater is found to affect human health with the high concentration of total dissolved solids along with the presence of Ca, Na, Mg, and Cl (Li et al 2020). Water contamination with heavy chromium ion concentrations is observed to affect children's health more than adults, leaving behind the water no portable (Wu et al 2020). Study the presence of trace elements in groundwater very essential to be alarming in another area (Suman et al 2017). The concentration of minerals is effectuated on soil water, and vegetation by means of irrigation sources, in Iran which in turn affects humans (Cheshmazar et al 2018). The groundwater quality is assessed for use in irrigation alone in some studies (Bhat et al 2016, Kumar et al 2019). The higher humus concentration in soil and the neutral pH values in the soil solution validate the presence of enough microorganisms to resist the pollutants. (Sidhu et al 2021). Hence it is highly important to identify the intrusion of minerals including high concentration of fluorides in groundwater (Jothimani et al 2017).

The progression of minerals in drinking water may harm the natural resources as well as the ecosystem and this alarming situation calls for an apt solution in which the effects can be predicted well before the degradation of the groundwater quality. To protect the ecosystem, future prediction of minerals contamination is necessary and it helps to take initiative measures prior by the policymakers. It is very essential to manage the water quality problem by prediction technique, particularly in urban areas. Future prediction is often executed with advanced forecasting methods such as Support Vector Machine (SVM), Artificial Neural Network (ANN), and Deep Learning methods. Neural networks are found to be effective in analyzing data in a simpler and faster way even for solving non-linear problems. (Xin et al 2004). Despite the accuracy in neural networks, Support Vector Machine that works on the principle of kernel technique is effectively used to solve complex issues faced in neural networks (Kramer et al 2011). Compared to both classification and regression approaches, deep learning methods showed outstanding performance serving as a traditional machine learning method (Doppalapudi et al 2021).

In this study Artificial Neural Network, Support Vector Machine and, Deep Learning methods were adopted for water quality prediction analysis by means of MSE, RMSE, MAPE using the data of dependent variable pH, Ec, Na, K, SO_4, TH, Ca, Cl and independent variable of rainfall, water level, population, year, temperature, humidity, wind speed, evaporation of the study region.

MATERIAL AND METHODS

Study area and data collection: Padmanabhapuram [8.1444N&77.1855E], in Southern India, is chosen as the study area for this research investigation owing to the varying annual rainfall and increasing groundwater.

The factors affecting the groundwater quality were identified as rainfall, water level, population increase, consecutive years, temperature, humidity, wind speed, and evaporation. The groundwater quality data were collected from the Central Ground Water Board, a government organization. Parameters such as pH, electrical conductivity (EC), sodium (Na), calcium, potassium(K), sulphate (SO4), and Total Hardness (TH)were found to be the major contributors to the accumulation of minerals in water sources (Table 1). The missed data were calculated based on time series analysis (Wilson et al 2002) as well as forecasting formulae. Though more minerals were discussed in the Bureau of Indian Standards for water, limited minerals that contributed more in the past two decades were only considered in this prediction analysis. As per the Bureau of Indian Standards, the minerals identified are listed along with their permissible limits for water usage by humans (BIS, 2012) are presented (Table 2). The concentration of minerals regarding these standards is taken over for the groundwater quality analysis.

Research methodology: Initially, identification of the accumulated minerals in groundwater is done followed by the prediction in the concentration of these minerals in the future. The collected factors of the study area are used as variables for executing the analysis process. The correlation method is carried out for the collected factors by using the standard formula. Correlation is taken over between individual factors that were collected and each mineral. The factors that correlate well with minerals are selected for further analysis. The ideal correlation factor value in this analysis is 0.75. The highly correlated factors are taken for further data analysis whereas correlated factors with a value of less than 0.75 are not considered for further analysis. These correlated factors are then analyzed for further prediction methods using ANN network, SVM technique, and Deep Learning methods in which correlated factors are analyzed for better results by developing models. The results of these prediction tools are compared for accurate results. The comparison is done with the errors that resulted in each prediction model such as MSE, RMSE, and MAPE. According to the results of the error obtained, prediction can be compared effectively. The

Table 1. Parameters involved for analysis

Dependent variable	Independent variable
pH	Rainfall
EC	Water level
Na	Population
K	Year
SO4	Temperature
TH	Humidity
Ca	Wind speed
Cl	Evaporation

Table 2. Permissible limit as per BIS

Minerals	Permissible limit (mg/L)
pH	6.5-8.5
EC	1000 μS/cm
Ca	75
Na	50
K	20
Mg	30
F	1
Cl	250
TH	200
NO_3	45
SO_4	200
HCO_3	120

prediction results can be used to analyze the future accumulation of minerals and thereby mitigating groundwater contamination. The detailed research methodology is presented as a flow chart in Figure 2.

Artificial neural network: Upon the selection of minerals based on high correlation with the variables, further analysis is carried out initially using an artificial neural network. Usually, a correlated value with a factor above 0.75 is considered as a highly correlated value and if it is 1, then those are very effective in prediction therefore the parameters which have a correlation factor above 0.75 are considered for further process. Correlated factors are selected based on formula 1 in which x, y is an

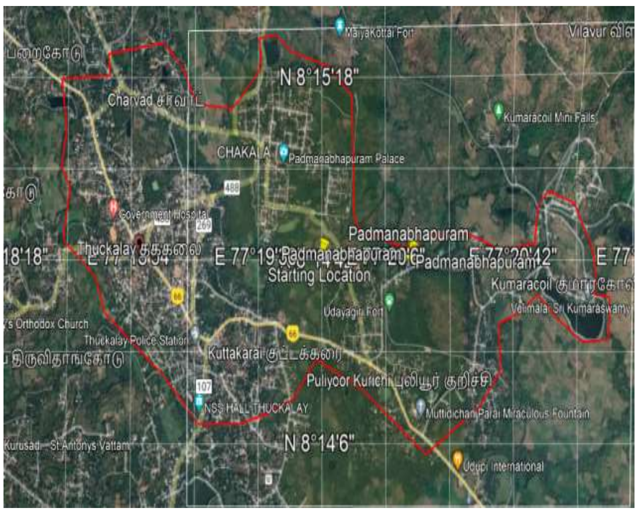

Fig. 1. Study area from Google earth (8.1444N & 77.1855E)

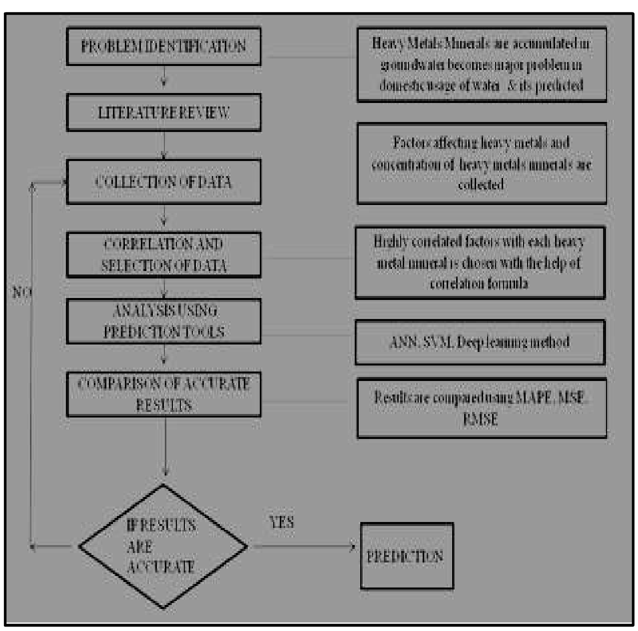

Fig. 2. Research methodology process chart

independent/dependent data and x's, y' is an average value of the data.

$$Correl\ (x, y) = \frac{\Sigma(x - x')(y - y')}{sqrt\ [\Sigma(x - x')^2\ \Sigma)(y - y')^2\ ]} .....(1)$$

The neural network tool seems to work as an analytical tool in this investigation that improved the accuracy in an efficient way for a lot of prediction models much similar to a previous investigation (Cetkovic et al 2018).

Support vector machine: Among the statistical methods, SVM is a proposed model and its learning process is used in finding prediction functions (Kramer et al 2011). The tool assigns to the class of Kernel methods is SVM. Time series analysis is adapted to use historical data (Zeng et al 2012). Since ANN shows better accuracy and perfect results, it is involved to predict output in various criteria whereas ANN also noted to have limitations in a few cases which show some inaccuracy in its results. Therefore, to overcome those disadvantages SVM tool is introduced in some cases (Zendehboudi et al 2018). The working process of SVM is presented in Figure 4.

Generally, SVM is classified into two methods namely the least square SVM and ƐSVM which were based on

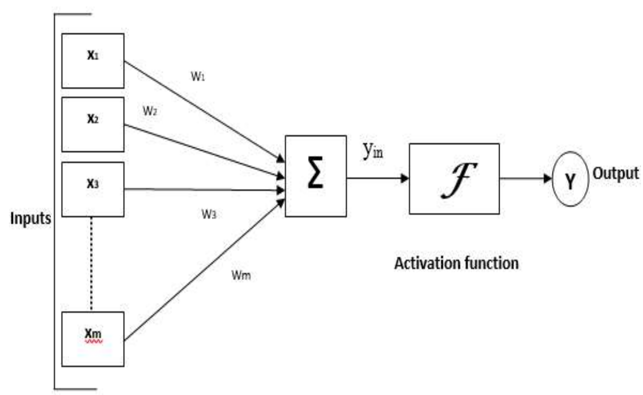

Fig. 3. Model of artificial neural network

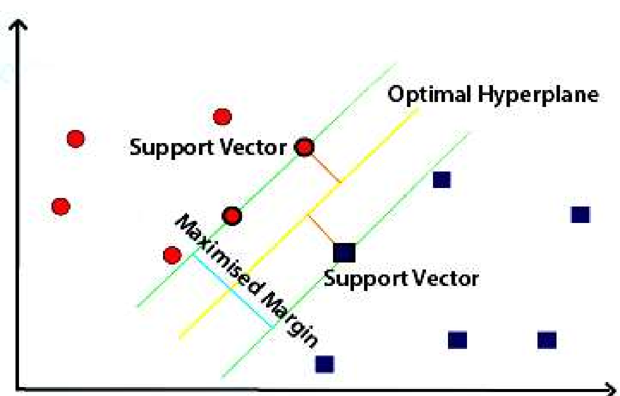

Fig. 4. Support vector machine working process

augmentation problem functions (Zeng et al 2012). Upon the prediction of wind power, SVM and ANN are then compared for results as well as better accuracy shown by SVM (Giorgi et al 2014). In this paper, the prediction of mineral accumulations was carried out with the help of the SVM technique, whereas the comparison is done with ANN and SVM results.

Deep learning: Deep learning is considered an important subset of all machine learning techniques and its models are set with the aid of neural networks. Neural networks intake input data which are processed in hidden layers and then are adjusted in the training model. Furthermore, the model takes into prediction and adjusted weights are used to make better results in prediction. The deep learning process includes a deeper level of knowledge as well as learning that takes place in two phases such as 1) nonlinear transformation of input with the output of statistical model 2) with the mathematical method, upon which the model is improved (Ingle et al 2021). A deep network with multiple layer process is shown in Figure 5.

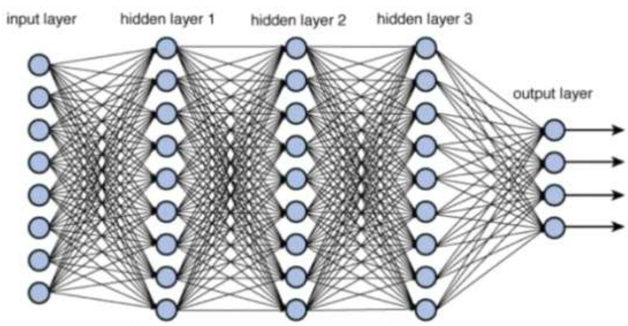

Fig. 5. Deep network with multiple layers

Complex and nonlinear relations that are hidden within huge data can be defined by deep learning algorithms. These algorithm works on the principle of neural networks which is composed of many layers (Patterson et al 2017). A neural network becomes complicated when it gets mixed by adding many weights in sub-layers which is called as deep. Some projects have used even more than 128 layers (Kumar et al 2020). Deep learning is found to be a trending method in machine learning because it executed few expected results where the processing function seems to be complex and the data used were very large (Ingle et al 2021). Conventional algorithms are surpassed by the deep learning method in terms of accuracy for most of the data types with less tuning and human works (Rajendrakumar et al 2019). Hence this study thrives to deal with the prediction of minerals accumulation for apposite results.

RESULTS AND DISCUSSION

MSE, RMSE, and MAPE are the errors that are used for developing the comparative analysis in this prediction. On comparing all the results, SVM shows more accurate results than neural networks and deep learning. Though all three techniques showcased an increased rate of mineral accumulation, SVM predicted the data with more accuracy. Table 3 shows the results of prediction tools whereas Figure 6 series presents the details of the relationship between the dependent variables and independent variables. The X-axis represents the independent variables whereas the Y-axis represents the dependent variables, such as pH, EC, Calcium, Chloride, Potassium, sodium, sulfate, total hardness.

The annual rainfall values are highly correlated with the mineral values in which the decreasing trend shows the mineral values when rainfall is higher and vice versa (Figure 6). An alternate location for safe disposal after proper segregation and appropriate treatment is mandatory for mitigating the further pollution of the study area. The best prediction tools are identified using MAPE, MSE, RMSE, and MAD. The line of best fit of data points is measured using MSE (Table 3). The smaller value of RMSE indicates the higher accuracy of the best fit for the data points. The behavior of MAPE and MAD remained much similar throughout the study. The difference between the actual and predicted values deviation is calculated using MAD and percentages were calculated using MAPE. The Prediction error and accuracy is measured widely using MAPE.

$$MAPE = \frac{100}{n}\Sigma_i^n\left(\frac{A-P}{P}\right)\text{.........}\ \text{...}(2)$$

$$MSE = \frac{1}{n}\Sigma_i^n(A-P)^2\text{..........}\ \text{..}(3)$$

$$RMSE = Sq.rt\left(\frac{1}{n}\Sigma_i^n A-P\right)^2\text{..........}\ \text{..}(4)$$

$$MAD = \frac{1}{n}\Sigma_i^n\left|A-P\right|\text{..........}\ \text{..}(5)$$

Where

n is a no of data

Table 3. Permissible limit and level of positioning

Minerals	Permissible limit	Increasing level
pH	6.5-8.5	Moderate
EC	0-800	Fluctuating & increase
Ca	75	Moderate
Na	50	Increasing
K	20	Fluctuating & increase
Cl	250	Extremely high
TH	200	Extremely high
SO_4	200	Increasing

A is an actual value

P is a predicted value

For the prediction analysis in this study, the average value of MAPE, MSE, and RMSE values of different minerals was chosen. These error values (Table 4) are compared with the results of three prediction tools and the average values are presented in table 3. The detailed value of error for the individual parameters obtained through prediction is given in Table 5.

The predicted groundwater mineral values using Artificial Neural Network, Support Vector Machine, and Deep

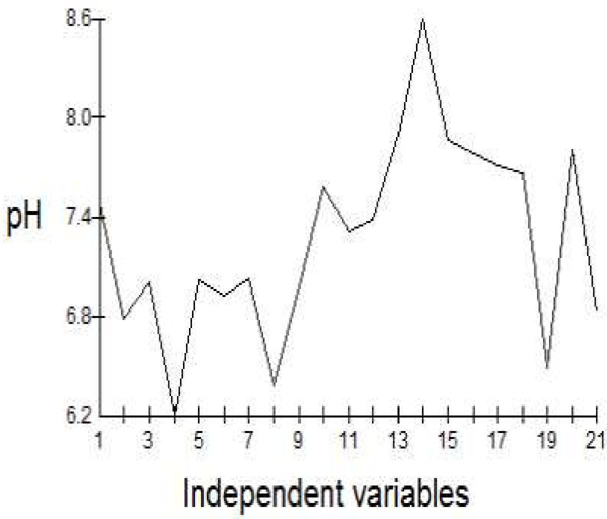

Fig. 6.1. Relationship between the dependent variables and independent variables for pH

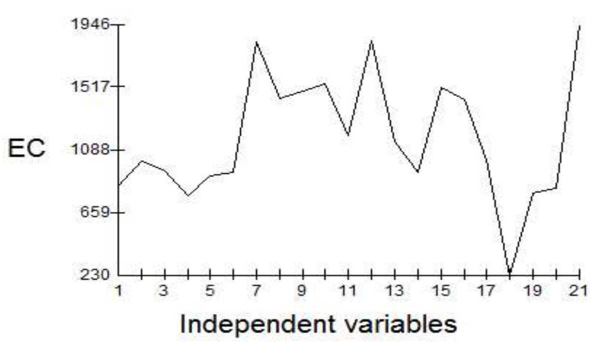

Fig. 6.2. Relationship between the dependent variables and independent variables for EC

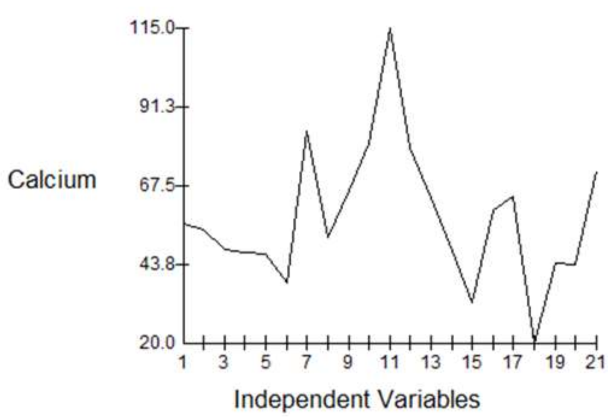

Fig. 6.3. Relationship between the dependent variables and independent variables for calcium

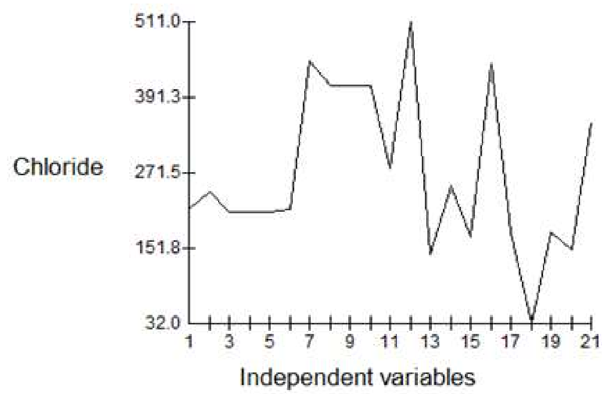

Fig. 6.4. Relationship between the dependent variables and independent variables for chloride

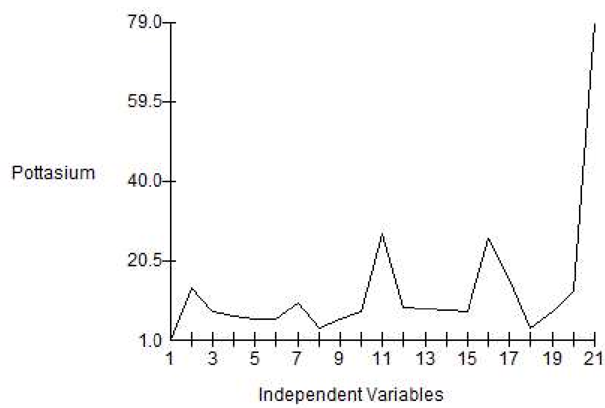

Fig. 6.5. Relationship between the dependent variables and independent variables for potassium

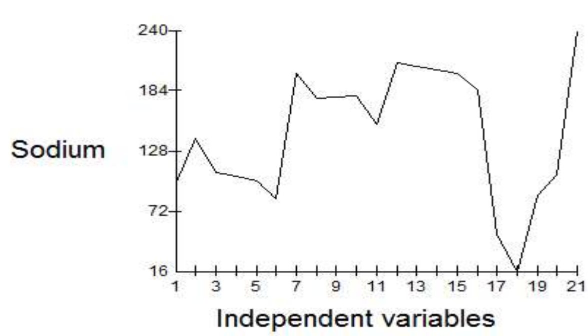

Fig. 6.6. Relationship between the dependent variables and independent variables for sodium

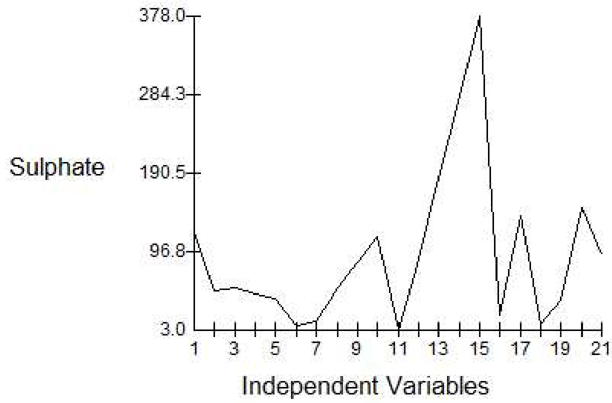

Fig. 6.7. Relationship between the dependent variables and independent variables for sulphate

Table 4. Error-values comparison for different tools

Error	Parameters	ANN	SVM	DL
MSE	pH	106.32	63.20	136.90
	EC	112.81	61.11	133.48
	Ca	109.76	62.97	132.73
	Na	110.49	70.34	140.67
	K	108.51	66.28	140.16
	Cl	107.37	63.83	138.25
	TH	113.92	61.72	134.79
	SO_4	109.55	65.04	138.98
RMSE	pH	10.62	7.82	11.55
	EC	10.32	8.12	13.27
	Ca	9.60	7.53	11.99
	Na	10.95	7.02	10.53
	K	10.98	8.54	15.17
	Cl	11.07	9.13	13.06
	TH	11.42	8.20	8.58
	SO_4	10.42	8.20	13.40
MAPE	pH	4.80	4.96	7.37
	EC	6.92	2.98	7.40
	Ca	4.72	3.46	7.51
	Na	5.67	2.99	8.86
	K	7.04	4.24	6.43
	Cl	4.85	5.00	7.44
	TH	6.99	3.01	7.47
	SO_4	6.01	4.74	6.50

Table 5. Value of error for the individual parameters

Prediction tools	Artificial neural network	Support vector machine	Deep learning network
MSE	109.84	64.31	137
RMSE	10.67	8.07	12.19
MAPE	5.88	3.92	7.37

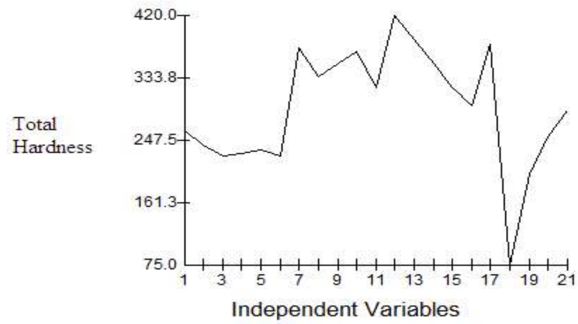

Fig. 6.8. Relationship between the dependent variables and independent variables for total hardness

Table 6. Predicted groundwater mineral values using ANN, SVM and DL

Parameter	Year	ANN	SVM	DL
pH	2021	7.75	7.74	8.28
	2022	7.79	7.78	8.32
	2023	7.83	7.81	8.36
	2024	7.87	7.85	8.40
	2025	7.91	7.89	8.44
EC	2021	1302.63	1278.52	1320.96
	2022	1308.66	1284.44	1327.08
	2023	1314.70	1290.36	1333.20
	2024	1320.73	1296.28	1339.32
	2025	1326.76	1302.20	1345.43
Ca	2021	58.57	57.48	59.39
	2022	58.33	57.25	59.15
	2023	58.09	57.02	58.91
	2024	57.86	56.78	58.67
	2025	57.62	56.55	58.43
Na	2021	163.08	160.06	165.37
	2022	164.03	161.00	166.34
	2023	164.99	161.93	167.31
	2024	165.94	162.87	168.28
	2025	166.90	163.81	169.25
K	2021	27.89	27.37	28.28
	2022	29.15	28.61	29.56
	2023	30.42	29.86	30.85
	2024	31.69	31.10	32.13
	2025	32.95	32.34	33.41
Cl	2021	254.75	250.04	258.34
	2022	252.04	247.37	255.58
	2023	249.32	244.70	252.83
	2024	246.60	242.04	250.07
	2025	243.88	239.37	247.32
TH	2021	313.71	307.90	318.12
	2022	314.10	308.29	318.52
	2023	314.50	308.68	318.92
	2024	314.89	309.06	319.32
	2025	315.29	309.45	319.72
SO_4	2021	147.96	145.22	150.04
	2022	152.39	149.57	154.54
	2023	156.82	153.92	159.03
	2024	161.25	158.27	163.52
	2025	165.68	162.61	168.01

Learning were observed to degrade the groundwater quality further and therefore apt suggestions were proposed (Table 6). Based on these error accuracy reports, the future value can also be predicted to control groundwater contamination in the future.

CONCLUSIONS

Based on the results obtained for the prediction of minerals in groundwater using Artificial Neural Network (MSE-109.84, RMSE-10.67, MAPE-5.88), Support Vector Machine (MSE-64.31, RMSE-8.07, MAPE-3.92), and Deep Learning (MSE-137, RMSE-12.19, MAPE-7.37) the following conclusions were obtained:

- An increased rate in the concentration of minerals over years is observed.
- Considering the number of data available and correlated data, SVM performed well with less error with the predicted values. (MSE-64.31, RMSE-8.07, MAPE-3.92)
- Since the foundation of minerals seems to be fluctuating as well as increasing, this results in serious harm to the ecosystem.
- This predicted mineral accumulation aids in creating awareness among the nearby residents and visitors to secure the groundwater quality, in the study area.
- The annual rainfall values are highly correlated with the mineral values in which the decreasing trend shows the mineral values when rainfall is higher and vice versa.

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