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Research Article

The Performance of Artificial Neural Network Approaches to Estimate the Nitrate Concentration in Groundwater

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Abstract

The estimation of the pollution concentration in groundwater is important, since it is one of the key resources of water supply. Nitrate (NO3-N) is one of the well-known indicator parameters in groundwater pollution. Using historical data, artificial neural networks can be utilized to estimate the nitrate concentration in groundwater. In this study, a sample dataset, which is derived from a survey analysis in the literature, is used to estimate the nitrate concentration of groundwater (i.e., target parameter) with respect to six different well characteristics (i.e., input parameters). The effect of different hydrogeological parameters of the wells on the nitrate concentration is focused for the first time in this study. The performance of two different ANN approaches, namely BPNN and GRNN, is evaluated comparatively by means of their regression performances. Considering regression results of ANN models, it can be concluded that the GRNN (R=0.99) algorithm works slightly better than the BPNN (R=0.98) algorithm with this dataset. Correlation results indicate that the most important characteristics of the wells to estimate the nitrate pollution are the well depth, depth below water table, clay above screen, and depth to well screen, respectively. Moreover, all these characteristics are inversely related to nitrate concentration of the well.

Keywords: Groundwater, Nitrate Pollution, Artificial Neural Network, Regression, BPNN, GRNN.

Yapay Sinir Ağı Yaklaşımlarının Yeraltı Suyundaki Nitrat Konsantrasyonunu Tahmin Etme Performansı

Öz

Su temininde temel kaynaklardan olduğu için yeraltı suyundaki kirlilik konsantrasyonunun tahmini önemlidir. Nitrat (NO3-N) yeraltı suyu kirliliğinde iyi bilinen gösterge parametrelerinden birisidir. Yapay sinir ağları (YSA) geçmiş veriler kullanılarak yeraltı suyundaki nitrat konsantrasyonunu tahmin etmek için kullanılabilir. Bu çalışmada, literatürdeki bir kuyu analizinden türetilen örnek bir veri seti, altı farklı kuyu özelliğine (girdi parametrelerine) göre yeraltı suyunun nitrat konsantrasyonunu (hedef parametre) tahmin etmek için kullanılmıştır. Kuyuların farklı hidrojeolojik parametrelerinin nitrat konsantrasyonu üzerindeki etkisine ilk kez bu çalışmada dikkat çekilmiştir. BPNN ve GRNN olmak üzere iki farklı YSA yaklaşımının performansı, regresyon performansları üzerinden karşılaştırmalı olarak değerlendirilmektedir. YSA modellerinin regresyon sonuçlarına bakıldığında, bu veri seti ile GRNN (R=0.99) algoritmasının BPNN (R=0.98) algoritmasından biraz daha iyi çalıştığı sonucuna varılabilir. Korelasyon sonuçları, nitrat kirliliğini tahmin etmek için kuyuların en önemli özelliklerinin sırasıyla kuyu derinliği, su tablasının altındaki derinlik, elek üstü kil ve kuyu ızgarasına derinlik olduğunu göstermektedir. Ayrıca tüm bu özellikler kuyunun nitrat konsantrasyonu ile ters orantılıdır.

Anahtar Kelimeler: Yeraltı Suyu, Nitrat Kirliliği, Yapay Sinir Ağı, Regresyon, BPNN, GRNN.

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1. Introduction

Groundwater is the most important drinking water supply throughout the world, especially where the water resources are limited or polluted. In general, groundwater supplies roughly half of all drinking water in the world [1]. Additionally, the groundwater contributes to surface water resources through the watershed. Agricultural practices, especially excessive use of fertilizers, causes the largest diffusion threat to groundwater quality on a global scale [2-3]. Since the nitrate (NO3-N) is one of the main groundwater pollutants and can directly affect human health, it is important to evaluate the nitrate concentration in groundwater.

The natural nitrate concentration in groundwater under aerobic conditions is very low (a few milligrams per liter) and relies upon heavily on soil type and on the geological situation [4]. However, it can rise high levels through agricultural runoff, refuse dump runoff, or contamination with human or animal wastes [2]. Wells, drilled into the aquifers, enable the groundwater to be pumped out. Hence aquifer/well characteristics are other important parameters affecting the nitrate concentration in groundwater. There are different driving parameters affecting the nitrate concentration in groundwater [5]. They can be chemical or hydrogeological variables. The well depth, depth to static water table, clay above screen, well density, depth to well screen, and depth below water table (i.e., depth to groundwater) can be classified as hydrogeological variables. The depth to static water table measures the depth to groundwater level and it is being a proxy to the time that contaminants require to reach the aquifer [6]. Higher density of wells means the spatial pattern of irrigation return and more pollutant leachate into the soil and groundwater consequently [5]. Higher density areas are where potential impacts to groundwater quantity and quality will be the greatest. The potential for groundwater pollution usually increases by lower depth to groundwater [5]. It is also known that groundwater pollution in clayey formations is higher than in well-drained sandy plains [7]. Wells with long screen lengths may facilitate cross-contamination between contaminated zones [8].

Artificial neural networks (ANNs) present an information-processing paradigm for pattern recognition which is generally used in situations where the relationships between data are not very complex and linear [9-10]. ANNs use input-output response patterns to estimate the underlying governing rules of the output responses considering specific inputs in a convoluted physical space [9]. The aim of the training process for ANNs is to calculate the optimal weights of the links in the neural net by minimizing the overall prediction error which is known as empirical risk minimization [9]. Different machine learning models have been investigated to estimate the groundwater nitrate concentration in the literature. Table 1 represents the summary of the reviewed studies reporting the implementation of machine learning models, namely ANN and SVM, for the purpose of nitrate concentration estimation in groundwater.

Different physical, chemical, and hydrogeological parameters can be used as input variables to estimate the nitrate concentration in groundwater. Considering research remarks of the reviewed studies, it can be concluded that the applied models are robust with promising results.

In this study, a sample dataset, which is derived from a survey analysis in the literature, is used to estimate the nitrate concentration of groundwater (i.e., target parameter) with respect to six different well characteristics (i.e., input parameters). The effect of different hydrogeological parameters of the wells on the nitrate concentration is focused for the first time in this study. The performance of two different ANN approaches is evaluated comparatively by means of their regression performances. The backpropagation neural network (BPNN) and the generalized regression neural network (GRNN) were chosen as ANN approaches for this study. A multilayer perceptron (MLP) is a class of feedforward ANN which utilizes a supervised learning method for training called backpropagation (BP). A MLP neural network trained by BP algorithms, also known as the BPNN, is the most typical type of ANN which is broadly employed in environmental pollution controls [25]. GRNN as a special variation of the radial basis function neural network is being used in the field of environmental pollution controls as well [24]. Relying on nonlinear Gaussian kernel regression, a GRNN has strong nonlinear mapping ability and is able to get decent results even when the data is ambiguous [24].

Table 1. The summary of the reviewed studies reporting the implementation of machine learning models (ANN and SVM)

Reference	Case study region	Applied models	Performance metrics
[11]	Sangamon River, USA	BPNN, RBFNN	RMSE
[12]	Harran Plain, Turkey	MLP with BP and Levenberg–Marquardt	R-value, MSE
[13]	Kutahya, Turkey	BPNN	MSE, MAPE
[14]	Kadava River basin, Nashik, Maharashtra, India	MLP with Levenberg–Marquardt	R^2, RMSE, MARE
[15]	Shandong, China	BPNN	R-value
[16]	Northern part of Iran	BPNN, RBFNN	MSE
[17]	Central Valley, California	BRT, ANN, Bayesian networks	R^2
[18]	Bethune, France	MLP with BP	R-value
[19]	African continent	RFR, MLR	R^2
[20]	Marvdasht watershed, Iran	SVM, Cubist, random forest, Bayesian-ANN	R^2, MAE, RMSE, Nash–Sutcliffe efficiency (NSE)
[21]	Gaza Strip, Palestine	MLP, RBFNN	RMSE, R-value, MAE
[22]	Gaza Strip, Palestine	MLP with BP and Levenberg–Marquardt, SVM	R-value, MAPE, NSE
[23]	Gaza Strip, Palestine	MLP, RBF, GRNN, and linear networks.	R-value
[24]	Arak plain, Iran	SVM	RMSE

2. Material and Method

The sample well survey data used in this study is adapted from a study in the literature [26]. Table 2 represents the nitrate concentration (NO3-N, mg/L) levels of different wells with respect to different well characteristics. Although there are different supervised machine learning approaches for regression, BPNN and GRNN are chosen for this study. Hydrogeological variables such as the well depth, depth to static water table, clay above screen, well density, depth to well screen, and depth below water table are considered potential factors influencing nitrate contamination in this study. Hence these six parameters are utilized as the input parameters whereas the NO3-N concentration is used as the target parameter.

Table 2. Sample well survey analysis

Well No	Well depth (m)	Depth to static water table (m)	Clay above screen (m)	Well density	Depth to well screen (m)	Depth below water table (m)	NO3-N (mg/L)
1	10.9	3.9	0.3	1.0	7.6	3.6	11.5
2	31.7	3.6	4.8	1.0	19.5	15.9	3.8
3	23.7	6.4	14.0	1.0	14.6	8.2	4.0
4	17.3	5.5	3.9	1.0	14.3	8.8	5.2
5	27.4	3.0	13.1	4.0	21.3	18.3	1.7
6	14.0	2.4	2.1	2.0	7.9	5.5	5.9
7	28.0	3.9	14.6	1.0	18.5	14.6	3.6
8	8.9	1.8	4.3	1.0	58.8	4.0	3.4
9	12.2	2.1	2.7	1.0	6.1	4.0	6.3
10	16.7	3.9	3.6	3.0	13.7	9.8	8.1
11	21.0	4.5	0.0	3.0	17.0	12.5	1.8
12	19.8	6.1	9.1	5.0	13.7	7.6	8.3
13	18.6	5.7	10.9	1.0	15.5	9.8	2.5
14	36.6	8.2	17.6	2.0	24.3	16.1	2.5
15	15.8	6.7	9.1	2.0	12.8	6.1	7.9
16	18.3	4.2	7.3	4.0	7.9	3.7	2.5
17	13.7	4.3	6.1	4.0	10.6	6.3	9.9
18	25.6	6.4	9.1	1.0	14.6	8.2	3.6
19	18.3	4.5	5.5	2.0	12.2	7.7	8.8
20	18.3	7.9	11.2	0.0	15.2	7.3	5.2
21	18.3	5.8	9.4	0.0	13.4	7.6	1.3
22	21.0	5.5	12.5	1.0	17.9	12.4	4.0
23	41.2	7.0	10.3	3.0	21.3	14.3	3.8
24	28.6	7.6	20.1	1.0	22.5	14.9	5.9
25	16.7	6.7	9.1	1.0	14.3	7.6	6.3
26	18.3	7.3	9.1	2.0	12.2	4.9	5.9
27	18.3	8.2	5.2	2.0	12.2	4.0	3.4
28	31.4	9.1	9.4	3.0	19.2	10.1	4.7
29	21.3	6.4	10.3	5.0	18.2	11.8	9.5
30	25.9	5.2	20.7	3.0	23.2	18.0	1.4
31	26.5	7.3	10.6	2.0	20.4	13.1	2.9
32	11.5	3.6	4.8	5.0	10.3	6.7	7.6

In BPNN method, data preprocessing is performed using minimum-maximum normalization which preserves the relationship between the original data [27]. The raw data is normalized before directing to training and testing through altering the data to the range of 0 to 1 to increase the speed and accuracy of ANN performance [28]. As stated in Table 2, six input parameters and one target parameter are used to perform the BPNN algorithm using MATLAB®.

The number of hidden layers and output layer are used in BPNN approach are given in Fig 1. The BPNN model is trained using the Levenberg-Marquardt function. Performance of the algorithm is determined using MSE parameter and the number of epochs is chosen as 40,000. The construction of the network (the number of neurons in hidden layers) are decided by trial and error.

As another approach GRNN is applied to the same dataset (raw data) including six input parameters and one target parameter using MATLAB®. The results of two different algorithms are compared by means of their R-values.

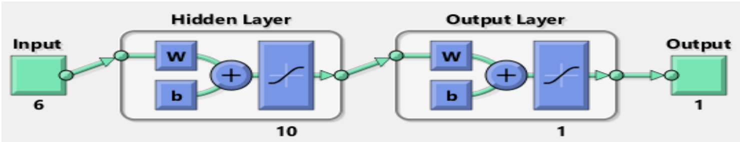

Fig 1. The architecture of the network

3. Results and Discussion

Linear regression analysis is performed for training, validation, and testing, to evaluate the relation among the outputs of the network and the targets. The training, validation, and test results of BPNN algorithm are given in Fig 2 with corresponding R-values.

In each plot, the dashed line describes the ideal result (i.e., outputs=targets), while the solid line presents the best fit linear regression. As the R-value reaches to 1, then there is an exact linear relationship. The regression results (i.e., R-values) are 0.98, 0.98, and 0.97 for training, validation, and test, respectively. Those results are approaching to a total response of 0.98.

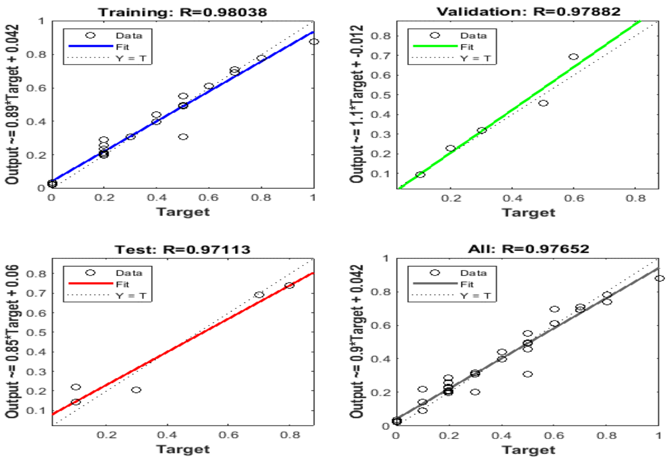

Fig 2. The training, validation, and test results of BPNN algorithm

The best validation performance of the model is given in Fig 3. In general, there is no correct value for MSE. The lower value is better and zero means the model is perfect and the predicted values are equal to measured values [29]. Considering R-values in Fig 2 and the MSE value (MSE=0.0024) in Fig 3, it can be concluded that the results of BPNN algorithm are promising for the estimation of nitrate concentration levels of wells if the hydrogeological parameters of the well are specified.

The result of GRNN algorithm is given in Fig 4. Considering regression results (R=0.99) in the Fig 4, it can be concluded that GRNN algorithm works slightly better than BPNN algorithm with this dataset.

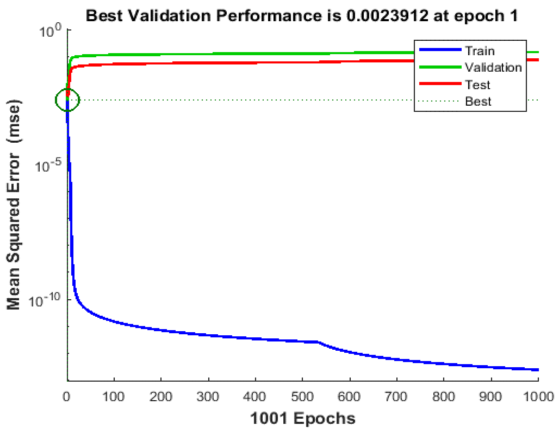

Fig 3. The best validation performance of the model

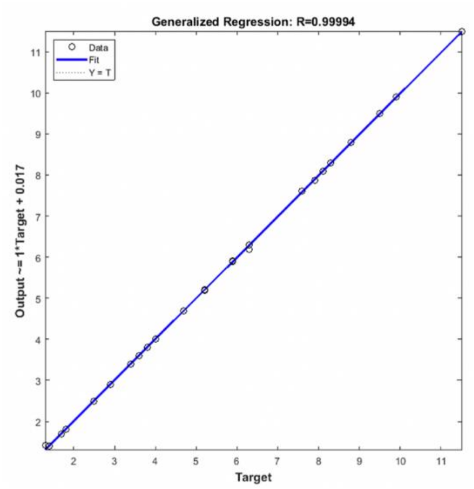

Fig 4. The result of GRNN algorithm

The R-values obtained in this study correlate with the literature values related to the nitrate concentration estimation using ANN approaches which are ranging from 0.58 to 0.99 [12-13, 16, 21-22, 24, 29, 32, 34]. Similarly, the MSE values also correlate with the literature values in the range of 0.001-0.121 [12-13, 17, 19, 24, 29-31, 33].

To interpret the effect of different characteristics of the well on the nitrate concentration, the raw data (Table 2) is utilized to prepare the correlation (Fig 5) and the correlation matrix (Table 3).

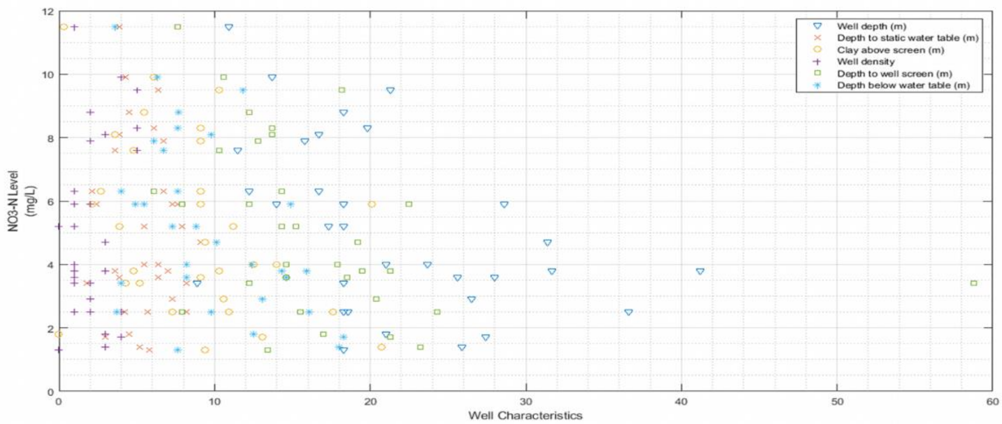

Fig 5. The correlation between well characteristics and NO3-N concentration

The correlation graph and correlation matrix are prepared using the MATLAB® and MS Office Excel software, respectively.

Considering Fig 5 and Table 3, it can be concluded that the most important characteristics of the wells to estimate nitrate pollution are the well depth, depth below water table, clay above screen, and depth to well screen respectively. Moreover, all these characteristics are inversely related to nitrate concentration of the well.

Table 3. The correlation matrix

	Well Depth (m)	**Depth to Static Water Table (m)**	**Clay Above Screen (m)**	**Well Density**	**Depth to Well Screen (m)**	**Depth below Water Table (m)**	**NO3-N (mg/L)**
Well Depth (m)	1						
Depth to Static Water Table (m)	0.4805	1					
Clay Above Screen (m)	0.5931	0.4847	1				
Well Density	0.0358	-0.0865	-0.0567	1			
Depth to Well Screen (m)	0.1735	-0.0771	0.2409	-0.1175	1		
Depth below Water Table (m)	0.7826	0.1511	0.6242	0.1020	0.2806	1	
NO3-N (mg/L)	-0.4598	-0.1077	-0.3749	0.2556	-0.3531	-0.4384	1

4. Conclusions and Recommendations

The results of two different ANN models are promising for the estimation of nitrate concentration levels of wells if the hydrogeological parameters of the well are specified. Considering regression results of ANN models, it can be concluded that GRNN (R=0.99) algorithm works slightly better than BPNN (R=0.98) algorithm with this dataset. Correlation results represent that the most important characteristics of the wells to estimate nitrate pollution are the well depth, depth below water table, clay above screen, and depth to well screen, respectively. Moreover, all these characteristics are inversely related to nitrate concentration of the well.

In conclusion, this study offers the nitrate concentration estimation based on hydrogeological parameters rather than water quality analysis parameters in contribution to the literature and confirms the applicability of ANN approaches in this area with different types of well parameters. Although a small dataset is used as a demonstration in this preliminary study, these ANN approaches can be applied to large datasets as well. The results can be improved after refining the input parameters using correlation as pre-modeling technique in addition to the normalization of the data.

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