

Adaptive Network-based Fuzzy Inference System-Genetic Algorithm Models for Prediction Groundwater Quality Indices: a GIS-based Analysis

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Abstract

The prediction of groundwater quality is very important for the management of water resources and environmental activities. The present work has integrated a number of methods such as Geographic Information Systems (GIS) and Artificial Intelligence (AI) methodologies to predict the groundwater quality in Kerman plain (including HCO_3^- concentrations and Electrical Conductivity (EC) of groundwater). In this research work, we investigate the abilities of the Adaptive Neuro Fuzzy Inference System (ANFIS), hybrid of ANFIS with Genetic Algorithm (GA), and Artificial Neural Network (ANN) techniques, and predict the groundwater quality. Various combinations of monthly variability, namely rainfall and groundwater levels in the wells, were used by two different neuro-fuzzy models (standard ANFIS and ANFIS-GA) and ANN. The results obtained show that the ANFIS-GA method can present a more parsimonious model with a less number of employed rules (about 300% reduction in the number of rules) compared to the ANFIS model and improves the fitness criteria and so the model efficiency at the same time (38.4% in R^2 and 44% in MAPE). This work also reveals the groundwater level fluctuations and rainfall contribution as two important factors in predicting indices of groundwater quality.

Key words: *Indices of Groundwater Quality, GIS, Genetic Algorithm, Neuro-Fuzzy, ANN.*

1. Introduction

Groundwater quality parameters are considered as serious issues in Iran, especially in areas of high-intensity agriculture and residence like Kerman plain. The impact of industrial effluents is also responsible for the deterioration of the physical, chemical, and bio-chemical parameters of groundwater [1]. Knowledge of water chemistry is important in assessing the quality of aquatic resources in order to understand its suitability for various needs. Factors controlling groundwater chemical parameters in aquifer may include water table fluctuations, factories or cities, topographic setting around the well, potential point sources near the well, and amount of rainfall. The development of optimal environmental management to prevent future groundwater contamination obviously requires knowledge of concentrations of chemical parameters such as Na^+ , Ca^{2+} , Mg^{2+} , Cl^- , HCO_3^- , and SO_4^{2-} and Electrical Conductivity (EC) of groundwater. Various numerical models are available for

predicting groundwater quality [2,3,4,5]. These models require physical descriptions concerning the porous media, suitable initial and boundary conditions for flow and transport processes, and the reactions occurring between soil and the porous matrix. Accurate quality prediction is beyond the capabilities these models provide, since the complex interaction between soil and the contaminants, the heterogeneity in physical and chemical properties of soil, and the uncertainty in estimating regional flow and transport parameters are difficult to account for in these models [2]. Although many of the models provide the required mathematical complexities to account for flow and transport processes, well-characterized soil, geology, and climatic data are not available in regional settings especially in Iran. Therefore, alternative methods are needed to predict groundwater quality from the available information. Adaptive neuro fuzzy inference system (ANFIS) and artificial neural network

(ANN) and hybrid of them with meta-heuristic optimization methods have been used for modeling and predicting non-linear and complex environmental problems such as water and air quality and quantity with reasonable accuracy [6,7,8]; Artificial intelligence methods are non-linear modeling tools, and do not need an explicit formulation of the physical relationship of the problem. In the recent years, successful applications of soft computing techniques in water engineering have been widely published[9,10]. The objectives of the present investigation include: (1) to examine the applicability of a hybrid model (ANFIS-GA) as a tool to predict the chemical parameters of groundwater (2) to examine the impact of input parameters on groundwater quality through sensitivity analysis of the parameters used in the hybrid model.

2. Materials and methods

In this research work, the following general equation was considered for predicting the concentration of chemical parameters in water:

$$Parameter_{t+1} = F_{non} (X, Y, L_t, L_{t-1}, R_t, R_{t-1}) \quad (1)$$

in which: X, Y: UTMX and UTM Y coordination of the observed wells, respectively, R_t : monthly rainfall in the time step of t at the location of wells, R_{t-1} : monthly rainfall in the time step of $t-1$: observed rainfall values were interpolated by inverse distance weighted method in GIS environment to find rainfall values at location of wells in two mentioned time steps. L_t : level of water in the well in the time step of t , L_{t-1} : level of water in the well in the time step of $t-1$. The three different models of ANN, ANFIS, and ANFIS-GA were employed in order for the extraction of F_{non} non-linear function for each one of the chemical parameters.

Two different types of standard statistics were considered in the statistical performance evaluation.

The correlation coefficients (R^2) and mean absolute percentage error (MAPE) were used. The two performance evaluation criteria used in this work can be calculated utilizing the following equations:

$$R^2 = \left(\frac{\sum_{i=1}^n (H_i^o - \bar{H}_i^o)(H_i^p - \bar{H}_i^p)}{\sqrt{\left[\sum_{i=1}^n (H_i^o - \bar{H}_i^o)^2 \right] \left[\sum_{i=1}^n (H_i^p - \bar{H}_i^p)^2 \right]}} \right)^2 \quad (2)$$

$$MAPE = \frac{1}{n} \sum_{i=1}^n \left| \frac{H_i^p - H_i^o}{H_i^o} \right| \quad (3)$$

where, H_i^o is the observed value at the present time, H_i^p is the predicted value and n is the number of values. The best fit between calculated values would have, respectively, been $R^2=1$ and $MAPE=1$.

2.1. Artificial neural networks

Artificial neural networks (ANNs) are widely used for simulation of cases where deterministic models are not available or fail in fitting the data. The model is known to be generic and it can be used for a variety of problems with minor adaptations. ANN learns the data pattern using an algorithm known as “training”, where many data rows [input/output] are presented to the net until it fits the data. Details about the neural network algorithm features and training process may be found in [11].

The structure of all network models that are used in this work are Multilayer Perceptron (MLP) with log-sigmoid and pure line functions as activation functions in hidden and output layers respectively. All networks are trained by Levenberg Marquardt (LM) training algorithm and the number of epochs wereset to 150.

2.2. Neuro-fuzzy structure

ANFIS is a multi-layer feed-forward network which uses neural network learning algorithms and fuzzy reasoning to map inputs into an output. Indeed, it is a fuzzy inference system (FIS) implemented in the framework of adaptive neural networks. As it can be seen in figure1, the architecture of a typical ANFIS consists of five layers. For simplicity, a typical ANFIS architecture with only two inputs leading to four rules and one output for the first order Sugeno fuzzy model is expressed [12,13].

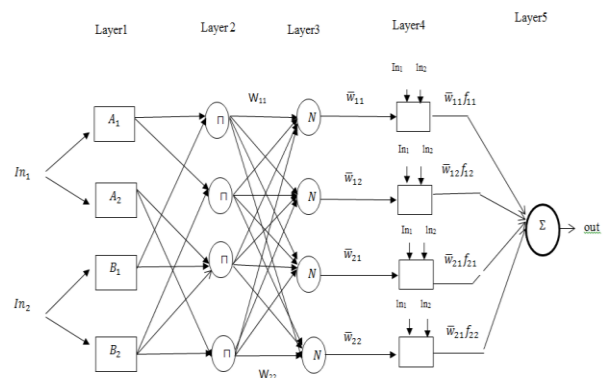


Figure 1. A typical ANFIS architecture for a two-input Sugeno model with four rules.

It is also assumed that each input has two associated membership functions (MFs). It is clear that this architecture can be easily generalized to our preferred dimensions. The detailed algorithm and mathematical background of the hybrid learning algorithm can be found in Reference [14].

2.3. Proposed method

A hybrid of canonical real-coded GA, subtractive clustering and ANFIS is utilized in order to produce suitable approximate fuzzy models in terms of accuracy and parsimony. The main modeling procedure is an optimization task performed by GA, where both the accuracy and compactness of fuzzy models are subjects of optimization simultaneously. The overall optimization process by GA consists of four steps, namely, 1- Fitness assignment 2- Selection 3- Crossover 4- Mutation. Generating a fuzzy model based on subtractive clustering method is carried out in the fitness assignment part of GA. The flow chart for modeling procedure is given in figure 2.

Subtractive clustering method can be used for generating a TSK fuzzy model in which the number of rules (i.e. the number of clusters) can be determined through radii parameters dedicated into dimensions. These radii are used for generating clusters. Each cluster represents a rule and regarding to the fact that clustering is carried out in multidimensional space, fuzzy sets for each rule must be obtained. The centers of MFs are obtained by projecting the center of each cluster in the corresponding dimension. The widths of MFs for each dimension are obtained on the basis of radius r_d that is considered for that dimension. Therefore, each chromosome in this work encodes radii values for all dimensions (inputs and outputs) of a fuzzy model. These radii of fuzzy model are then employed by subtractive clustering for generating a Takagi-Sugeno-Kang (TSK) Fuzzy-Inference- System (FIS).

2.4. Simulation setup

After testing different sets of parameters in order to find the optimized one, the following optimized parameter set is derived.

The population size (PZ) and generation numbers (G) for GA are set to PZ = 100 and G = 50, respectively. These parameters were derived by a try and error procedure. The 1-point cross-over with the probability of 0.7 is employed. Classical mutation with probability 0.02 is used, and selection method is the roulette wheel. Number of epochs and learning rate are set to 100 and 0.2 for ANFIS.

The Gauss Membership Function (MF) is used in the ANFIS model, and the Takagi-Sugeno-Kang (TSK) subtractive clustering method is used in all proposed models. Ranges of radii are considered to be in the interval [0.1, 2]. These values were derived from a try and error procedure.

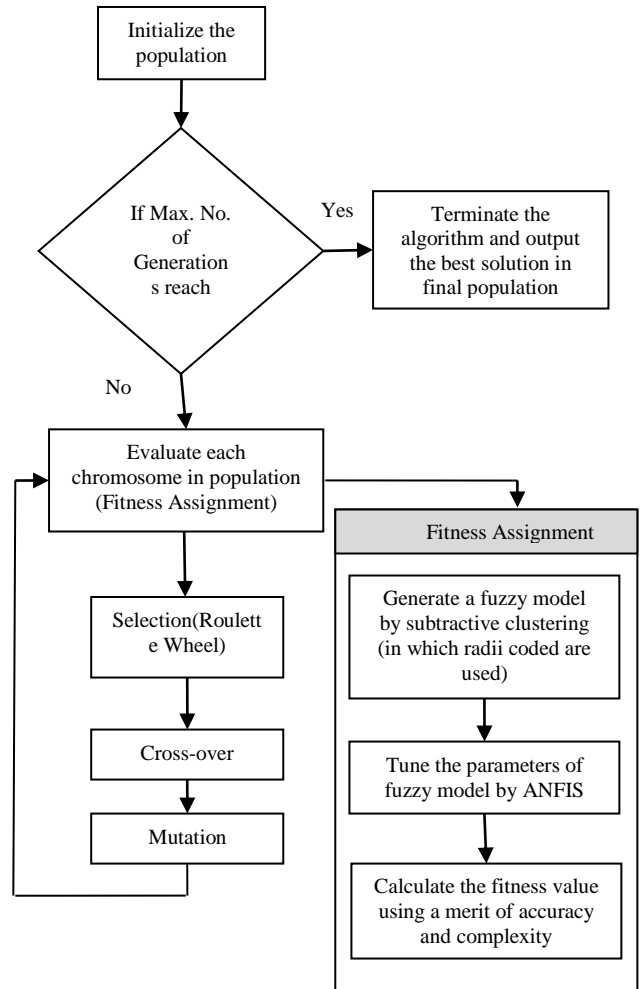


Figure 2. Steps of modeling procedure.

2.5. Spatial data analysis using spatial statistics

Geographic Information systems (GISs) are powerful computer-aided tools for varied applications ranging from sophisticated analysis and modeling of spatial data to simple inventory and management. In groundwater studies, the spatial statistics can be applied to study the distributions of non-point source contamination of groundwater on a regional scale. Spatial statistics method has also been used for various purposes such as groundwater potential, quality mapping and determination of spatial distribution of major and minor ions present in the water and has been applied in diversified applications in medical diagnosis, geology and other fields. These maps are being used as preliminary screening tools for policy and decision-making in groundwater

management strategies on a regional scale[6]. We used ArcGis software to carry out our spatial analysis. This software is a standard GIS analysis tool which is used in about all water resources spatial analysis around the world. We used this software for performing geo-statistics computation along with preparing maps for the observed (real) and predicted data.

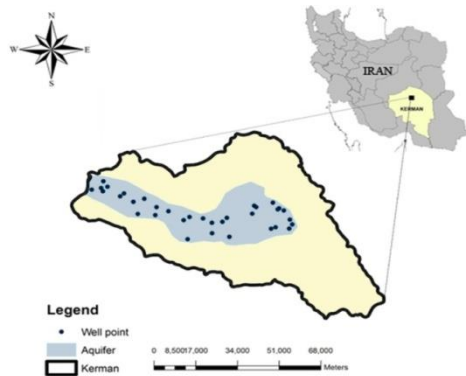


Figure 3. Location of wells in Kerman plain.

2.6. Studied area

The area studied in this research work is the aquifer of Kerman plain, which is a part of Kerman province located in the SE of Iran and in the SW of Loot desert, as shown in figure 3.

Its longitude is between 56°18" and 57°37" east and its latitude is between 29°30" and 30°31" north. This plain is a part of Iranian central plateau super watershed. The area of Kerman plain is 5420 km², 3200 km² of which is alluvium and the rest of it (2220 km²) is mountains and foothills.

In this plain, no permanent river exists. Therefore, the supply of water demands in agriculture, industry, domestic, and municipal sectors in 3200 km² highly depends on groundwater resources. Consecutive droughts and increasing the number of pumping wells in two recent decades has been the main cause of groundwater decline that is happening at a rate of 1 to 3 m per year.

Over-exploitation of groundwater storage has caused serious problems regarding the groundwater quality indices. The depth of wells in the plain is about 57 m in average, and the mean areal precipitation is about 130 mm annually. The rainfall time series data was acquired from Kerman airport station (latitude: 30°16' N, longitude: 56°54'E. Other data sets were collected from the Iranian Ministry of Energy (IMOIE).

2.7. Data preparation

Groundwater table fluctuations is, undoubtedly, one of the most important factors in changing the concentration of chemical parameters extant in ground water. Due to the lack of quality control, data from only 27 quality-controlled wells were used for interpolation.

Further, to assess the impact of rainfall on groundwater quality, the monthly rainfall from 9 rain gage stations were estimated using the Thiessen polygon method. The present study utilized groundwater information and average monthly rainfall in different lag times in order to anticipate effective qualitative factors in groundwater table using the AI methods. Table 1 presents the statistical specifications of the utilized set of variables in the modeling procedure.

Table 1. Statistical parameters of data.

Variable	Mean	St.Dev	Min	Max	Skewness
water table(m)	57.04	27.22	8.92	113.88	0.22
EC(μmoh/cm)	2371	2344	240	13990	2.54
TH(mgr/lit)	533.1	405.1	100	2680	2.21
Ca(meq/lit)	4.48	3.52	0.8	25	2.16
Mg(meq/lit)	6.19	5.41	0.7	43.6	2.81
Na(meq/lit)	15.23	19.7	0.2	115	2.77
Cl(meq/lit)	14.03	18.97	0.2	120	2.84
SO₄(meq/lit)	7.78	8.02	0	49	2.49
HCO₃(meq/lit)	4.07	2.55	1	28.1	5.17

3. Result and discussion

3.1. Input Combinations

Lack of decent qualitative information in different locations of groundwater table is considered as one of the complications in the way of quality analysis of groundwater aquifer.

To this end, the present study attempted to extract the qualitative groundwater information from limited information of the aquifer such as groundwater levels, average rainfall, and local coordinates of the location. Subsequent to preparation of the information, the author attempted to predict the qualitative changes of groundwater in Kerman plain in different locations for the next month, using artificial intelligence models and the mentioned different important combinations.

Table 3. Details of ANN model architecture in test and train

chemical parameters	Input variable	No. of Hidden neurons	Train(tr) / Test(ts)	
			R^2_{tr}/R^2_{ts}	$MAPE_{tr}/MAPE_{ts}$
EC	4	15	0.98/0.98	0.14 / 0.13
TH	5	20	0.95/0.9	0.18 / 0.16
Mg	4	25	0.88/0.65	0.3 / 0.4
Na	4	15	0.98 / 0.93	0.4 / 0.14
Ca	4	30	0.92 / 0.8	0.23 / 0.97
Cl	6	30	0.96 / 0.97	0.6 / 0.29

Table 2. Best input combinations for each chemical parameter.

	$L_{(t)}$	$L_{(t-1)}$	$R_{(t)}$	$R_{(t-1)}$
EC	×			×
TH		×	×	×
Mg	×	×		
Na	×			×
Ca		×	×	
Cl	×	×	×	×
SO_4	×	×		
HCO_3	×	×		×

The feature selection results in table 2 show that except for ‘TH’ and ‘Ca’, ‘ L_t ’ (water level in the current month) of the rest of the parameters is one of the effective factors on the anticipation of concentrations of the mentioned chemical parameters. Likewise, except for parameters of ‘Mg’ and ‘ SO_4 ’, the effect of rainfall in either of (t) or (t-1) time steps was recognized to be among the effective factors on the prediction of concentration of parameters. The experience of technicians at Well Water Quality Assessment Lab of Kerman approves the foregone results, although, considering relatively great depth of wells (an average of 57 m) and fairly low annual rainfall (an average of 130 mm annually), the discussed effect seemed unlikely at first glance. However, although recharging of aquifer by rainfall on its surface within monthly periods seems unlikely, the discussed rainfall portrays favorable changes with quality change, in such a manner that it can be utilized for quality prediction.

3.2. AI models

Considering the limited volume of qualitative information of the aquifer in Kerman plain and the relatively large number of parameters pertaining to AI models, the development of such models is associated with a fairly significant uncertainty in calibration parameters. The modeling strategy of the present study, therefore, was based on the

development of AI models maintaining the minimum possible parameters for reaching a logical and favorable fit. The three models (ANN, ANFIS, and ANFIS-GA) were employed. For the first two models to achieve acceptable functionality, we extract the number of optimal parameters including hidden layer neurons in ANN as well as the number of rules and membership functions for ANFIS through trial and error, while our model, ANFIS-GA, by employing GA, achieves the best and most accurate neuro-fuzzy model by optimization of the clustering.

3.2.1. ANN models

Table 3 shows the best ANN structures for chemical parameters along with their goodness of fitting criteria. Besides, the scatter plots of the observed values compared to the predicted values were also analyzed in selecting the most appropriate structure. To extract the mentioned table, a total number of 1620 data (5 monthly recorded years (2005-2010) for 27 different wells was utilized, from which 70% (1134 data) were used for training and 30% (486) for testing the models. As it will be presented later, based on fitness criteria, the models show a relatively high performances, and thus the number of data used to train and test them are enough. All the networks were Multilayer Perceptron (MLP) with the function of Log-sigmoid and Levenberg-Marquardt (LM) training algorithm.

3.2.2. ANFIS model

The following table contains the best ANFIS extracted models through trial and error and also employing GA. Gaussian membership function was used for the entire models stated in table 4. Based on this table, the ANFIS-GA model improved the performance of the model by changing the clustering radius and consequently the number of rules. Thus, the proposed combinational model reduced the number of parameters. The number of employed rules in the ANFIS-GA model decreased by 300%, compared to the ANFIS model, which resulted in an average increase of 38.4% for R^2 and 44% decrease for MAPE.

Table 4. Details of ANFIS and ANFIS-GA model architecture in test and train period.

Chemical parameter	Model	No. of input variable	No. of rules	No. of MF	Train		Test				
					R ²	MAPE	R ²	MAPE	Percent of improve R2	Percent of improve MAPE	Percent of decrease rules
EC	ANFIS	4	32	128	0.78	0.33	0.82	0.2			
	ANFIS-GA	4	8	32	0.99	0.1	0.99	0.1	20.7	50	300
TH	ANFIS	5	26	130	0.71	0.31	0.65	0.4			
	ANFIS-GA	5	7	35	0.95	0.15	0.91	0.14	40	65	270
Mg	ANFIS	4	17	68	0.78	0.39	0.43	0.59			
	ANFIS-GA	4	6	24	0.97	0.12	0.68	0.37	58.1	37.3	180
Na	ANFIS	4	23	92	0.77	0.8	0.85	0.25			
	ANFIS-GA	4	7	28	0.98	0.29	0.98	0.09	15.3	64	228
Ca	ANFIS	4	28	112	0.59	0.39	0.64	0.27			
	ANFIS-GA	4	4	16	0.82	0.3	0.89	0.18	39	33.3	600
Cl	ANFIS	6	21	126	0.73	0.89	0.84	0.48			
	ANFIS-GA	6	4	24	0.99	0.17	0.99	0.14	17.9	70.8	425
SO ₄	ANFIS	4	27	108	0.64	0.93	0.44	0.26			
	ANFIS-GA	4	7	28	0.8	0.78	0.8	0.24	81.8	7.7	285
HCO ₃	ANFIS	5	15	75	0.72	0.22	0.58	0.21			
	ANFIS-GA	5	6	30	0.94	0.13	0.78	0.16	34.5	23.8	150

Two model performance indices of R² and MAPE are compared in figures 4 and 5, respectively. Based on these figures, the ANFIS_GA model is preferable for all parameters over the other ones, except for the SO4 factor.

Figures 6 and 7 show the mapping of the two parameters of EC and Na, respectively as sample, and in order to compare with the prediction results and also to present some sorts of validation procedure for September 2010 in Kerman plain.

Figures 6 and 7 indicate the high accuracy and compactness of the ANFIS-GA model in predicting the mentioned parameters regarding the observed values. The analysis of mapping graphs of chemical parameters in the surface of the plain indicates the existence of a logical pattern of changes in the concentration. Therefore, the mentioned effect cannot be created due to local changes of concentration of chemical parameters in the location of the well caused by infiltration of pollutants from surface to the well.

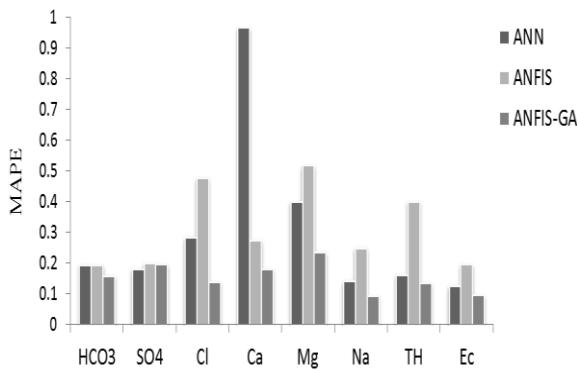


Figure 4. MAPE of chemical parameters analysis

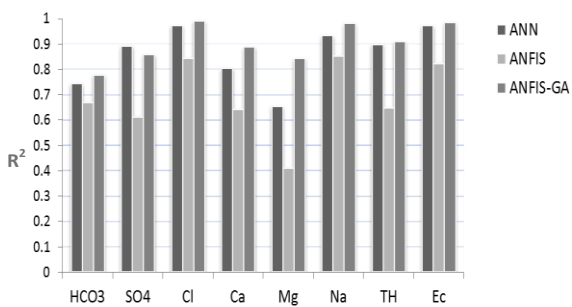


Figure 5. R² of chemical parameters analysis

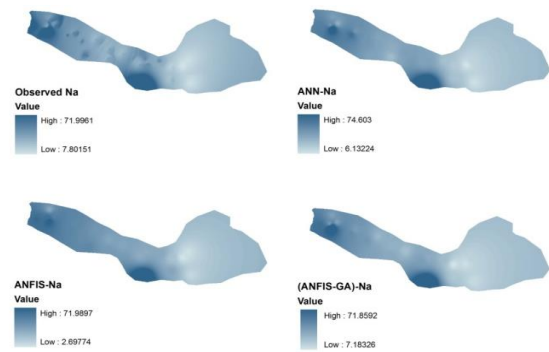


Figure 6. Observed and predicted (Na) for test period on Kerman's aquifer.

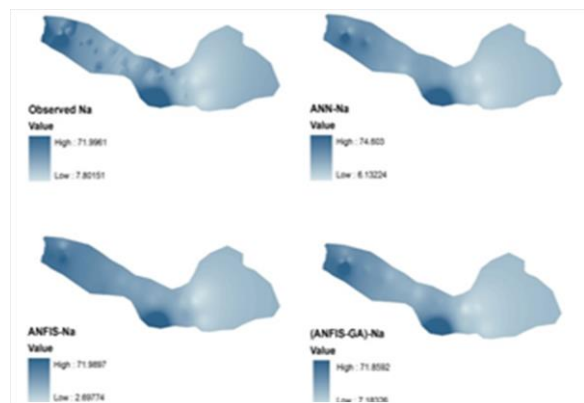


Figure 7. Observed and predicted (EC) for test period on Kerman's aquifer.

4. Conclusions

Sensitivity analysis of different input compositions in AI models in the present work showed that the concentrations of chemical parameters were significantly affected by water level fluctuations. Furthermore, though the effect of rainfall in the under studied plain was not significant on aquifer recharge, rainfall affected the changes in the qualitative parameters of aquifer, except for Mg and SO₄. Thus, it can be concluded that changes in the groundwater chemical parameters in Kerman plain depend on the level fluctuations of groundwater, location under investigation, and mean areal rainfall. The results of the studied models indicated their acceptable function in the prediction of qualitative parameters of the aquifer with a one-month lead time. Analysis of the ANFIS-GA model with objective function showed an increase in the accuracy and compactness of this model in the testing step compared to the ANFIS model. Our proposed method aimed at providing us with an optimized composition in the structure of the ANFIS model through trade-off rise and fall between the accuracy and the number of parameters. The results maintained that a new hybrid algorithm provided both accuracy and complexity of a neuro-fuzzy model. Concerning the comparison of ANN and ANFIS models, it can be concluded that although the ANN method presented acceptable results for prediction objectives, the obtained accuracy of ANN model, being based on trial and error, cannot reach that of the ANFIS-GA hybrid model.

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چکیده:

پیش بینی کیفیت آب های زیرزمینی در مدیریت منابع آب و محیط زیست حائز اهمیت بسیار زیادی می باشد. در تحقیق حاضر با به کارگیری تعدادی از روش ها نظیر سامانه اطلاعات جغرافیایی (GIS) و هوش مصنوعی (AI) کیفیت آب زیرزمینی (مشمول بر غلظت HCO_3^- و هدایت الکتریکی آب EC) در دشت کرمان پیش بینی شده است. در این کار تحقیقاتی، توانایی سامانه تطبیقی استنتاج نورو فازی (ANFIS)، ترکیب (ANFIS) با الگوریتم ژنتیک (GA) و شبکه عصبی مصنوعی (ANN) در پیش بینی کیفیت آب زیرزمینی مورد سنجش قرار گرفت. ترکیبات متفاوتی از تغییرات ماهانه متغیرها از جمله بارش و سطح آب زیرزمینی در چاه ها در دو مدل مختلف نورو فازی (ANFIS استاندارد و ترکیب ANFIS و الگوریتم ژنتیک) استفاده شد. نتایج حاصل شده حکایت از این دارد که روش ترکیبی سامانه استنتاج نورو فازی و الگوریتم ژنتیک در مقایسه با روش سامانه تطبیقی استنتاج نورو فازی استاندارد به طور همزمان توانایی ارائه مدلی با تعداد پارامترهای کمتر (حدود ۳۰٪ کاهش در تعداد قوانین) و بهبود معیارهای برازش (۳۴٪ بهبود در ضریب تعیین و ۴۴٪ بهبود در میانگین قدرمطلق درصدخطا) را دارد. هم چنین این تحقیق مشخص نمود که نوسانات سطح آب زیرزمینی و بارش دو عامل مهم در پیش بینی شاخص های کیفیت آب زیرزمینی می باشند.

کلمات کلیدی: شاخص های کیفیت آب زیرزمینی، سامانه اطلاعات جغرافیایی، الگوریتم ژنتیک، نورو فازی، شبکه عصبی مصنوعی.