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Estimation of Nitrate Concentration Using Fuzzy Regression Method and Support Vector Machines

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Abstract: Groundwater pollution by nitrate is a worldwide problem. To evaluate the performance of fuzzy regression method and support vector machines (SVM) for estimating the nitrate concentration, an analysis was conducted. In this research, 175 observation wells in Isfahan province, Iran, were selected and the concentration of nitrate, potassium, magnesium, sodium, chlorine, bicarbonate, sulphate, calcium and hardness of water samples was determined in laboratory. Electrical conductivity and pH were also measured and the sodium absorption ratio was calculated from the measurements. The average concentration of water quality parameters, including bicarbonate, calcium, magnesium, hardness and electrical conductivity was introduced as input data and nitrate concentration as output. The results showed that R^2 of fuzzy and SVM models were 0.94 and 0.936, whereas the root mean squared error values were 1.5 and 1.3, respectively. Both fuzzy and SVM approaches work well for the data set used from this region, but the SVM technique works better than the fuzzy model for estimation of nitrate concentration in the groundwater.

Key words: Nitrate pollution · Fuzzy regression method · Support vector machines

INTRODUCTION

Nowadays, nitrate pollution of groundwater is an important environmental and agricultural problem in Iran. Due to occurrence of droughts in recent years, over-exploitation of groundwater for agriculture, urban and rural water supplies has become an important issue in water resources management of this water-scarce region. Nitrates, being extremely soluble in water, move easily through the soil and into the groundwater. Leaching of excessive amounts of nitrate has some adverse effects on infants and susceptible adults. It causes blue-baby syndrome or methemoglobinemia, which can lead to brain damage and sometimes death. The maximum permissible level for nitrate in public drinking water is established by the USEPA as 45 *mg/lit*.

Isfahan province is undergoing great land use changes due to population growth and the accompanying industrial, commercial and agricultural developments. These activities produce multiple sources of contaminants such as manure and chemical fertilizers, landfills, accidental spills and domestic or industrial effluents. Among these sources, agriculture-related activities are well-known non-point source pollution. Agricultural activities may deteriorate the groundwater quality in small to large watersheds, especially due to excessive use of fertilizers and various pesticides [1, 2]. Variation in groundwater quality is a function of physical and chemical parameters that are greatly influenced by geological formations and anthropogenic activities as well [3]. Because of development of farmlands and over-application of chemical fertilizers, particularly nitrogen fertilizers, nitrate has become one of the main sources of soil and water pollution. Therefore, it is necessary to investigate nitrate pollution of groundwater.

Artificial neural network has been used to predict the pesticide and nitrate contamination in rural private wells [4]. Depth to aquifer materials from soil surface, well depth and distance to cropland were used as input parameters and concentration of pesticides or nitrate was the output. A set of neural networks were used to predict soil water content at a given depth as a function of soil temperature and soil type and was compared with a multiple regression model [5]. Neural networks were generally able to predict

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the soil water content over time but the regression model did not perform well to follow the trend of data over time. The probabilistic, statistical and stochastic approaches require large amounts of data for modeling purposes and therefore are not practical in local studies. It is therefore necessary to adopt a better approach for nitrate modeling. Support vector machines and fuzzy regression method are used in this paper.

In this research, the collected well-water data are used to: 1) estimate nitrate concentration in an arid region (Isfahan province, Iran) and 2) investigate the effective parameters on nitrate concentration, for controlling pollution of groundwater, using Fuzzy regression and SVM in MATLAB software version 7.1.

MATERIALS AND METHODS

Study Region and Data: Isfahan province is located at 30° 43' to 34° 27' N latitude and 49° 36' to 55° 31' E longitude. Isfahan has arid and semiarid climate, mostly characterized by low rainfall and high potential evapotranspiration. The main river of the province (Zayandehrud), runs for some 350 km roughly west-east from the Zagros Mountains to the Gavkhuni swamp. The average annual rainfall of Isfahan is about 120 mm, which falls mostlt in November to April. Severe droughts are recognized as a feature of Isfahan climate. In 2009-2010, the province has suffered severe dryness and this lack of rainfall has resulted in extensive damages. The region under investigation is a part of Isfahan province, located between northern latitude of 31° 54' 21? to 34° 05' 31? and eastern longitude of 51° 05' 30? to 52° 38' 31?. This area includes the city and suburbs of Najafabad, Shahreza, Natanz, Kashan (Figure 1), north of city of Isfahan and the vicinities of Zayandehrud river [6].

In this research, 175 observation wells were selected and the concentration of nitrate (NO_3^-), potassium (K^+), magnesium (Mg^{2+}), sodium (Na^+), chlorine (Cl^-), bicarbonate (HCO_3^-), sulphate (SO_4^{2-}), calcium (Ca^{2+}), hardness (TH), electrical conductivity (EC) and pH were determined in laboratory from the taken water samples. Sodium absorption ratio (SAR) was calculated from these measurements.

Support Vector Machines: A support vector machine (SVM) uses a linear model to separate the sample data through some nonlinear mapping from the input vectors into the high-dimensional feature space. The linear model constructed in the new space can represent a nonlinear decision boundary in the original space. SVM aims at finding a special kind of linear model, the so-called optimal separating hyperplanes. The training points that are closer to the optimal separating hyperplane are called support vectors, which determine the decision boundaries. In general cases where the data is not linearly separated, *SVM* uses the nonlinear machines to find a hyperplane that minimizes the errors on the training set.

Consider a training set $D=\{x_i,y_i\}^N_{i=1}$ with input vectors $X_1 = \{ X^1_1 , \ldots X^N_1\}$ ° R^n and target labels y_i ° {-1, + 1}. *SVM* binary classifier satisfies the following conditions [7]:

$$y_i(w^T\phi(x_i) + b \geq) \; i = 1,\ldots..., N \qquad (1)$$

Fig. 1: Map of Isfahan province and the location of the chosen wells

where w represents the weighting vector and b is the bias. The nonlinear function $\Theta(0)$: $R^n \rightarrow R^{nk}$ maps the input vectors into a high-dimensional feature space. From Eq. (1), it can be seen that it is possible for multiple solutions to separate training data points. From a generalization perspective, it is the best to choose two bounding hyperplanes at opposite sides of a separating hyperplane $w^T \Phi(X) + b = 0$ with largest margin $2/(|w|^2)$. However, most of the classification problems are linearly non-separable cases. Therefore, it is common to introduce slack variables æ$_i$ to permit misclassification. Thus the optimization problem becomes as follows:

$$\underset{w,b,\xi}{Min}\left(\frac{1}{2}w^T W + C\sum \xi_i\right) \tag{2}$$

$$s.t.\begin{cases} y_i(w^T\phi(X_I)+B \geq 1-\xi_I) \\ \xi_I \geq 0 \end{cases} i = 1,....N \tag{3}$$

where C is the penalty parameter of the error term. The solution of primal problem is obtained after constructing the Lagrangian. Then, the primal problem can be converted into the following QP-problem:

$$Max_a\left(e^T\alpha - \frac{1}{2}\alpha^T Q\alpha\right) \tag{4}$$

$$s.t.\begin{cases} 0 \leq \alpha_i \leq C, i=1,...N \\ \sum_{I=1}^{N} \alpha_i y_i = 0 \end{cases} \tag{5}$$

where α_i is Lagrange multipliers, $Q_{ij} = yy_j\Phi(X)^T \Phi(X)$. Due to a large amount of computation, inner product is replaced with kernel function which satisfies Mercer's condition, $K(x_i,x_j) = (X)^T \Phi(X)$. Finally, we get a nonlinear decision function in primal space for linearly non-separable case:

$$y(x) = \text{sgn}\left(\sum_{i=1}^{N} \alpha_i y_i k(x,x_i) + b\right) \tag{6}$$

Four common kernel function types of *SVM* are given as follows: Linear kernel: $k(x_i, x_j) = x^T_i x_j$, Polynomial kernel: $k(x_i, x_j) = (\tilde{O}x^T_i x_j + r)^d$, Radial basis kernel: $k(x_i, x_j) = exp(-\tilde{O}|x_i - x_j|^2)$ and Sigmoid kernel: $k(x_i, x_j) = tanh(\tilde{O}x^T_i x_j + r)$ where $d, r \circ N$ and $\tilde{O} \circ R^+$ are constants [8, 9].

SVM Modeling: Model selection and parameter search plays a crucial role in the performance of *SVM*. However, there is no general guidance for selection of *SVM* kernel function and parameters so far. In general, the radial basis function (*RBF*) is suggested for *SVM*. The RBF kernel nonlinearly maps the samples into the high-dimensional space, so it can handle nonlinear problem. Furthermore, the linear kernel is a special case of the *RBF*. The sigmoid kernel behaves like the *RBF* for certain parameters. However, it is not valid under some parameters. The second reason is the number of hyper parameters which influence the complexity of model selection. The polynomial has more parameters than the *RBF* kernel. Finally, the RBF function has less numerical difficulties. While *RBF* kernel values are $0 < K_{ij} = 1$, polynomial kernel value may go to infinity or zero when the degree is large. In addition, polynomial kernel takes a longer time in the training stage and is reported to produce worse results than the *RBF* kernel in the previous studies [10].

The linear kernel SVM has no parameters to tune except for C. For the nonlinear SVM, there are additional parameters, the kernel parameters c to tune. Improper selection of the penalty parameter *C* and kernel parameters can cause over-fitting or under-fitting problems. Currently, some kinds of parameter search approach are employed such as cross-validation via parallel grid-search, heuristics search and inference of model parameters within the Bayesian evidence framework. For median-size problems, cross-validation might be the most reliable way for model parameter selection. In v-fold cross-validation, the training set is first divided into v subsets. In the ith *(i = 1,2, . . . , v)* iteration, the ith set (validation set) is used to estimate the performance of the classifier trained on the remaining *(v -1)* sets (training set). The performance is generally evaluated by cost, e.g. classification accuracy or mean square error (*MSE*). The final performance of classifier is evaluated by mean costs of v folds subsets. In grid-search process, pairs of *(C, c)* are tried and the one with the best cross-validation accuracy is picked up. In this study, a grid-search on (C, c) is preferred using 10- fold cross-validation for the following reasons. Firstly, the cross-validation procedure can prevent the over-fitting problem. Secondly, computational time to find good parameters by grid-search is not much more than the other methods. Furthermore, the grid-search can be easily parallelized because each *(C, c)* is independent, while other methods are iterative process, which might be difficult for parallelization. The LIBSVM software was used to conduct SVM experiment. The overall procedure of modeling SVM is illustrated in Figure 2.

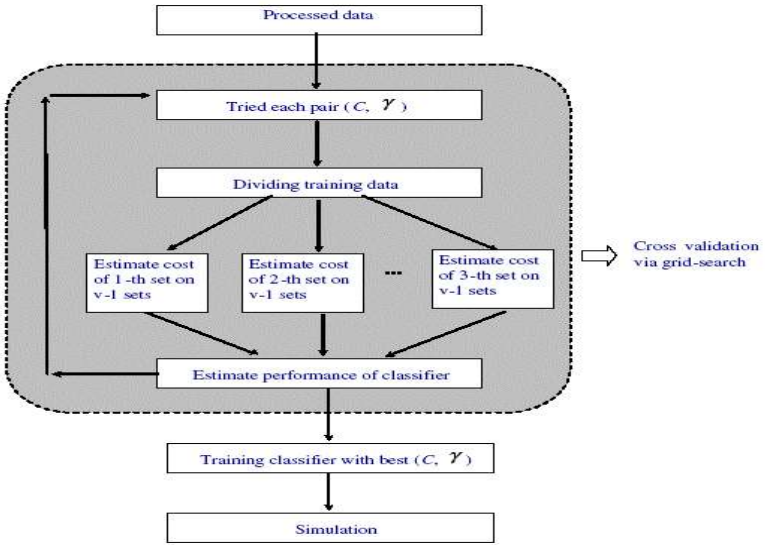

Fig. 2: Overall procedure of SVM modeling

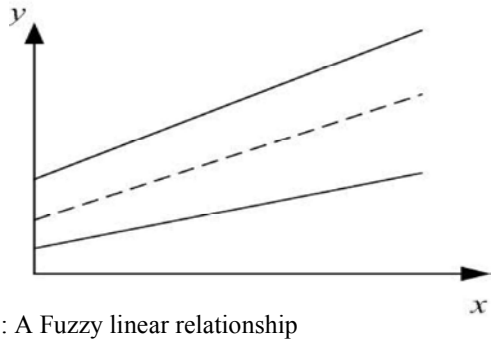

Fig. 3: A Fuzzy linear relationship

Fuzzy Linear Regression Method: Fuzzy regression analysis was first proposed by Tanaka *et al.* [11]. Since membership functions of fuzzy sets are often described as possibility distributions, this approach is usually called possibility regression analysis. The basic concept of fuzzy theory of fuzzy regression is that the residuals between estimators and observations are not produced by measurement errors, but rather by the parameter uncertainty in the model and the possibility distribution is used to deal with real observations [12, 13]. This method provides the means by which the goodness of a relationship between two variable, y and x, may be evaluated on the basis of a small sample size. In this approach, the regression coefficients are assumed to be fuzzy number [14, 15].

The fuzzy linear regression (FLR) model can be expressed as:

$$\tilde{Y} = \tilde{A}_0 + \tilde{A}_1 x_{i1} + \cdots + \tilde{A}_n x_{in} = \tilde{A} x_i \qquad (7)$$

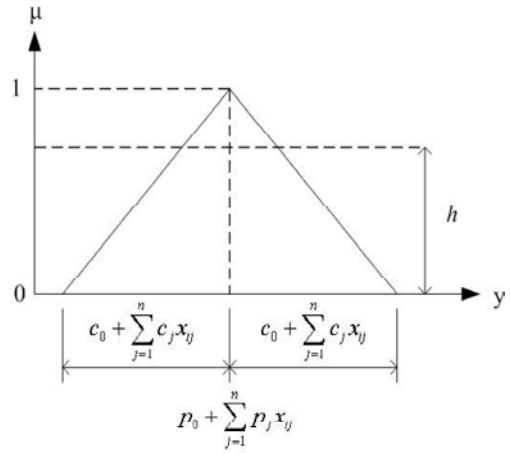

Fig. 4: Triangular membership function of fuzzy output

where *xi* [x_o. x_{i1},.....x_{in}] is a vector of independent variables in the *i*th data *i* = 1,.....m; $\tilde{A} = [\tilde{A}_0, \ldots, \tilde{A}_n]$ is a vector of fuzzy parameters exhibited in the form of symmetric triangular fuzzy numbers denoted by $\tilde{A}_j = (p_j, c_j), j = 1, \ldots, n$, with its membership function depicted as equation (8) bellow, where P_j is its central value and C_j is its half width (Fig. 3).

A fuzzy linear relationship can be represented by a band (the bold lines having membership=0) with a centre line (the dashed line having a membership=1) as in Fig 4.

$$\mu_{\tilde{A}j}(a_j) = \begin{cases} 1 - \dfrac{|a_j - p_j|}{c_j}, & p_j - c_j \le a_j \le p_j + c_j, \\ 0, & \textit{otherwise}. \end{cases} \qquad (8)$$

Therefore, formula (7) can be written as:

$$\tilde{Y} = (p_0, c_0) + (p_1, c_1)x_{i1} + \ldots + (p_n, c_n)x_{in}. \quad (9)$$

Since the regression coefficients are fuzzy numbers, the estimated dependent variable $\tilde{Y}$ is a fuzzy number.

Finally, the method uses the criterion of minimizing the total vagueness, S, defined as the sum of individual spreads of the fuzzy parameters of the model.

$$Minimize\ S = mc_0 + \sum_{i=1}^{m}\sum_{j=1}^{n} c_i \left|x_{ji}\right| \quad (10)$$

The fuzzy coefficients are determined such that the estimated fuzzy output $\tilde{Y}$ has the minimum fuzzy width C_j, while satisfying a target degree of belief *h*. The term *h* can be viewed as a measure of goodness of fit or a measure of compatibility between the regression model and data. Each of the observed data sets must fall within the estimated $\tilde{Y}$ at *h* levels (Fig. 4). The value of *h* is between 0 and 1, *h*=0 indicates that the assumed model is extremely compatible with the data, while *h*=1 illustrates that the assumed model is extremely incompatible with the data; *h* is chosen by the decision maker. A choice of the *h*-level value influences the widths *c* of the fuzzy parameters:

$$\mu_{\tilde{Y}}(y_i) \geq h \qquad i = 1,2,\ldots,m. \quad (11)$$

Taheri *et al.* [14] proposed a method of sensitivity analysis based on credible level *h*. Their results showed that as the credible level *h* increases, the mean of predictive capability (MPC) increases, too. On the other hand, by increasing *h*, the total vagueness of model, *S*, increases as well. For selecting a suitable *h* we would analyze the variations of *S* and *h*. Variations of *S* is gradual from *h* equal zero up to optimal *h*. After optimal *h*, increasing of *h* makes an abrupt variation in *S* value.

The problem of finding the fuzzy regression parameters was formulated by Tanaka *et al.* [11] as a linear programming problem:

$$Minimize\ S = mc_0 + \sum_{i=1}^{m}\sum_{j=1}^{n} c_i \left|x_{ji}\right| \quad (12)$$

Subject to

$$p_0 + \sum_{j=1}^{n} p_j x_{ij} - (1-h)\left[c_0 + \sum_{j=1}^{n} c_i x_{ij}\right] \leq y_j \quad (13)$$

$$p_0 + \sum_{j=1}^{n} p_j x_{ij} + (1-h)\left[c_0 + \sum_{j=1}^{n} c_i x_{ij}\right] \geq y_j \quad (14)$$

Equations (13) and (14) are linear, thereby allowing the optimization problem to be solved by linear programming.

Application: To evaluate the performance of ANFIS model in nitrate estimation, two performance criteria were used including root mean squared error (RMSE) and determination coefficient (R^2). These criteria are defined as [16, 17]:

$$RMSE = \sqrt{\frac{1}{N}\sum\nolimits_{i=1}^{n} \left(X_k - Y_k\right)^2} \quad (15)$$

$$R^2 = \left[\frac{\sum_{K=1}^{n}\left(X_k - \bar{X}\right)\left(Y_k - \bar{Y}\right)}{\sum_{K=1}^{n}\left(X_k - \bar{X}\right)^2 \sum_{Y=1}^{N}\left(Y - \bar{Y}\right)^2}\right]^2 \quad (16)$$

where X_k is measured value, Y_k is predicted value, $\bar{X}$ is mean of observed values and $\bar{Y}$ is mean of predicted values. The linear regression was used between the measured (*X*) and predicted (*Y*) values of nitrate as follows:

$$Y = pX + q \quad (17)$$

where *p* is slope of the line and q is distance from the origin. If the value of *q* is not significant at 5% level, it is considered zero.

RESULTS AND DISCUSSION

The applicability of fuzzy regression method was investigated to predict the nitrate concentrations in 175 observation wells in Isfahan province. The groundwater quality in the observation wells was previously described in detail by Jafari Malekabadi [6]. In the present study, we have used the easily measurable water quality parameters (Table 1) in the prediction of nitrate concentration. The data set was divided into two groups: 122 observations (70% of the data set) for building the model (training data set) and 53 observations (30% of the data set) for validating the model (validation data set). This selection was done randomly. The relationships between input variables and output were investigated first using

Table 1: Relationship between nitrate concentration and input variables

Correlation with nitrate	Min	Max	Mean	Variable
Not significant	7.45	8.73	8.05	PH
Not significant	0.53	148.96	7.029	SAR
Not significant	1.12	64.12	11.89	SO_4
Not significant	19.4	7042.5	445.58	Na
5 percent level	0.78	54.88	5.91	K
1 percent level	1.4	287.75	18.64	Cl
0.1 percent level	180	3091	680.24	TH
0.1 percent level	0.33	25.92	3.14	EC
0.1 percent level	0.84	30.66	5.902	Mg
0.1 percent level	0.73	31.16	4.166	Ca
0.1 percent level	2.3	7.9	3.87	HCO_3

Table 2: Comparison between one-class SVM, epsilon-SVR and nu-SVR for NO_3 estimation

	Training			Validation		
SVM	RMSE (mg/lit)	MSE (mg/ lit)^2	R^2	RMSE (mg/lit)	MSE (mg/ lit)^2	R^2
One-class SVM	1.46	2.13	0.72	1.38	1.90	0.74
Epsilon SVR	1.19	1.41	0.89	1.17	1.36	0.93
Nu-SVR	1.22	1.48	0.85	1.19	1.41	0.88

Table 3: Comparison between linear, polynomial, RBF and sigmoid kernel for NO_3 estimation

	Training			Validation		
Kernel function type	RMSE(mg/lit)	MSE(mg/lit)^2	R^2	RMSE(mg/lit)	MSE(mg/lit)^2	R^2
Linear	1.23	1.51	0.87	1.19	1.41	0.89
Polynomial	1.22	1.48	0.89	1.17	1.36	0.91
RBF	1.16	1.34	0.90	1.13	1.27	0.93
Sigmoid	2.20	4.84	0.70	2.00	4.00	0.74

statistical analyses according to correlation coefficients by Keskin *et al.* [18]. Kisi [8] asked that there should be used a non-linear method instead of correlation analysis for determination of the degrees of effectiveness between the output and each input parameter and different input combinations could be tried using fuzzy models in order to chose the best one, in a non-linear manner. Table 1 shows the performance and statistical coefficients of input variables vs. nitrate concentration. The inputs were hardness, EC, Mg, Ca and HCO_3.

Support Vector Machines: The architecture of the SVM model used for this paper and the results obtained from employing statistical criteria of performance, are given in Table 2. Three types of SVM were compared including one-class SVM, epsilon-SVR and nu-SVR. The results are shown in Table 2. In this study, epsilon-SVR model showed better results. Also among the four kernel functions (linear, polynomial, radial basis function (RBF) and sigmoid), the RBF kernel indicates better performance, as given in Table 3. The table presents the four SVM models used in this research as well as their corresponding performance criteria of RMSE, MSE and R^2. It is concluded that the best input combination should include variables in the order of their importance (that is, TH, EC, Mg, Ca and HCO_3). Actual and predicted values of NO_3 by SVM are plotted in Figure 5.

Fuzzy Linear Regression Method: Since in the present study, the nature of variables has been expressed ambiguous and sensed in a sequential scale, the fuzzy logic was used for the analysis [11]. The employed scale contains a range of literal variables from “none” to “very high” and the membership function is shown in Figure 6.

Based on the Input Data, Three Fuzzy Regression Models Were Obtained as Follows:

Fuzzy 1: NO_3= (0.5431, 0)+(0.1733, 0.1271) EC+(0.08652, 0) Mg +(0, 0.03544) Ca+ (0.0588, 0) Hardness+ (0.165, 0) HCO_3

Fuzzy 2: NO_3= (0.76, 0)+(0.1833, 0.1684) EC +(0.089, 0) TH + (0, 0.1653) Mg +(0, 0) Ca + (0.1938, 0.0847) HCO_3

Fuzzy 3: NO_3 = (0.0734, 0)+(0.1637, 0.1356) EC ++(0, 0) Ca +(0,0) Mg +(0.3668, 0.093) HCO_3+ (0.1813, 0) TH

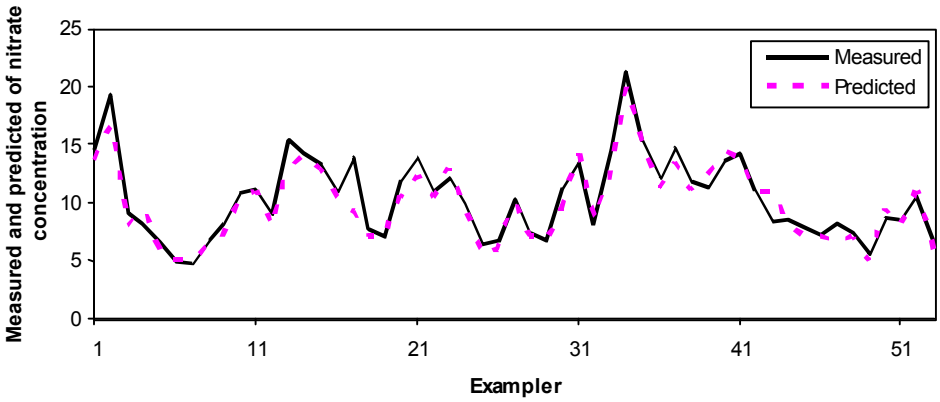

Fig. 5: Measured and predicted nitrate concentrations in different wells using SVM

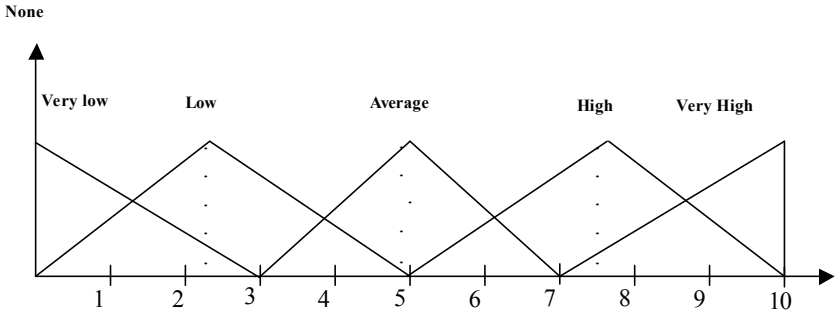

Fig. 6: Membership functions

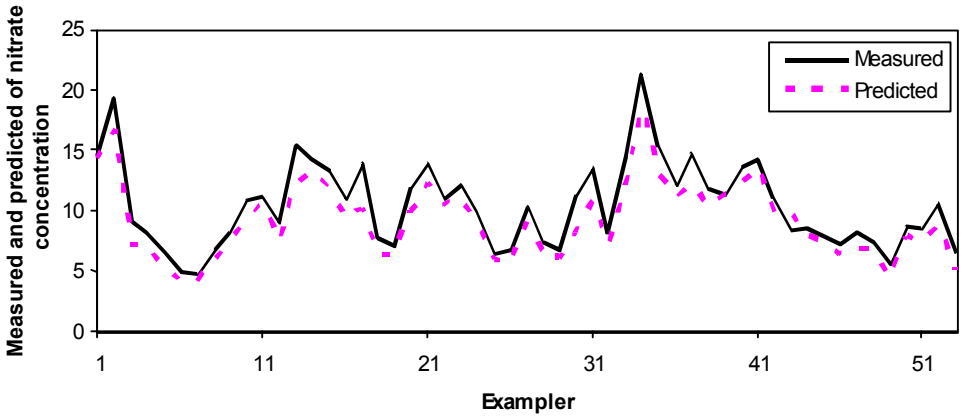

Fig. 7: Predicted nitrate concentration using fuzzy regression method

Table 4: Regression equation of different models compared to measured nitrate

Method	Input	Equation	R^2	RMSE	Performance
SVM	EC, HCO_3, Ca, Mg, TH	$N_{measured}=1.05N_{SVM}$	0.93	1.3	Very good
Fuzzy Regression	EC, HCO_3, Ca, Mg, TH	$N_{measured}=1.14N_{FUZZY}$	0.94	1.5	Good

By using the input data in the above models, nitrate concentration was obtained as a fuzzy number and with the use of area-center method, it was turned into a classical number. These numbers were the estimated NO_3^-. To evaluate the estimation of nitrate concentration by these models, two criteria of RMSE and R^2 were used. The results showed that the best model to estimate NO_3^- is fuzzy1 with inputs of HCO_3^-, TH, EC, Ca^{2+} and Mg^{2+} with RMSE=1.5 mg/lit and R^2 =0.94.

In Figure 7, the measured NO_3 values and the ones calculated by fuzzy regression method are compared. The performance and the statistical coefficients obtained for each model are shown in Table 4.

CONCLUSIONS

In Iran, public concern over the deterioration of groundwater quality from nitrate contamination has grown significantly in recent years. This concern has focused increasingly on anthropogenic sources. Evidences indicate that the NO_3^- levels routinely exceed the maximum contaminant level of 45 mg/lit in many aquifers. Nitrate pollution in groundwater of some regions in Isfahan province, Iran, was investigated. The correlation between NO_3 concentration and other measurable water quality parameters in groundwater was analyzed. In this study, the suitability of Fuzzy regression method and SVM models was examined for estimating NO_3 concentration with observed data as the input. Eleven water quality variables including K, Mg, Ca, Na, Cl, HCO3, SO4, TH, pH, EC and SAR were used as inputs for the models. The results showed that SVM provided the best estimates of NO_3 with lower RMSE and higher R^2 values, followed by fuzzy regression. Generally, the results of the current research could be useful for management purposes and also for beneficiaries of groundwater. Application of SVM could save cumbersome laboratory expenses.

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