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# Estimation of nitrate concentrations in well and spring water using ANFIS and SVM models (Case study: Golestan province)

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**Abstract**

Groundwater contamination by nitrate is a globally growing problem due to the population growth and increase of demand for food supplies. Increasing nitrate concentrations in soil solution and leaching into the ground water table cause water pollution and disturbs the ecological balance. In addition to natural nitrogen cycle, nitrate can be entered to soil and water from the human waste, urban and industrial wastes and agricultural activities and cause undesirable effects on human health. Because of Iran's semi-arid climate, groundwater is one of the most important water resources. Ground water supplies are always at risk of nitrate contamination. An adaptive network-based fuzzy inference system (ANFIS) and support vector machine (SVM) as models that analyze the available information, provide the possibility of extracting nonlinear and unknown relationships, and have applied successfully in many branches of science, especially in water science. In this study, intelligent techniques such as ANFIS and SVM used as a quite flexible tool in simulation of nitrate concentration changes in well and spring waters. The advantage of this approach is high flexibility of intelligent systems against complex functions and use of inputs that are readily available. The results showed that the simulation of nitrate using the ANFIS system was better than the SVM and also this simulation for spring water was better than the simulation for well water. Determination coefficient of ANFIS method was obtained as 0.93 and 0.95 for well and spring waters, respectively. Furthermore, determination coefficient of SVM method was obtained as 0.88 and 0.91 for well and spring waters, respectively.

***Keywords:*** Nitrate pollution, Support vector machine, ANFIS model, Well water, Spring water.

## 1. Introduction

Annual average rainfall of Iran is 252 mm that is less than one third of global annual average rainfall, making Iran’s climate as dry. Population growth, improve living standards and urban, industrial and agricultural developments increase the demand for water supply. Water shortage has become an increasingly serious problem in Iran, especially in the arid and semi-arid regions (Jalali, 2006). Groundwater has become the major source of water supply for domestic, industrial, and agricultural sectors of many countries. It is estimated that approximately one third of the world’s population uses groundwater for drinking purposes (UNEP, 1999). The monitoring of water quality is important for sustainable development and provides valuable information for water management practices. The importance of water quality in human health has recently attracted a great deal of interest. In the developing world, 80% of all diseases are directly related to poor drinking water quality and unsanitary conditions (Jalali and Kolahchi, 2008).

The connection between agricultural and groundwater pollution is well established (Hamilton and Helsel,1995) and groundwater contamination by anthropogenic activities, such as urbanization and agricultural activities, is a problem in arid and semiarid regions (Jalali, 2005).Groundwater contamination by nitrate is a globally growing problem (Bhatnagar and Sillanpää, 2011).Nitrate(NO3-) is probably the most widespread contaminant in groundwater (Goulding, 2000) and its contamination of groundwater in Iran has also been increasingly reported (Jalali and Kolahchi, 2005).

Nitrate is the main form of N in groundwaters. Manyresearchers (Antonakos and Lambrakis, 2000) have related groundwater nitrates to different sources such as leaching of organic and inorganic fertilizers, animal waste, domestic effluents and industry. Fertilizers are considered to be the principal source in the intensively cultivated areas. The amount of nitrate that leaches from agricultural lands is influenced by natural factors such as the soil type and climatic conditions (Mikkelsen, 1992).When any nitrogen is added to the soil, either from organic or inorganic sources, becomes a part of the soil nitrogen cycle. The total amount of nitrogen generated through the processes of the nitrogen cycle is not necessarily used by plants. When the nitrogen supply is greater than the amount used by plants, potential for accumulation of nitrates in the soil and loss from the system exists, regardless of the original source (Tyson et al., 1992).

Babies under six months of age are most affected by excess nitrates in the water. They may develop a condition called methemoglobinemia(blue baby syndrome), caused a bluish color around the lips, spreads to the fingers, toes and face, and eventually covers the entire body. If the problem is not dealt with immediately, the baby can die (Tyson et al., 1992).Sources of nitrate, the most common pollutant found in shallow aquifers, may be point and non-point sources and it can be easily lost from soil, especially in sandy soils, by leaching processes due to its high mobility (Almasri and Kaluarachchi, 2005; Yesilnacar et al., 2008).

Fuzzy sets, created to be easily understood, and used to model non-linear functions, build deduction systems based on the experience of experts, and to trade with indefinite data (Romano et al., 2004). These benefits have been applied to view water dependent complex environmental problems (Ghosh and Mujumdar, 2006).

Neuro fuzzy methods have appeared from the combination of artificial neural networks (ANN) and fuzzy inference systems (FIS) and form a popular framework for solving the real world problems. A neuro-fuzzy system is based on a fuzzy system which is ordered by algorithms conclude from neural network theory. But the learning ability is a benefit from the opinion of FIS, the foundation of linguistic rule base will be benefit from the viewpoint of ANN. There are several methods to identify ANN and FIS (Jang et al., 1997; Tsoukalas and Uhrig, 1997).

Fuzzy set has been expanded for modeling complex systems in uncertain and imprecise environment (Ross, 2004). Fuzzy logic can be used for mapping inputs to appropriate outputs. The fuzzy inference system and its dependent network are a Sugeno fuzzy inference system (Takagi and Sugeno, 1985; Sugeno and Kang, 1986) and an adaptive network-based fuzzy inference system (ANFIS) (Jang, 1993).

The fuzzy system generator assists the user to design a Sugeno fuzzy system order for each system output, either from explicit knowledge or from training data. Once a fuzzy system order is available, the ANFIS algorithm will tune and optimize the fuzzy system by learning from the training data, and finally produce a Sugeno fuzzy system with the same structure as the order. Also each output has a dedicated fuzzy system and corresponding ANFIS with the same inputs. Therefore, totally calculation result is a group of Sugeno fuzzy systems. It was called "resulting model" in Tay and Zhang (1999).

ANFIS depend to the category of rules extracting systems using an analysis strategy, where rules are extracted at the level of individual nodes and then aggregating these rules to form global behavior descriptions (Denal et al., 2004).

Yesilnacar et al. (2008) investigated an artificial neural network model for predicting concentration of nitrate. The samples from 24 observation wells were monthly analyzed for 1 year and easily measurable parameters such as electrical conductivity, groundwater level and pH were used as input parameters in the ANN-based nitrate prediction. Recently, ANFIS was used to construct water level forecasting systems in reservoir management (Chau et al., 2005; Chang and Chang, 2006). ANFIS explored for prediction of pesticide occurrence in rural domestic wells with low information (Sahoo et al. 2005). ANFIS model was presented to predict groundwater electrical conductivity based on the concentration of positively charged ions (Tutmez et al., 2006). Also, ANFIS has been used to modeling of nutrient loads in watersheds (Marce et al., 2004).Mousavi and Amiri (2012) estimated nitrate concentration of groundwater using ANFIS model. The results showed that ANFIS model is recommendable for prediction of nitrate level in groundwater.

During the last decades, many researchers have been working on SVM in different fields, and it has a very active field. The review of Cristianini and Shaw-Taylor (2000) and Bishop (2006) can help to learn of SVM.

SVMs have the ability to generalize well in high dimensional feature spaces and besides, SVMs are robust, outperforming other conventional methods. Compared to other grouping methods, SVMs have benefits in avoiding over-fitting, slow calculation speed and rough precision of the result.

Recently, SVMs have been used in water resources and hydrological areas as a novel method of learning. Liong and Sivapragasam (2002) used SVM in the flood stage forecasting. Asefa et al.(2005) used SVMs for different water resources modeling, including optimal design of the groundwater monitoring networks for both the head observation and contamination networks.

The main advantage of the SVM over the MLP or neuro-fuzzy network is its good generalization ability, acquired at the relatively small number of learning data and at the large number of input nodes. Due to different problem formulation, the learning is simplified to the solution of the quadratic problem of a single minimum point. Therefore, it is very important to predict the nitrate concentration in such areas by means of cost-effective technologies. The goal of this study was to modeling of nitrate by using ANFIS and SVM systems.

## 2. Materials and Methods

### 2.1. Study area

In this study, Golestan province, Iran, was selected to evaluate the nitrate pollution. This province is located the north part of Iran (Fig. 1). The numbers of 218 wells and 111 springs have been used for sampling nitrate that have four years data. The observational wells, located in the region with geographic coordinates27 06’20”-36 64’50” N and 40 83’57”- 41 39’19” E. In addition, the observational springs, located in the region with the geographic coordinates 28 20’70”- 37 21’56” N and 40 93’93”- 41 39’39” E.As regards that the main activities of people in this region is agriculture, the use of agricultural pesticides and fertilizers is common for the increasing of the efficiency of agricultural products that cause the pollution of groundwater. In addition, wastewater of Industrial, poultry, livestock are the other resources of groundwater pollution. According to studies, the most toxic elements in groundwater are Arsenic, bohr, Magnesium and Nitrate. In this study, the applicability of ANFIS and SVM as estimation models for well and spring nitrates was investigated.

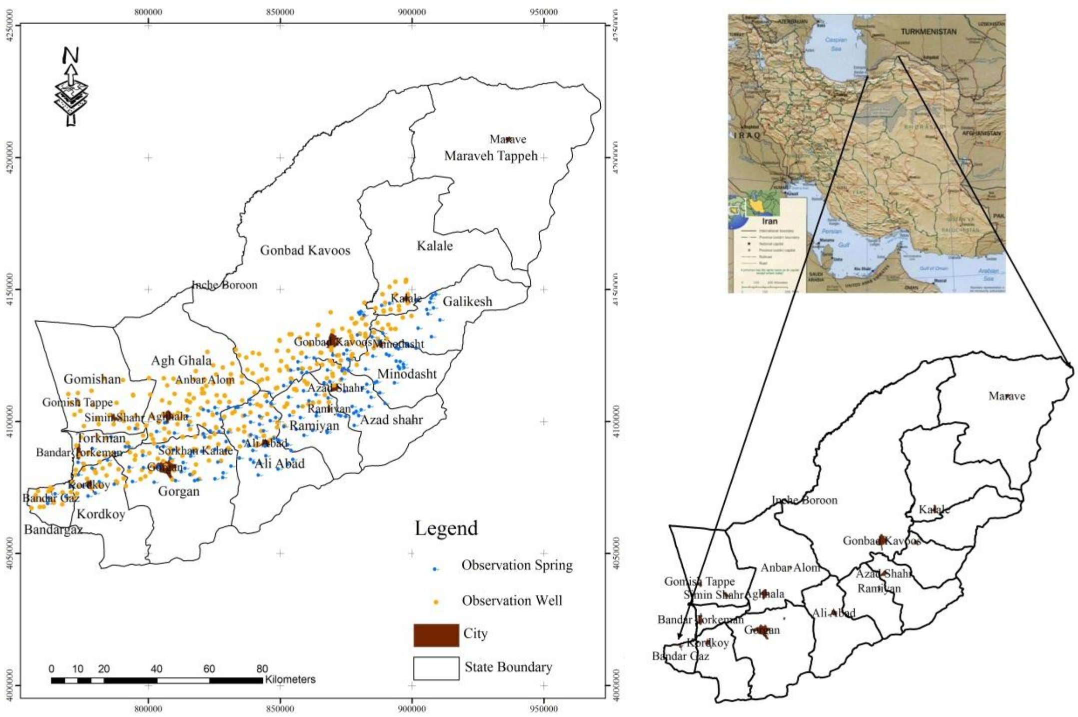


Fig. 1. Study Area

## 2.2. ANFIS model

For designing the ANFIS system, the measured field data were used. The number of available data collected in this study was 218 and 111 for well and spring, respectively. The data set were shuffled; 80% of them were used for the learning process that was 174 and 44 for well and spring, respectively. The 40% sets were used for testing those were 89 and 22 for well and spring, respectively. The data set for learning and testing processes were selected randomly at different points on the landscape in the field to avoid biasness in estimations. In this study, ANFIS models were performed using MATLAB software package (MATLAB version 7.6 with the neural network toolbox). The number of input and output parameters depends on independent and dependent variables, respectively. The network of well was designed with 4 parameters as input, including well water depth, water electrical conductivity (EC), rainfall (Rain) and pH. Also, the network of spring was designed with 3 parameters as input, including water electrical conductivity (EC), rainfall (Rain) and pH. For evaluation of the developed model by ANFIS, the statistical parameters including the determination coefficient (R2) and root mean square error (RMSE) were used.

## 2.3. Overview of ANFIS architecture

ANFIS architecture (Hines 1997) consists of five layers with the output of the nodes in each respective layer is represented by Oi,1 where i is the ith node of layer 1 (Fig. 2).

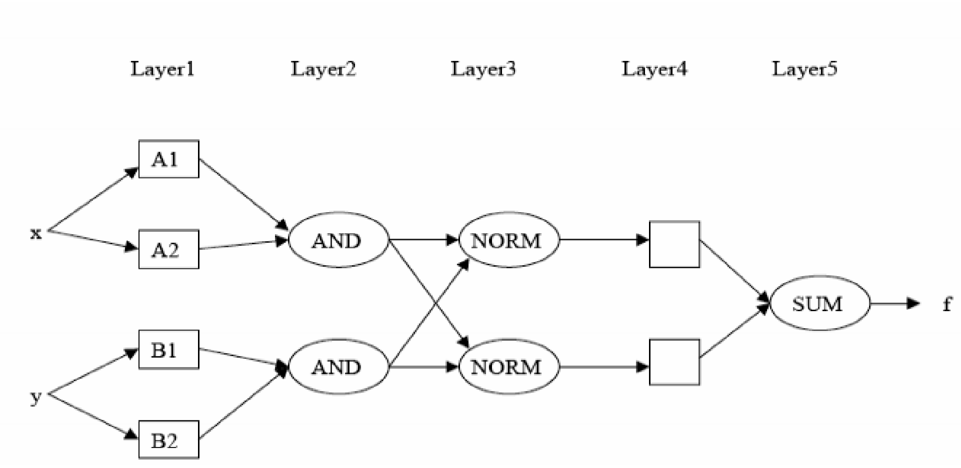


Fig. 2. Structure of an ANFIS network

Layer 1: Generate the membership grades

$O_{l,i} = \mu_{Ai}(x)$ i=1,2 (1)

$O_{l,i} = \mu_{Ai-2}(y)$ i= 3,4 (2)

Where x (ory) is the input to the node and $A_i$ (or $B_{i-2}$) is the fuzzy set associated with this node such us the generalized bell function

$$\mu_{A_i}(x) = \frac{1}{1+\left(\frac{x-c_i}{a_i}\right)^{2b_i}} \quad (3)$$

Where {$a_i$, $b_i$, $c_i$} is the parameter set referred to as premise parameters.

Layer 2: Generate the firing strengths by multiplying the incoming signals and outputs the t-norm operator result, e.g.

$$O_{2,i} = w_i = \mu_{A_i}(x).\mu_{B_i}(y) \text{ i = 1, 2} \quad (4)$$

Layer 3: Normalize the firing strengths

$$O_{3,i} = \overline{W_i} = \frac{w_i}{\sum_{i=1}^{n} w_i} \text{ i = 1, 2} \quad (5)$$

Layer 4: Calculate rule outputs based on the consequent parameters {$p_i$, $q_i$, $r_i$}

$$O_{4,i} = \overline{w_i} f_i = \overline{w_i}(p_i x + q_i y + r_i) \text{ i = 1, 2} \quad (6)$$

Layer 5: Computes the overall output as the summation of incoming signals

$$O_{5,i} = \sum_i \overline{W_i} f_i = \frac{\sum_i w_i f}{\sum_i w_i} \text{ i = 1, 2} \quad (7)$$

The structure of ANFIS model implemented is based on a first order Sugeno fuzzy model so the consequent part of fuzzy if-then rules is a linear equation (Jang et al. 1997; Denal et al. 2004).

In ANFIS model, the simulation has been correctly done when premise parameters of $S_1$ and consequent parameters of $S_2$are estimated so that the amount of error functions of the model in training and testing parts are minimized. The function that makes the lowest error in the least training time will be chosen as the membership function.

The final computed output of the network was prepared to compare with the target output. In this regard, an appropriate objective function such as the sum of square error (SSE) or the root mean square error (RMSE) was calculated as follows (Degroot, 1986).

$$SSE = \sum_{i=1}^{n}(O_i - E_i)^2 \quad (8)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(O_i - E_i)^2}{n}} \quad (9)$$

Where, $O_i$, $E_i$ and n are measured value, predicted value and the number of patterns, respectively.

After calculating the objective function, the second step of the BP algorithm, i.e. the backward process, was started by back propagation of the network error to the previous layers. Using the gradient descent technique, the weights were adjusted to reduce the network error by performing the following equation (Rumelhart and McClelland, 1986).

Kumar et al. (2002, 2008 and 2009) used the normalized scheme such that the difference between the original data and mean was divided by the range of the data series (Equation 10).

$$x_{norm} = 0.5\left(\frac{x_0-\bar{x}}{x_{max}-x_{min}}\right) + 0.5 \qquad (10)$$

Where, $x_{norm}$, $x_0$, $x_{min}$, and $x_{max}$ are normalized value, real value, minimum value, and maximum value, respectively.

## 2.4. SVM model

The Support Vector Machines is categorized, proposed by Vapnik (Vapnik, 1995) that finds an optimal separating hyperplane between two groups of data. SVM is a kind of grouping method based on statistical theory that shows many benefits for solving of questions with high dimension and non-linear shape. When SVMs have been selected for categorization, the essential purpose is to detect the best separating hyperplane between the positive and negative patterns (Zhang and Peng, 2004). The examples nearest to the separating hyperplane are called Support Vectors. By detecting optimal hyperplane, new examples can be classified simply by checking which side of the hyperplane they fall on. A simple two-dimensional example is shown in Fig.3.

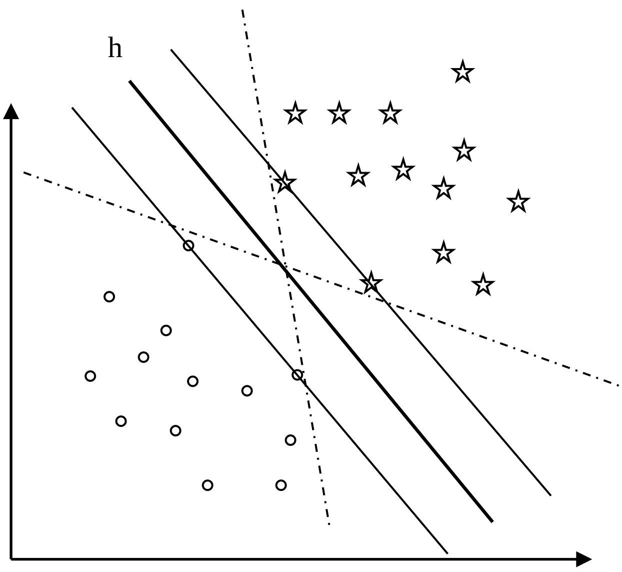


Fig. 3. Support Vectors in SVM algorithm

In Fig.3 there are only two dimensions. The dotted lines represent the limits of linear planes that would correctly classify the training examples. The bold line labeled with an "*h*" represents the plane that provides the maximum separation between the two classes. The four support vectors in the figure can be used to completely define "*h*". SVMs can be combining many statistical methods and machine learning algorithms. Some types of these methods are such as polynomials, radial basis functions, or neural networks.

For classification, the best separating hyperplane, *h* is defined by the values of *x* where the decision function *D(x)* is equal to zero (Cooley, 1999). With a set of training data like $(x_i, y_i)$, the decision function will be defined as:

$$D(x) = \sum_{i=1}^{n} a_i^* y_i H(x_i, x) \quad (11)$$

The $a_i^*$ 's is the maximal solution to the following quadratic problem:

$$Q(a) = \sum_{i=1}^{n} a_i - \frac{1}{2}\sum_{i,j=1}^{n} a_i a_j y_i y_j H(x_i, x) \quad (12)$$

Subject to the constraints:

$$\sum_{i=1}^{n} y_i a_i = 0, \qquad 0 \le a_i \le \frac{C}{n},\ i = 1,...,n \quad (13)$$

Where $H$ is the inner product kernel and $C$ is the regularization parameter.

If radial basis functions be of a form like, with $\sigma$ as width:

$$f(x) = \sin(\sum_{i=1}^{n} a_i \exp\{-\frac{|x - x_i|^2}{\sigma^2}\}) \quad (14)$$

The inner product kernel is equal to:

$$H(x, x') = \exp\{-\frac{|x - x'|^2}{\sigma^2}\} \quad (15)$$

For polynomials of degree $q$, the inner product kernel is equal to:

$$H(x, x') = \left[(x.x') + 1\right]^q \quad (16)$$

The Support Vector Machines is based on these three ideas (Cooley, 1999):

Minimize the structural risk by minimizing the Vapnik-Chervonenkis dimension.

Find a kernel function in an inner product space by mapping input samples onto a high-dimensional space.

Make estimates of model parameters in a high-dimensional feature space and maximizing the distances between classes.

In each step of experiments, number of examples in training and test sets is different, thus we selected 20 percent of all data for test and other for training. In this experiment, the kernel function that is used for SVM is a radial basis function with $\sigma$ equal to 0.1 and the regularization parameter C is set to one. It is essential to mention that the values in SVM are based on experience and are selected by some tests.

## 3. Results and Discussion

### 3.1. ANFIS model

For development of ANFIS model for nitrate prediction of well, four bell membership function for each input parameter, and 3 bell membership function for spring nitrate for each input parameter, linear membership function for output data and back propagation learning rule was used.

The ANFIS model is evaluated based on its performance in training and testing sets. It may be noted that the models are trained using non-transformed data. It appears that the ANFIS models are accurate and consistent in different subsets, where all the values of RMSE are smaller, and all correlation coefficients are very close to unity. It also showed that the value of the RMSE for well is 0.0606 and for spring is 0.0293. To evaluate the ANFIS system, the amount of nitrates in the study area by this method was plotted versus observed values and the best passing line was fitted through the data. Figs. 4 and 5 show the normalized predicted values of nitrate versus the normalized measured values of nitrate for testing data set for well and spring, respectively and the coefficients of determination ($R^2$) were determined. The correlation coefficients of well and spring are 0.93 and 0.95, respectively (Table 1).

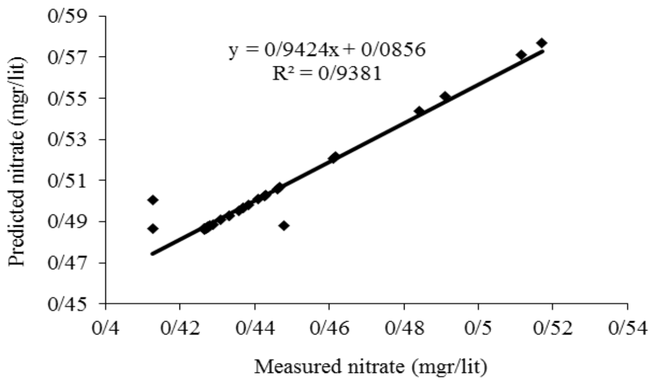


Fig. 4. The comparison of predicted nitrate versus measured values by the ANFIS model for the well

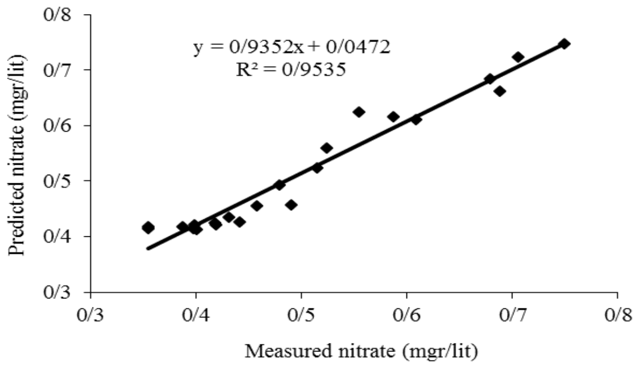


Fig. 5. The comparison of predicted nitrate versus measured values by the ANFIS model for the spring.

Table 1. Statistical parameters of the ANFIS system for nitrate prediction

| Developed model of ANFIS | $R^2$ | RMSE |
|---|---|---|
| model of well nitrate | 0.93 | 0.0606 |
| model of spring nitrate | 0.95 | 0.0293 |

The results showed that the ANFIS model could more carefully simulate the spring nitrate than the well nitrate. Namely, the nitrate model of spring has more determination coefficients and less error than nitrate model of well. Considering the obtained results in this study, could be stating that use of ANFIS model can predict the amount of nitrates in ground water, and this application can be added to the other applications of ANFIS model.

Marcé et al., (2004) stated that the parameters fitted during the ANFIS modeling could be valuable tool to describe features of modeled data and to understand historical changes in human impact on watersheds.

The efficiency of the ANFIS, artificial neural networks and ordinary kriging are investigated for interpolation of transmissivity in an unconfined aquifer. The results indicate that ANFIS model is more efficient than ANN and kriging models to estimate the transmissivity. With these results, we can propose ANFIS model to interpolate the transmissivity values in groundwater modeling processes (Kholghi and Hosseini, 2006).

Cakmakci (2007) used ANFIS to predict the effluent volatile solids (VS) and methane yield from the anaerobic digestion system of primary sludge in municipal hospital wastewater treatment plant (WWTP). The results indicated that the $R^2$ value of effluent VS concentration was 0.80 for testing; the value of methane yield was 0.90. $R^2$ values showed good results

### 3.2. SVM model

The results of SVM model showed that the value of the RMSE for well is 0.05005 and for spring is 0.05017. To evaluate the SVM model, the amount of nitrates in the study area by using this method was plotted versus observed values and the best passing line was fitted through the data. Figs. 6 and 7 show the normalized predicted values of nitrate versus the normalized measured values of nitrate for testing data set for well and spring, respectively and the coefficients of determination ($R^2$) were determined. The correlation coefficients of well and spring are 0.88 and 0.91, respectively (Table 2). The simulation results showed a reasonably accurate prediction of nitrate well and spring. This result is nearly similar to Mousavi et al., (2011).

SVMs are one of the best and superior algorithms in pattern recognitions. However, with some improvements like selecting a large dataset for training can obtain a better performance.

The regression SVM model developed recently, due to its ability to approach nonlinear function in an arbitrary precision degree and the feature of having global minima, has been successfully applied in the fields of short-term forecast (Zhao et al., 2002), biological protein structure forecast (Ward et al., 2003) and time series estimation (Mukheijee et al., 1997; Van Gestel et al., 2001) etc., having solved many practical project problems.

Support Vector Machines (SVMs) are used to estimate aqueous solubility of organic compounds. A SVM equipped with a Tanimoto similarity kernel estimates solubility with accuracy comparable to results from other reported methods where the same data sets have been studied. Complete cross-validation on a diverse data set resulted in a RMSE = 0.62 and $R^2$ = 0.88 (Lind and Maltseva, 2003).

Comparing the two estimation models, it can be seen that the values of the RMSE of the ANFIS model for well is higher than SVM model and the RMSE of the ANFIS model for spring is lower than the SVM model. Also, correlation coefficients of SVM model is lower (5.37% for well and 3.19% for spring) compared to the ANFIS model during testing.

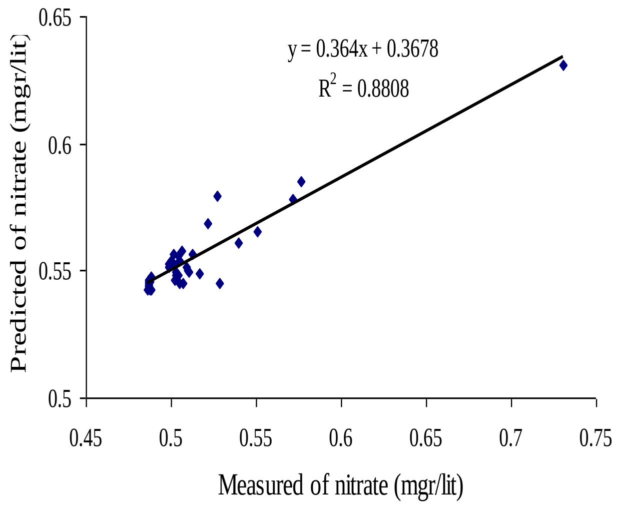


Fig. 6. The comparison of predicted nitrate against measured values by the SVM model for the well

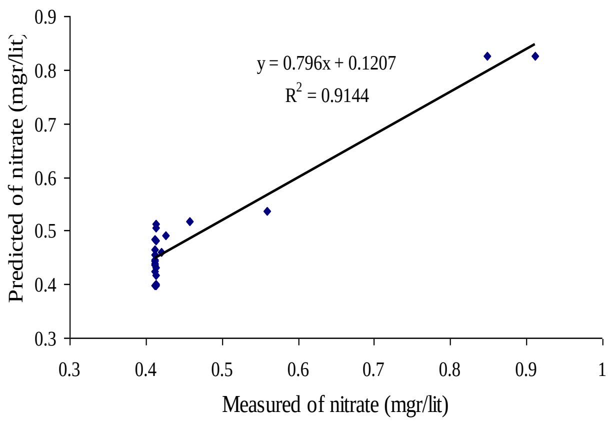


Fig. 7. The comparison of predicted nitrate against measured values by the SVM model for the spring.

Table 2. Statistical parameters of the SVM model for nitrate prediction

| Developed model of SVM | $R^2$ | RMSE |
|---|---|---|
| model of well nitrate | 0.88 | 0.05005 |
| model of spring nitrate | 0.91 | 0.05017 |

## 4. Conclusions

The paper has presented the prediction methods of well and spring nitrates pollution by applying the ANFIS and support vector machine. As shown, one of the most important features of intelligent techniques is the ability to learn through example without requiring the equations of governing the phenomenon. The obtained results of predictions are in good agreement with the actual measurements made at well and spring. The results showed that the accuracy of ANFIS system was greater than the SVM method in estimation the amount of nitrates. Namely, the ANFIS method has more determination coefficients and less error than SVM method. While, the computation cost involved with SVM is significantly smaller than the ANFIS algorithm. Furthermore, intelligent techniques could more carefully simulate the spring nitrate than the well nitrate. Because of considering the nonlinear relationship between environmental factors and the amount of nitrates and then increase the accuracy in estimating the predictions, ANFIS and SVM models can be a good substitute for regression conventional models for modeling the amount of groundwater nitrates. Therefore, can be controlled many of the existing problems with examining the quality of ground water and surface water resources.

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