Journal of Spatial Hydrology
Vol.6, No.2, Fall 2006

Estimation of Aquifer Transmissivity using Kriging, Artificial Neural Network, and Neuro-Fuzzy models

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Abstract

In interpolation of groundwater properties such as transmissivity, due to the unknown distributed values of the variables and heterogenity, the best and the unbiased aspects are frequently difficult to obtain. Therefore, applying a modern technique is necessary to obtain a real estimation of transmissivity. To gain the transmissivity values as an input data in groundwater modelling, the ordinary log kriging method has been used. In this study, the efficiency of the Adaptive Network based Fuzzy Inference System (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 to estimate the transmissivity in comparison with the ANN and kriging models. With these results, we can propose ANFIS model to interpolate the transmissivity values in groundwater modelling processes.

Keywords: Transmissivity**,** Kriging, Artificial Neural Network, ANFIS.

Introduction

The permeable ground materials are highly heterogeneous in terms of their hydraulic properties, such as the transmissivity of aquifer (Gelher, 1993). Geostatistical techniques such as log kriging are often used to estimate the transmissivity at unsampled sites. This linear and unbiased technique applies a deterministic mathematical tool called “variogram”, which describes the spatial variability structure of the transmissivity (Lin and Chen, 2004). The determination of the structure type of variogram has the most effect on the estimations. Marsily and Ahmed (1987) compared the universal kriging, cokriging, and kriging combined with linear regression methods to estimate the transmissivity and specific capacity. Their research showed that cokriging method with minimum standard deviation error is the most efficient method in comparison with other geosatistical methods. Lin and Chen (2004) presented a method for quantifying the uncertainty of the semivariogram of transmissivity, and determinining the required number of sufficient measurments.

In interpolation of groundwater charactristics such as transmissivity due to the unknown regional values of the variables and the unknown variances, the best and the unbiased aspects are frequently difficult to obtain. In these cases in order to attain the best and the unbiased aspects, the assumed variogram model must be used. Considering the importance of transmissivity in groundwater modelling, the role of modern techniques such as artificial neural networks (ANNs) and fuzzy inference system (FIS) are evident because of the non-linear structure in the first model and the ambiguity in variables in second model (Piotrowski et al. 1996, Mukhopadhyay 1999). Recently, researchers are attracted in the use of hybrid models such as Adaptive Network based on the Fuzzy Inference System (ANFIS) to analysis the variables, which are spatially distributed. Lee (2000)

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suggested the ANFIS model for handling the variogram in kriging method, and various computational methods are proposed to solve the resulting spatially distributed problems.
In this study, efficiency of the log kriging, ANN, and ANFIS models are investigated to estimate the transmissivity in a confined aquifer using measured data of Ghazvin plain in the west of Tehran (Iran).

Kriging
Transmissivity values show a log normal frequency distribution, hence the logarithm of their values must be used. Therefore, at first observed data were transformed to the logarithm values, and estimation were conducted and finally, the estimated values were transformed. kriging is a linear weighted-average technique, which is unbiased for expected values of estimators and random variables, and used to find the linear unbiased estimation of a second-order stationary random field with an unknown constant mean as follows:

$$\hat{Z}(x_0) = \sum_{i=1}^{n} \lambda_i Z(x_i) \quad (1)$$

where $\hat{Z}(x_i)$ is kriging estimate at location x_0; $Z(x_i)$ sampled value at x_i; and λ_i is weighting factor for $Z(x_i)$. The estimation errors are:

$$E(x_0) = \sum_{i=1}^{n} \lambda_i Z(x_i) - Z(x_i) \quad (2)$$

where $Z(x_0)$ is unknown true value at x_0; and $E(x_0)$ is the estimation error. In an unbiased estimator the mean of the estimates must be equal to the true mean as follows:

$$E\{R(x_0)\} = 0 \quad (3)$$

In ordinary kriging, the weighting factors (λ_i) can be calculated by solving an optimization problem with minimizing the variance of estimation error as follows

$$\textit{Minimize } Var\left[\sum_{i=1}^{n} \lambda_i Z(x_i) - Z(x_0)\right] \quad (4)$$

Subject to

$$\sum_{i=1}^{n} \lambda_i = 1 \quad (5)$$

by using the Lagrange multiplier μ, solving an equation set which can be expressed in matrix form is nesessary :

$$\begin{bmatrix} \gamma_{11} & \gamma_{12} & \dots & \gamma_{1n} & 1 \\ \gamma_{21} & & \dots & \gamma_{2n} & 1 \\ \vdots & & & \vdots & 1 \\ \lambda_{n1} & \gamma_{n2} & \dots & \gamma_{mn} & 1 \\ 1 & 1 & \dots & 1 & 0 \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \\ \mu \end{bmatrix} = \begin{bmatrix} \gamma_{01} \\ \gamma_{02} \\ \vdots \\ \gamma_{0n} \\ 1 \end{bmatrix} \quad (6)$$

The variogram γ can be defined as one-half the variance of the diffrence between the attribute values at all points seperated by *h* as follows:

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} \left[Z(x_i) - Z(x_i + h) \right]^2 \quad (7)$$

where $\gamma(h)$ is estimated variogram at distance *h*, and *N*(*h*) is the total number of pairs of attributes that are seperated by a distance *h* (Isaaks and Srivastava, 1989). The important charactristics or properties of the traditional variogram are range, sill, and nugget effect. The most commonly used models which applied to compute the variogram, are spherical, gaussian, and exponential models. In this study, the Geostatistics for the Environmental Science Software (GS^+) was used for geostatistical computations.

Artificial Neural Network (ANN)

An ANN consist of a number of interconnected computational elements called neurons that are arranged in a number of layers. There are a wide arrange of ANN architecture, among them the three-layer feedforward architecture with bach propagation algorithm, is widely used (Fig. 1).
This network contains three distinct modes (Daka and Chandramouli 2005):

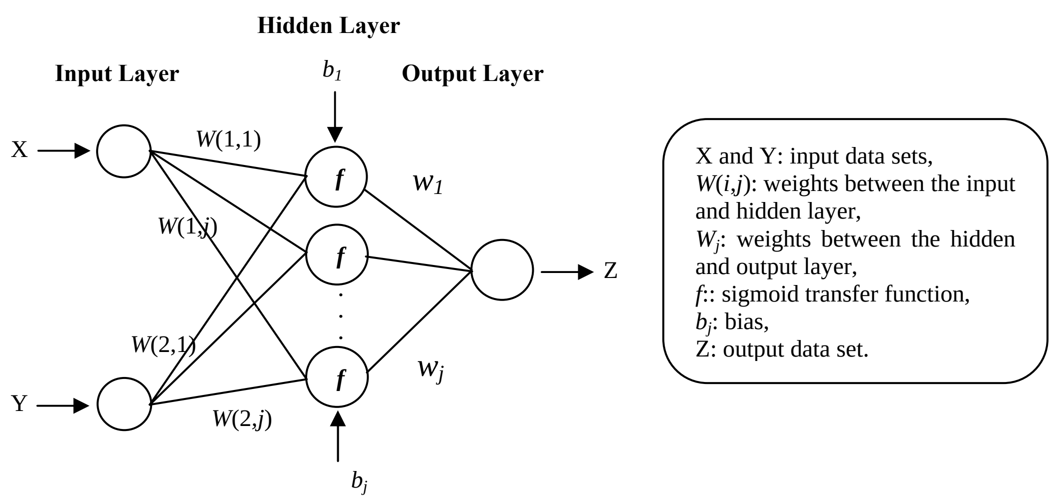

Fig. 1. Arcitecture of three-layer feedforward network

Training mode: In training mode, the training data sets are presented to the network. The weights are computed through an iterative processes based on back propagation algorithm such as the difference between the computed and given output is sufficiently small (or every error criterion such as mean square error). Algorithm, which results a very small difference between the computed and given output.

Cross validation mode (checking mode): this mode monitors the error to find the optimal termination point for training and also avoid overtraining.
Testing mode: this mode is to determine how accurately the network can simulate the input-output relationship.

Neuro-Fuzzy Approach
Adaptive Network based on the Fuzzy Inference System (ANFIS) is a powerful universal approximator for vague and fuzzy systems (Lee, 2000). The basic structure of adaptive network consist of two main conceptual parts: a fuzzy inference system (FIS) which includes three components a rule base, a data base, a reasoning mechanism (which is showed in Fig. 2, schematically), and a learning mechanism consist of a multilayer feedforward network (Nayak et al. 2004).

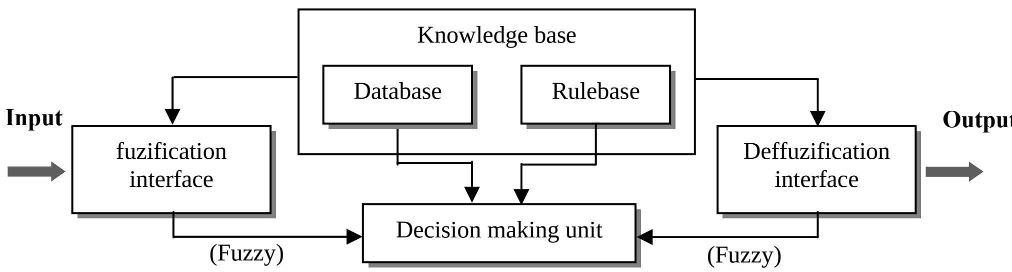

Fig. 2. Fuzzy Inference System with crisp output

The adaptive network based on Sugeno fuzzy inference model provides a deterministic system of output equations thus parameters can be easily estimated (Takagi and Sugeno, 1985). The architecture of ANFIS consists of five layers (Fig. 3), a brief sketch of the operation of these layers is as following (Chen et al. 2005, Nayak et al. 2000):

The first layer, input nodes: is composed of nodes which generates membership grades according to the appropriate membership functions and the set of parameters to minimize are determined accordingly.

The second layer, rule nodes: which the AND or the OR operator is applied to compute every possible conjunction of the decision rules.

The third layer, average nodes: the main purpose is the normalization of the conjuctive membership functions in order to rescale the inputs.

The fourth layer, consequent node: it is a standard perceptron (Rosenblatt, 1958) which Sugeno fuzzy inference model is used to associate the normalized membership function toward the total output, in other words, the contribution of the each rule is computed.

The fifth layer, output nodes: compute the overall output by summing the incoming evidences.
The output of adaptive network is a real number. The consequent parameters and the membership function parameters are learned by standard bachpropagation.

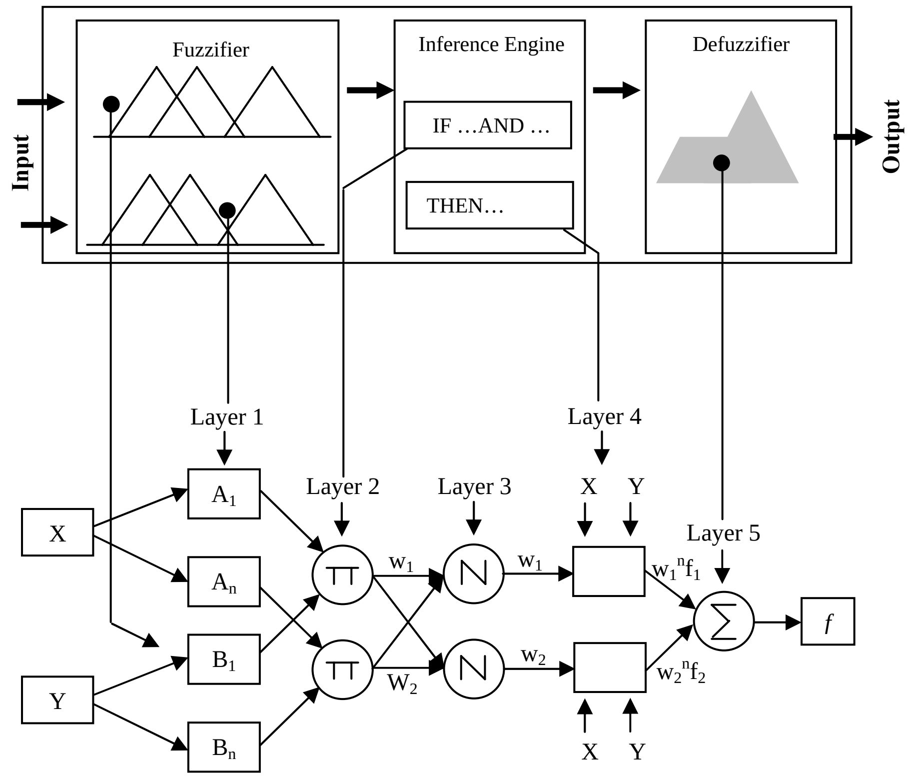

Fig. 3. Adaptive ANFIS architecture (Nayak et al. 2004)

In the ANFIS model, each input variable, which vary within a range, might be clustered into several class values in first layer to build up fuzzy rules. Accordingly, as the number of rules increased, the number of parameters that must be optimized, become enormous.

To prevent this problem, subtractive fuzzy clustering is used to establish the rule base relationship between the input and output variables (Chen et al. 2005).

Study Area and Datasets

Our study area is Qazvin plain aquifer with area of 3850 km^2, which is a part of Qazvin province, that is located in the north of Iran. The 230 measured values of transmissivity which was collected by the Iranian Ministry of Power (IMP) have been used in this study (Fig. 4). The descriptive statistics of transmissivity and log-transmissivity data are summarized in Table 1.

Table 1. Summary descriptive statistics for water table measured

Statistics	T(m^2/h)	Log T (log m^2/h)
Minimum	1.25	0.097
Maximum	520.83	2.717
Mean	80.59±5.863[1]	1.657±0.033[1]
Median	52.60	1.721
Standard deviation	88.92	0.509
Skewness	2.243	-0.455

[1] Standard error of mean (SE).

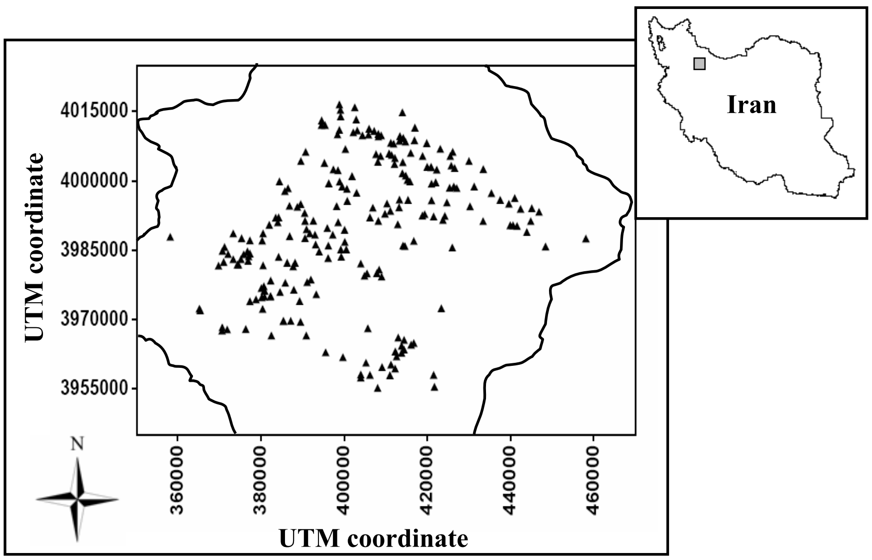

Fig. 4. The Study area and the location of the sample sites (MP 2000)

Results and Discussion

Data analysis indicate that transmissivity values which were used, did not follow the normal distribution, but transformed values have followed the normal distribution. The Kolmogrov-Smirnov test was chosen to test the normality of data (Fig. 5 (a,b)).

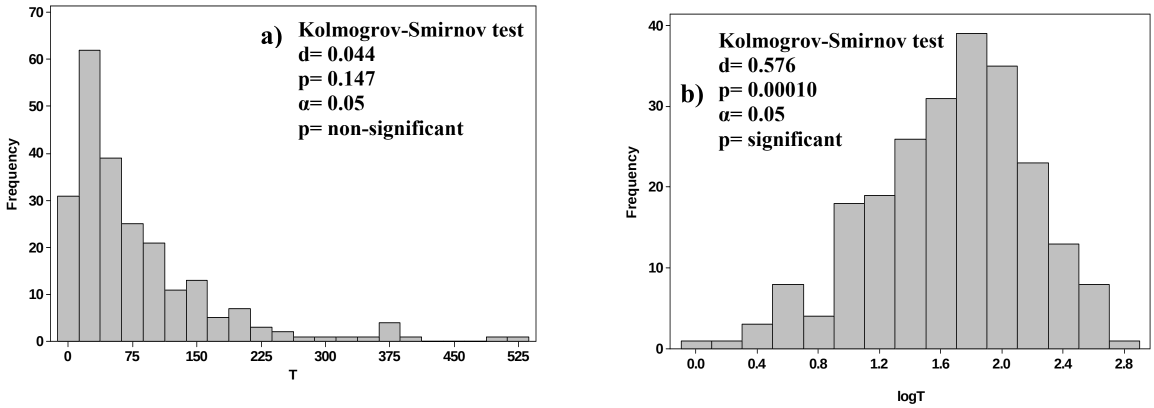

Fig. 5. Frequency histogram of tranmissivity (a) and its transformed values (b)

For investigating correlation of the transmissivity, the appropriate variogram must be determined. Three non-linear models, Gaussian, spherical and exponential were applied, as follow:

1. Gaussian model:

$$\gamma(h)=\begin{cases} C_0+C_1\left(1-\exp(-\frac{h^2}{a^2}\right), & h\le a \\ C_1, & h>a \end{cases}$$

2. Spherical model:

$$\gamma(h)=\begin{cases} C_0+C_1\left(1.5\times\frac{|h|}{a}-0.5\times\left(\frac{|h|}{a}\right)^3\right), & h\le a \\ C_1, & h>a \end{cases}$$

3. Exponential model:

$$\gamma(h)=\begin{cases} C_0+\frac{C_1|h|^2}{\left(1+\frac{|h|^2}{a}\right)}, & h\neq 0 \\ 0, & h=0 \end{cases}$$

where the C_0 is the nugget, the C_0+C_1 is the sill; a is the range; and h = lag distance.

The correlation coefficient between estimated values and observed values and residual sum of squares criteria are used to select the best model. Table 2. indicate the properies of fitted variograms and the criteria which were considered to determine the goodness of fit for each variogram.

Table 2. Properties of variogram for transformed transmissivity values

Model	Nugget	Sill	Range (km)	R^2	*R.S.S.*
Spherical	0.0001	0.2082	24.80000	0.88	0.00046
Exponential	0.0001	0.2222	12.3000	0.83	0.00066
Gaussian	0.0254	0.2098	12.5000	0.89	0.00043

The results in Table 2. indicate that best fitted variogram has gaussian form, as follows:

$$\gamma(h)=\begin{cases}0.0254+0.1844\left(1-\exp(-\dfrac{h^2}{(12.50)^2}\right), & h\leq a\\ 0.1844, & h>a\end{cases} \tag{8}$$

The plot of the gaussian semivariogram and the samples are shown in Fig. 6 and the three dimension surface plot of semivariance are shown in Fig. 7.

In ANN model, the x-coordinate and y-coordinate set each sampled sites, in UTM unit they are considered as input data sets and transformed values of transmissivity (log T) are considered as output data set. the observed data divided three sets randomly, training set (65% of total data), checking set (15% of total data), and testing set (20% of total data). In training process, the optimum number of nodes in hidden layer are obtained by trial and error. Considering three nodes in hidden layer recognized as the most efficient structure. The root mean square error in the training, checking, and testing mode were calculated as 0.012, 0.093, and 0.098 respectively in 450 epochs.

In the ANFIS model, the input and output variables are considered according to the ANN model. In training step, the influence clustering radii of input variables have been evaluated by trial and error. The range of influence 0.5 and squash factor 0.415 have the best performance, which produced 12 membership functions in the first layer. This model reach convergence in just 9 epochs.

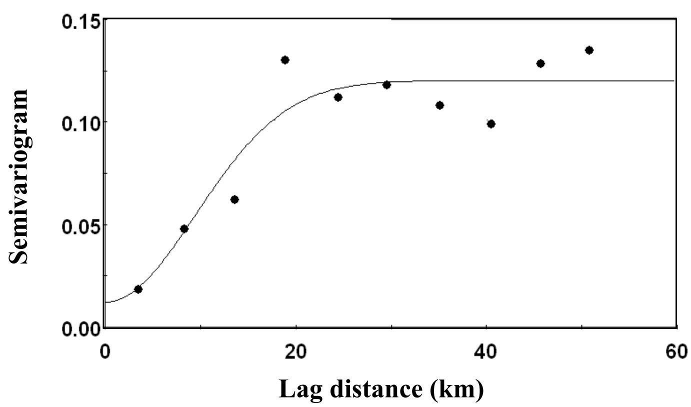

Fig. 6. Fitted variogram of log T

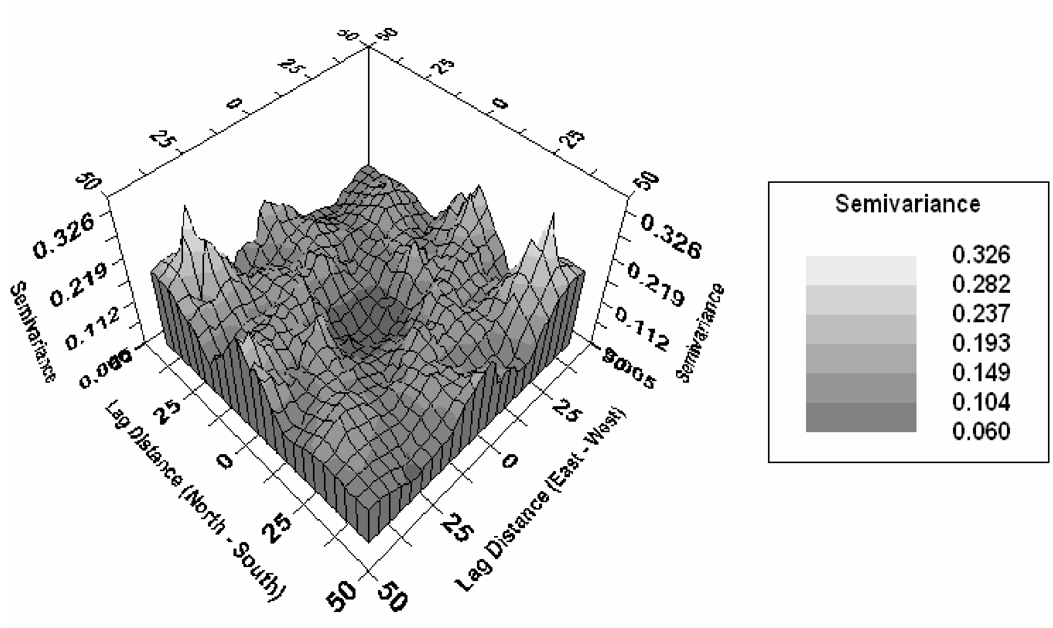

Fig. 7. Three dimensional surface plot of fitted semivariance of log T

The testing data set which is selected in ANN model are considered to evaluate the validity of three models. To investigate the degree of similarity between estimated and measured values, the determination coefficient (R^2) were computed. R^2 values between estimated values by kriging, ANN, and ANFIS methods and observed values are obtained 0.84, 0.78, and 0.75 and 0.76, 0.51, and 0.47 in transformed condition, respectively. Vieire et al. (1981) suggested that R^2=0.64 as an acceptable criterion in assessing the estiamtion process. In both condition transformed and un-transformed transmissivity the R^2 of ANFIS model was acceptable. Three-dimensional surface plot of the observed and estimated values of log T and transformed T based on ANFIS, ANN, and kriging methods are shown in Fig. 8(a, b, c, d) and Fig. 9(a, b, c, d), respectively.

The comparison of 3-D surface plots in Fig. 8 and 9 indicates that estimations based on the ANFIS model have better agreement in all points of aquifer in two states, in comparison with other models. Both ANFIS and kriging models maintain the overall shape of 3-D plot of observed, in transformed state better than ANN model.

To evaluate the suitability of the model for the estimation of transmissivity, three criteria were chosen to analyze the degree of goodness of fit. These criteria can be defined as follow:

1- root mean square error (*RMSE*)

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[Z(x_i) - \hat{Z}(x_i)\right]^2} \tag{9}$$

Where $Z(x_i)$ is the observed value at location *i*, $\hat{Z}(x_i)$ is the predicted value at location *i*, and *n* equals the number of samples. The smallest *RMSE* determines the method having the most accurate local or small-scale estimates (Schloeder et al., 2001).

2-mean absolute error (*MAE*)

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left[\left|Z(x_i) - \hat{Z}(x_i)\right|\right] \quad (10)$$

The smallest *MAE* is indicative of the most accurate global estimates (Schloeder et al., 2001).

3- the coefficient of efficiency

$$CE = 1 - \frac{\sum_{i=1}^{n}\left[Z(x_i) - \hat{Z}(x_i)\right]^2}{\sum_{i=1}^{n}\left[Z(x_i) - \overline{Z}\right]^2} \quad (11)$$

where $\overline{Z}$ is average of the observed values (Nash and Sutcliffe, 1970). The better the fit, the closer *CE* is to one.

4- standard error (*SE*)

$$SE = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[Z(x_i) - \hat{Z}(x_i)\right]^2}}{\overline{Z}} \quad (12)$$

The better the fit, the closer *SE* is to zero.

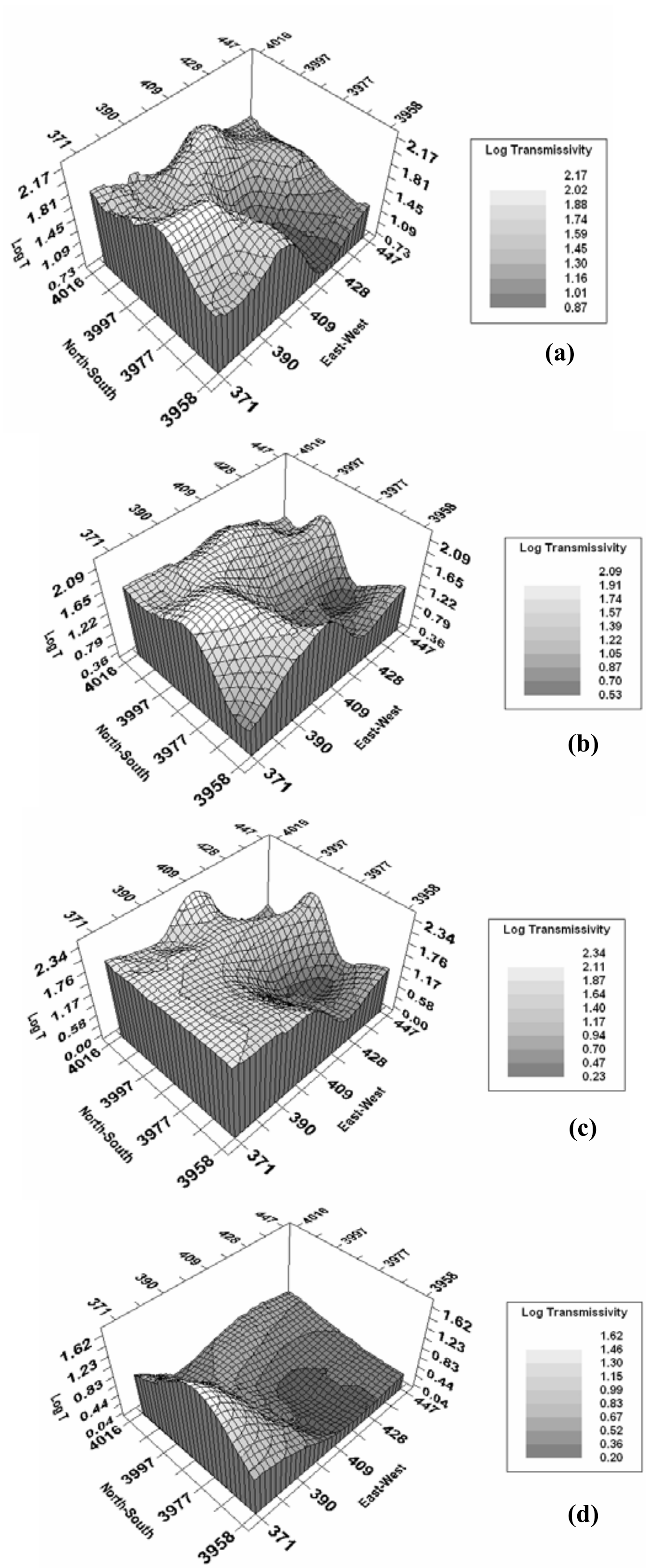

Fig. 8. The observed values of log T (log m^2/h) in x and y coordinate (km) (a) based on (b) ANFIS, (c) ANN, and (d) kriging models

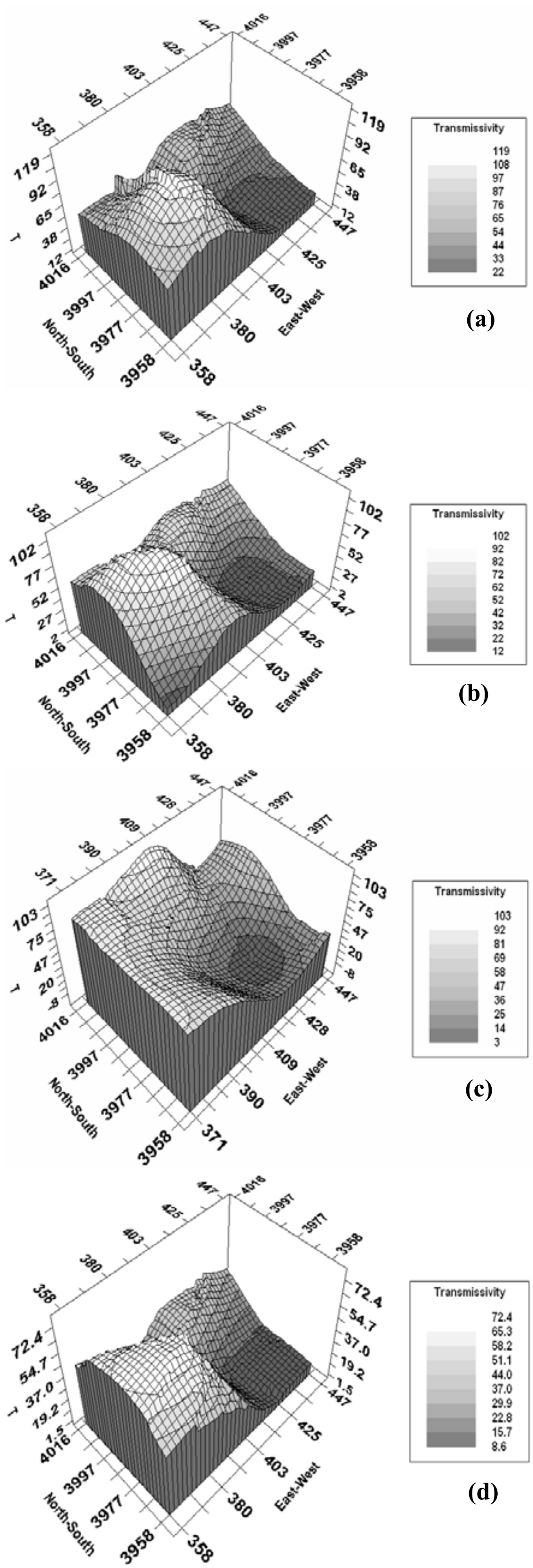

Fig. 9. Thr observed values of transformed T (m^2/h) in x and y coordinate (km) (a) based on (b) ANFIS, (c) ANN, and (d) kriging models

The criteria (9)-(12) were applied to the sampled data which were considered for evaluating the models verification. Table 3 indicate the summary of the results of applying these criteria.

The results of Table 3 indicate that, minimum value of *RMSE*, *MAE*, and *SE* are related to estimations based on the ANFIS and ANN model, respectively. The most efficient model is the ANFIS and ANN model. The ANFIS model modified the model efficiency, 17% and 60% and standard error, 21% and 48% related to the ANN and kriging methods.

Table 3. The performance of estimations with ANFIS, ANN, and ordinary kriging models

Model	*RMSE*	*MAE*	*CE*	*SE*
ANN	49.28	32.94	0.52	0.75
ANFIS	38.93	25.45	0.61	0.59
Kriging	75.51	56.67	0.38	1.156
ANN(Transformed)	0.27	0.21	0.60	0.17
ANFIS(Transformed)	0.23	0.19	0.69	0.14
Kriging(Transformed)	1.09	1.03	0.36	0.67

Summary and Conclusion

In this study, three methods (ANFIS, ANN, and kriging) are used to investigate the estimation of transmissivity in Qazvin confined aquifer (Iran). The results are summarize as follow:

1. In kriging method, searching for semivariograms and determining the best fitted semivariogram model and preparing the required statistical assumptions is a time-consuming and trial and error procedure. While both ANN and ANFIS models are not require to these assumptions.

2. The main adventage of kriging method over ANFIS and ANN methods, is providing a value of the estimation error at each point. Be aware of the residuals in a domain, give a set of measurements. In addition, the estimation error from the kriging technique can provide guidance for new sampling sites to reduce estimation errors.

3. It may be noted that for an ANN model, we have to perform a trial and error process to develop the optimal network architecture, while the ANFIS model does not require such a procedure. Another aspect of superiority for ANFIS model in comparison with ANN model, is the lower number of epochs which is needed to reach convergence. This adventage reduces the computing-cost widely.

4. The results indicate that the ANFIS model offers a promising step towards elevating ANN model from purly emperical model due to considering the ambiguity and vaguness of transmissivity for applying the FIS. This model is more efficient than the kriging method which is a deterministic linear model and developed based on mathematical hypotheses.

In conclusion,with these results, we can propose ANFIS model to interpolate the transmissivity values in groundwater modelling procrsses.

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