

## Assessment of Spatial Structure of Groundwater Quality Variables Based on the Geostatistical Simulation

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### Abstract

Our main objective in the present study was to assess the spatial variation of chemical and physical water properties. Prior to the design of groundwater quality monitoring networks, it is essential to investigate the spatial structure of the groundwater quality variables. A case study is presented which used ground water quality observations from groundwater domestic wells in the Dameghan, Iran. The analyses of the spatial structure used the following variables: Electrical Conductivity (EC), PH, SAR, TDS, Sodium (Na), Calcium (Ca), Magnesium (Mg). For all these variables the spatial structure is described by means of geostatistical simulation, used to yield a series of stochastic images characterized by equally probable spatial distributions of the chemical and physical water properties across the area. The data set including 5 years of annual observations. At first normality and homogeneity of data are examined. Then variographic analysis using two techniques including kriging, Weighted Moving Average (WMA) were applied for presenting spatial variation of water properties. Finally comparison of the results using statistical techniques showed that for more groundwater quality variables (e.g. TDS, EC, Cation, Na, Ca) kriging technique performed better than WMA-2 technique in characterizing the spatial variability. WMA-2 technique only for some groundwater quality variables like SAR and Mg has better result than kriging to simulate groundwater quality variables.

**Keywords:** Water properties; Interpolation; Geostatistics; Spatial variation; Dameghan; Iran

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### 1. Introduction

Pollution from agriculture and industrial origin threatens the groundwater quality in Iran. Since groundwater is the main source of fresh water, pollution causes a decrease in the long-term resources of water suitable for human consumption. Furthermore, since most groundwater finally flows to the surface, a deterioration of groundwater quality affects the ecohydrological conditions of the receiving seepage areas as well as the receiving seas.

Prior to the design of groundwater quality

monitoring networks, it is essential to investigate the spatial structure of the groundwater quality variables to be monitored. Generally, the objective of monitoring, introduces these variables. For example, greater monitoring effort is required for groundwater to be used for domestic (municipal) purposes than for agricultural use. The aim of characterizing the spatial structure of the variables is not only to assess their monitoring, which is needed to assess the cost of monitoring, but also to give a clear picture about their spatial variability or structure. The spatial structure of the groundwater quality variables can produce, for example, contour maps of the variable means. These maps can be used for predicting and signifying pollution areas. Accordingly, protection

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measures and management and planning decisions can be made to minimize the deterioration in the polluted areas.

Geostatistical methods were developed to create mathematical models of spatial correlation structures with a variogram as the quantitative measure of spatial correlation. The variogram is commonly used in geostatistics and the interpolation technique, known as kriging, provides the “best”, unbiased, linear estimate of a regionalized variable in an unsampled location, where “best” is defined in a least-squares sense. The emphasis is set on local accuracy, i.e. closeness of the estimate to the actual, but unknown, value without any regard for the global statistical properties of the estimates. The kriging estimation variances are independent of the value being estimated and are related only to the spatial arrangement of the sample data and to the model variogram.

One development of geostatistics, that has become more popular in the last decade, is the stochastic simulation which represents an alternative modelling technique, particularly suited to applications where global statistics are more important than local accuracy. Application of geostatistics techniques in hydrological sciences is a useful approach to avoid some errors and increase of calculation accuracy as well. In classic statistics samples taken from a population are lack of spatial properties. Therefore the calculated values of a parameter in a homogeneous sample do not include any information of the same parameter in another sample with a defined distance. Geostatistics consider the value as well as location of the sample. Then it is possible to analyze value and location of the samples together. To achieve this purpose it is necessary to relate spatial properties (distance, direction) of different samples using mathematical formula called spatial structure.

Obviously geostatistical methods use various variables and then produce different results. In many cases a method which is selected to reach the prediction process but it is vital to find out the most appropriate interpolation technique for precipitation prediction. Amini (2002) applied kriging and co-kriging techniques for predicting Cl<sup>-</sup> concentration of soil in Roudash, Isfahan which showed that kriging method provides more accurate and low cost results.

Azimzadeh et al. (2005) used kriging technique to estimate the area of desert pavement and threshold velocity of wind erosion in Mehriz,

Yazd. The results indicated that common kriging is a precise and relevant method to produce the map of the effective factors of wind erosion including Reg area and iso-velocity threshold lines. Campling et al (2007) were used kriging method to estimate spatial distribution of rainfall as well as to optimize the number and location of rain gages in Spain. Kriging techniques are employed to assess the spatial dependencies of the water quality variables such as TDS (e.g. Jager et al, 1990), groundwater level (e.g. Hudak and Loaiciga, 1993; Geo et al, 1996; Ahmed, 2002) and groundwater quality variables such as NO<sub>3</sub> and Cl (e.g. Rohani and Hall, 1988; Loaiciga, 1989). Ahmed (2002) applied kriging to assess the spatial dependencies of the water quality variables such as TDS and concluded that kriging has high capability for this purpose. Torabi (1999) investigated the groundwater table in Qom plain.

Jager et al. (1990) also used geostatistical tools like kriging to simulate groundwater quality variables and they result kriging is better than other geostatistical tools for simulating groundwater quality variables. Cressie, N (1985) introduced kriging method as most acceptable and strongest tool to interpolate data for preparation of contour maps of groundwater. Mohammadi et al (1999) used geostatistical tools to prepare hazard zonation maps of ecological pollution. Misaghi et al (2002) estimated groundwater table by using geostatistics methods. Nazarizadeh et al (2005) used geostatistical tools to investigate the spatial structure of groundwater quality variables and stated that the variograms of EC, Cl, So<sub>4</sub><sup>-2</sup> have spherical structure.

For correct watershed management planning the maps of important characteristics of water resources such as: EC, Ca, Mg, Cat ion, ... should be used. The use of current and traditional methods for investigation of changes of spatial structure of groundwater quality variables are expensive and time-consuming methods. On the other hand classic statistics can not consider spatial changes of variables. Physical and chemical characteristics of water resources change in time and place, even spatial structure of water variables change in various geographic directions. Therefore in this research geostatistical methods are used that consider spatial structure and changes of groundwater quality variables.

In the current study, kriging and Weighted Moving Average with the power of 2 were applied for presenting spatial variation of water properties in Dameghan plain, Iran.

## 2. Materials and Methods

### 2.1. Study area

The study region located in north eastern of Iran in Semnan province with 35° 36' 14" to 36° 5' 9" latitudes and 54° 5' 44" to 54° 58' 16" longitude which covers 15600 ha. Temperature variation in the region is high. The minimum

temperature in the area is -12°C in winter while it reaches to higher than 44° C in summers. The annual pan evaporation varies between 1250-4200 mm. The climate of study area is mostly semi-arid and the annual precipitation is 148.4 mm. In this study we used groundwater quality observations since (1999-2006) from 58 domestic wells in Dameghan plain (Figure 1).

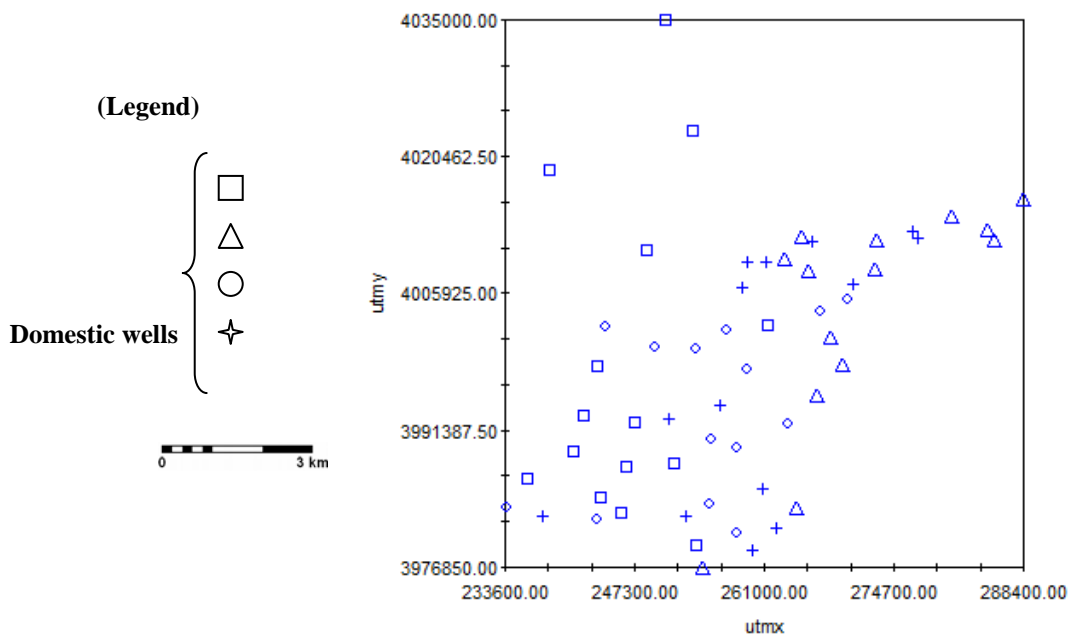


Fig.1. Distribution of domestic wells in the study area

### 2.2. The method of data collecting

This research has been done by using the data of 58 observed wells that have been gathered by Ministry of Power and Electricity. The depth of the wells is 35-55 meters. Because of high cost of data collecting from the other wells (no observed wells) and difficulty of the data gathering, the prepared data by mentioned Ministry have been used in the current study.

### 2.3. Methods

Geostatistical prediction includes two stages which is first identification and modeling of spatial structure. At this stage continuity, homogeneity and spatial structure of a given variable is studied using variogram. Second stage is geostatistical estimation using kriging technique

which depends on the properties of the fitted variogram which affects all stages of the process.

### 2.4. Variogram analysis

Variogram method is a suitable technique for estimating spatial variability of a variable. Calculation of variogram graph is one of essential stages in geostatistics which is defined as follow:

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

Where:

$\gamma(h)$ : value of variogram for pair points with distance h

$n(h)$ : Number of pair points with distance h

$Z(x_i)$ : observed value of variable x

$Z(x_i+h)$ : Observed value of the variable with distance h from x

For variogram plotting it is necessary to compute  $\gamma(h)$  for different values of  $h$  and then to plot the values for different distances of  $h$ . In another word variogram is the variance of different points with distance  $h$ . The obtained variograph of measured samples is called experimental variogram which is a vector value that is a dependent of distance and direction.

The properties variogram include threshold (sill=C0). The threshold is the maximum value of variogram which is spatial variance of the variable. The lowest value of variogram includes partial effect which shows variance of errors of measurements. The effective distance demonstrates the distance. That variogram has the highest value. Instead of variance, covariance shows the similarity of variables. Since arithmetic summation of similarity and dissimilarity is constant then it is possible to replace it with the average difference of points of distance  $h$ . The relation between variogram and co-variogram is defined as:

$$\gamma(h)+c(h)= \sigma^2 \tag{2}$$

Where:

$\sigma^2$ =threshold

$\gamma(h)$ : variogram value

$c(h)$ : co-variance value

### 3.4. Theory of common kriging

Kriging is a prediction method that considers values of a variable in unsampled points as a linear composition of the values of surrounding points. Considering the values of variable  $Z$  in  $n$  measured points as follow:

$$Z = (z(x_1), z(x_2), \dots, z(x_n)) \tag{3}$$

Estimation of  $Z$  in point  $X_0$  using kriging estimation is defined as:

$$Z^*(x_0) = \sum_{i=1}^n \lambda_i z(x_i) \tag{4}$$

The most important part of kriging is statistical weights assigned to  $\lambda_i$ .

To avoid bias of estimation, the weights should be determined in a way that summation is equal to one ( $\sum_{i=1}^n \lambda_i = 1$ ) and the variance of estimates should be minimized-as:

$$\text{var} [z^*(x_0)] = E [(z^*(x_0) - z(x_0))^2] = \text{Min} \tag{5}$$

### 3.5. Weighted Moving Average (WMA)

In WMA technique, the value of weighting factor ( $\lambda_i$ ) is estimated based on the following equation.

Where:

$$\lambda_i = \frac{D_i^{-\alpha}}{\sum_{i=1}^n D_i^{-\alpha}} \tag{6}$$

$D$ : the distance between observed and estimated points

$\alpha$ : equation order

$n$ : Number of observed points:

Three mentioned methods were validated using follow criteria:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (z^*(xi) - Qz(xi))^2} \tag{7}$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |z^*(xi) - z(xi)| \tag{8}$$

It should be mentioned that the results of three described methods were obtained using GS<sup>+</sup> software.

## 4. Results

Since the first step for geostatistical application for a set of data is variogram analysis then the results of variogram analysis in the study area were calculated (Table 1). Then kriging, and WMA methods were applied for the data (Table 2).

It is necessary to keep in mind that normality test was examined for the data and logarithm of the data were used to avoid skewness.

Table 1. The properties of suitable variogram model of variables

Variable	Mean	Sd	Skewness	Kurtosis	Model	Nugget	Sill	R <sub>o</sub> (effective range)	C <sub>o</sub> /C <sub>o</sub> +C
SAR (me/l)	5.29	2.6	0.86	1.71	Spherical	0.087	1.458	112100	0.94
EC (ds/m)	2630	1635	3.47	9.02	Linear	0.001	1.611	10200	0.999
pH	8.2	0.24	0.96	1.87	Spherical	0.014	0.0857	40400	0.83
TDS (mg/l)	1734	1100.6	2.51	9.16	Linear	0.001	2.011	101900	0.999
Cat ion (me/l)	26.6	17.001	2.58	9.72	Linear	0.001	1.61	10200	0.999
Na (me/l)	49.6	17.47	1.37	2.68	Spherical	1	2.77	53900	0.999
Mg (me/l)	6	4.62	1.35	1.01	Linear	0.001	2.01	55200	1
Ca (me/l)	8.4	9.43	4.45	24.66	Linear	0.001	2.01	54300	1

Table 2. The results of estimation of different geostatistical techniques

Variable	Method of estimation	r	RMSE	MAE
SAR (me/l)	Kriging	0.13	2.95	2.01
SAR (me/l)	WMA-2	0.017	2.86	1.99
EC (ds/m)	Kriging	0.53	1402.6	866.8
EC (ds/m)	WMA-2	0.50	1484	877.2
pH	Kriging	0.73	0.17	0.12
pH	WMA-2	0.70	0.173	0.121
TDS (mg/l)	Kriging	0.52	942.9	580
TDS (mg/l)	WMA-2	0.42	1020	585
Cation (me/l)	Kriging	0.015	6.8	5.9
Cation (me/l)	WMA-2	0.04	6.54	5.7
Na (me/l)	Kriging	0.04	6.98	4.9
Na (me/l)	WMA-2	0.14	7.57	5.1
Mg (me/l)	Kriging	0.49	9.1	4.67
Mg (me/l)	WMA-2	0.73	3.1	2.25
Ca (me/l)	Kriging	0.52	7.1	2.5
Ca (me/l)	WMA-2	0.49	8.5	3.7

The spatial variations of the mean of the variables are presented in Fig.2 where the contour lines were drawn using the kriging technique. In Fig.3 Average concentration distribution maps of: Ca, EC, Cat ion, Mg, Na and pH in Dameghan plain have been shown.

## 5. Variograms

In the references, spatial interrelationship of data is assessed by  $(C/C+C_0)$ , and if this parameter is close to 1, spatial interrelationship is suitable and if the mentioned parameter is close to 0 spatial interrelationship is weak and the value of nugget effect is high. All of physical and chemical soil factors that have been investigated in this research (according to table 1), have high value of mentioned parameter  $(C/C+C_0)$ , and this issue justifies the use of geostatistical techniques. According to table 1 spatial interrelationship of Mg and Ca data are higher than the other variables.

As seen in the variogram results (Table 1) the most appropriate models fitted to groundwater quality variables are spherical and linear models. However the results of current study show high spatial structure of the variable data but the most appropriate results based on the statistical comparisons showed high capability of kriging technique.

Figure 2 shows the variograms of physical and chemical soil factors that have been investigated in this research.

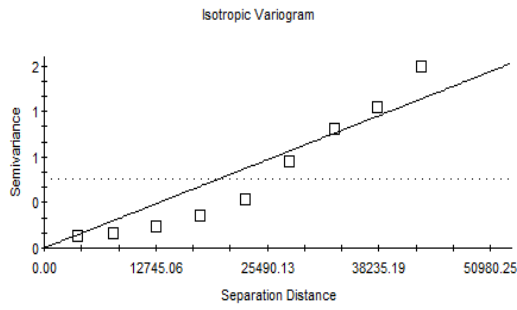
Assessment of effective range of various parameters show that some variables like EC and TDS have short effective range and for their assessment, we should prepare grading with short distance, If we want to calculate sampling distances (grading) for these two variables (EC and TDS) is 2/3 effective range (about 7 km), for Mg, Ca and pH, sampling distance is about 37 km and for SAR, Na and cation, it is about 74 km. (7)

All of physical and chemical soil factors that have been investigated in this research have high value of  $(C/C+C_0)$  parameter, and this issue justifies the use of geostatistical techniques.

In Fig. 3 average concentration distribution maps of: EC (a), Ca (b), Cat ion (c), Mg (d), Na (e) and pH (f) in Dameghan plain, over 1999-2006 have been shown.

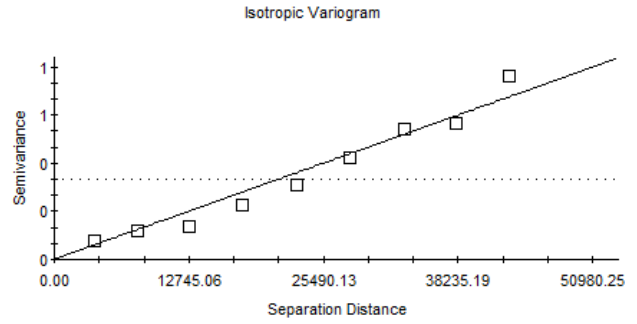
This study has attempted to predict the spatial distribution and uncertainty of groundwater quality variables in the north Eastern of Iran Semnan Province using the geostatistical techniques (kriging and WMA-2). Pollution from agriculture and industrial origin threatens the groundwater quality in Iran. Since groundwater is the main source of fresh water, pollution causes a decrease in the long-term resources of water suitable for human consumption. Furthermore, because most groundwater finally flows to the surface, a deterioration of groundwater quality affects the ecohydrological conditions of the receiving seepage areas as well as the receiving seas.

Ca



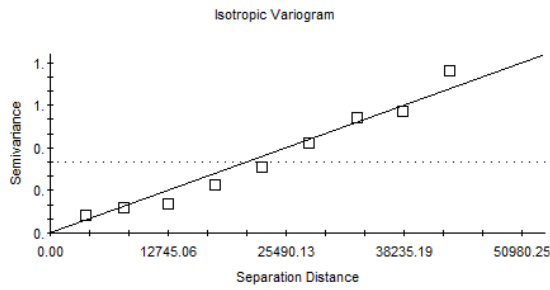
Linear model ( $C_0 = 0.0010$ ;  $C_0 + C = 2.0100$ ;  $A_0 = 54300.00$ ;  $r^2 = 0.934$ ;  $RSS = 0.427$ )

EC



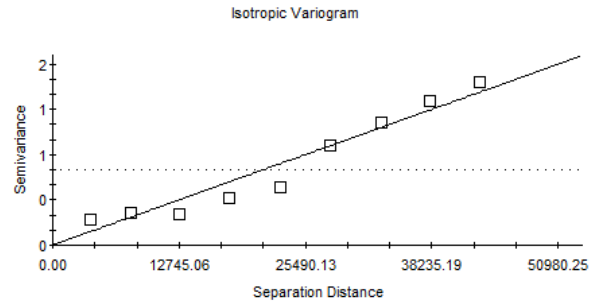
Linear model ( $C_0 = 0.0010$ ;  $C_0 + C = 1.6110$ ;  $A_0 = 102000.00$ ;  $r^2 = 0.966$ ;  $RSS = 0.0194$ )

Cat ion



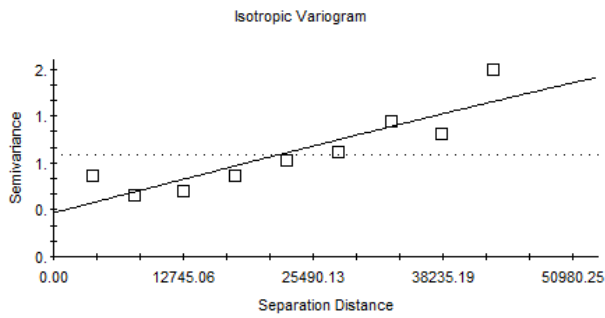
Linear model ( $C_0 = 0.0010$ ;  $C_0 + C = 1.6140$ ;  $A_0 = 102000.00$ ;  $r^2 = 0.966$ ;  $RSS = 0.0194$ )

Mg



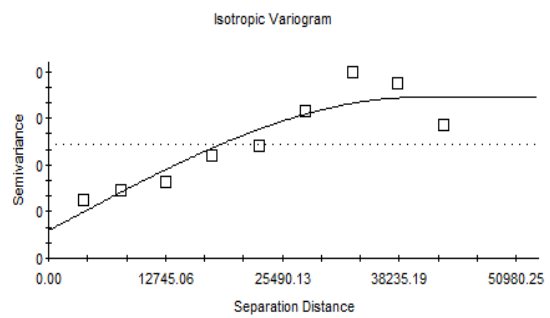
Linear model ( $C_0 = 0.0010$ ;  $C_0 + C = 2.0110$ ;  $A_0 = 55200.00$ ;  $r^2 = 0.941$ ;  $RSS = 0.147$ )

Na



Spherical model ( $C_0 = 0.3800$ ;  $C_0 + C = 2.7700$ ;  $A_0 = 155700.00$ ;  $r^2 = 0.796$ ;  $RSS = 0.196$ )

pH



Spherical model ( $C_0 = 0.0146$ ;  $C_0 + C = 0.0857$ ;  $A_0 = 40400.00$ ;  $r^2 = 0.849$ ;  $RSS = 7.372E-04$ )

Fig. 2. Variograms of variables

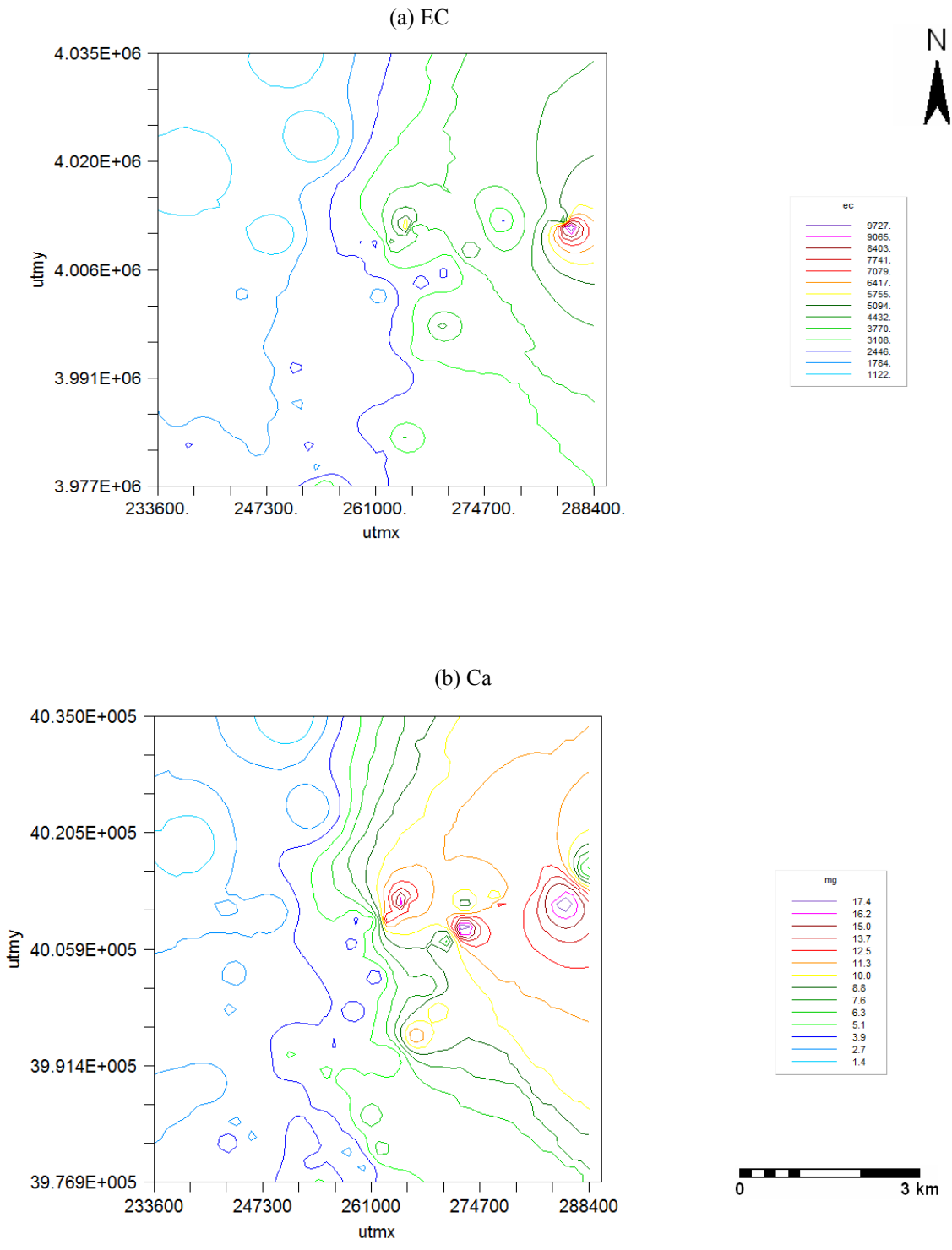


Fig. 3. Average concentration distribution maps of: EC (a), Ca (b), Cat ion (c), Mg (d), Na (e) and pH (f) in Dameghhan plain, over 1999-2006

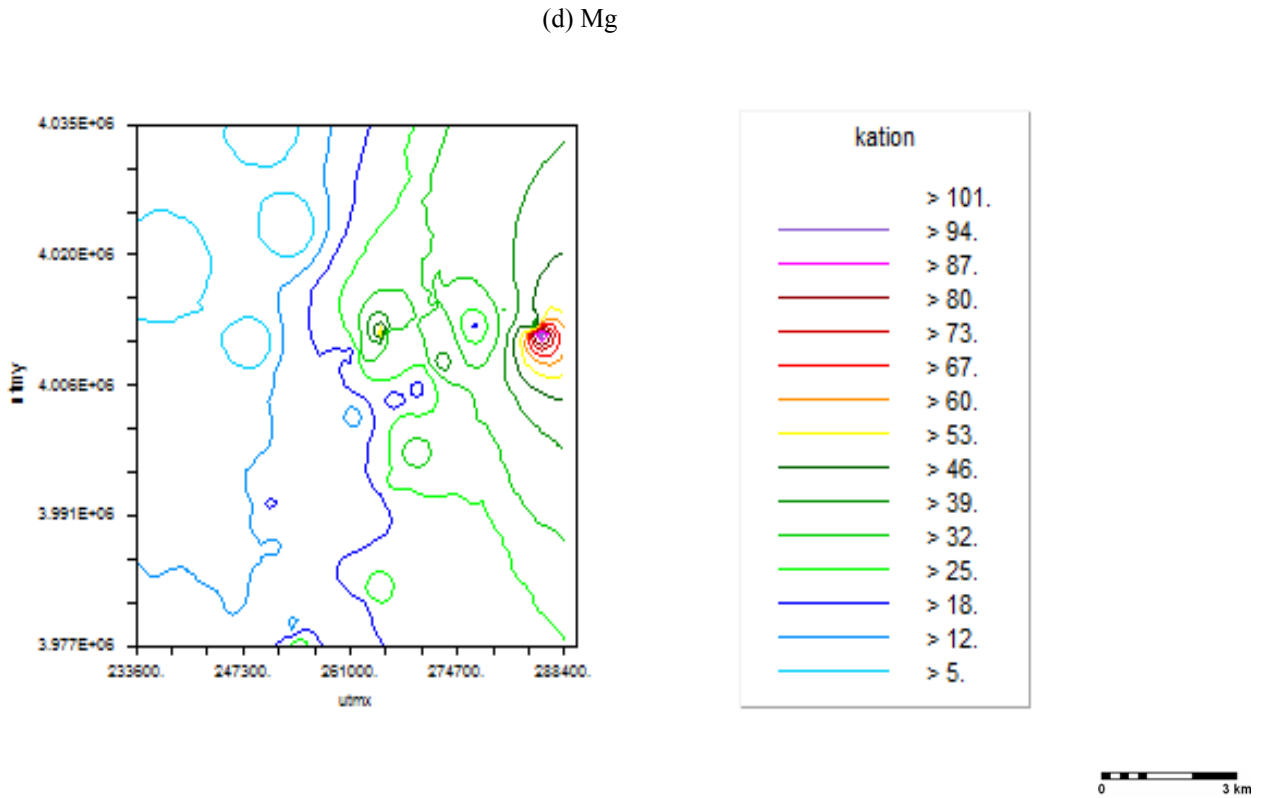
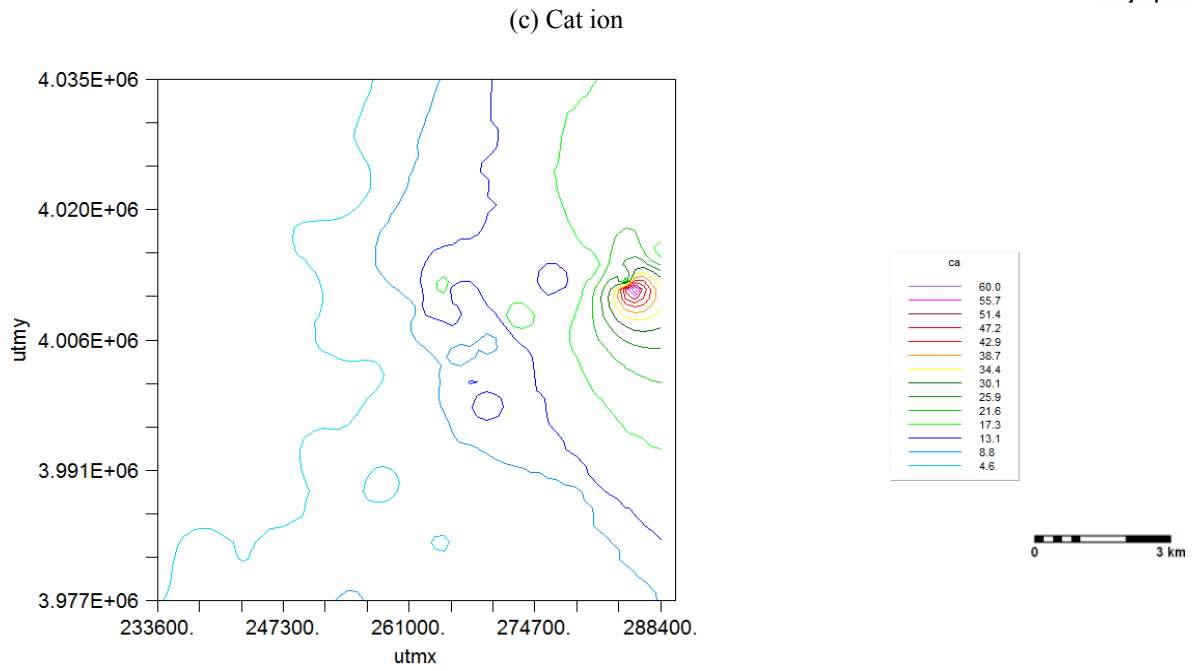
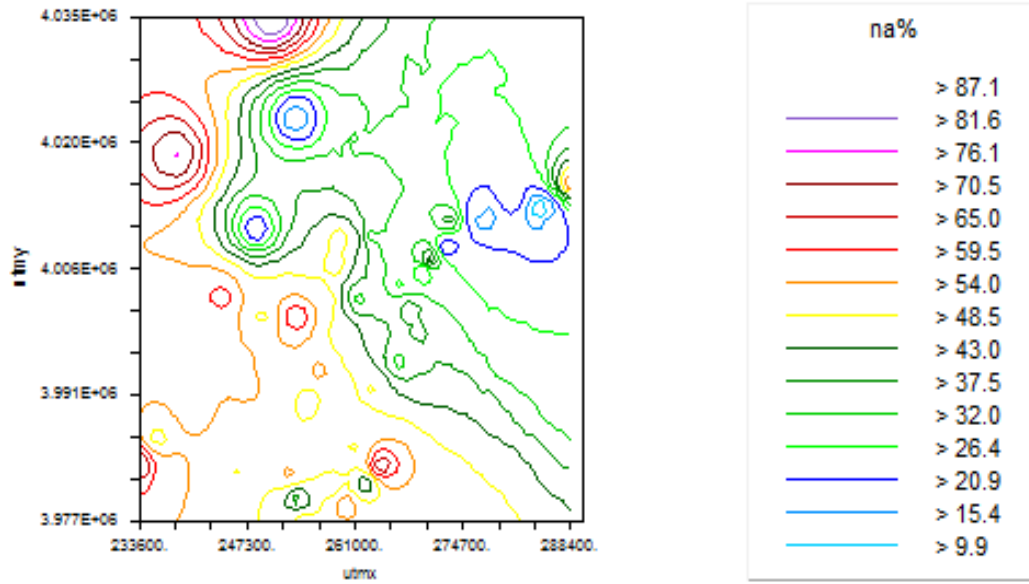


Fig. 3. Average concentration distribution maps of: EC (a), Ca (b), Cat ion (c), Mg (d), Na (e) and pH (f) in Dameghhan plain, over 1999-2006





(e) Na



(f) pH

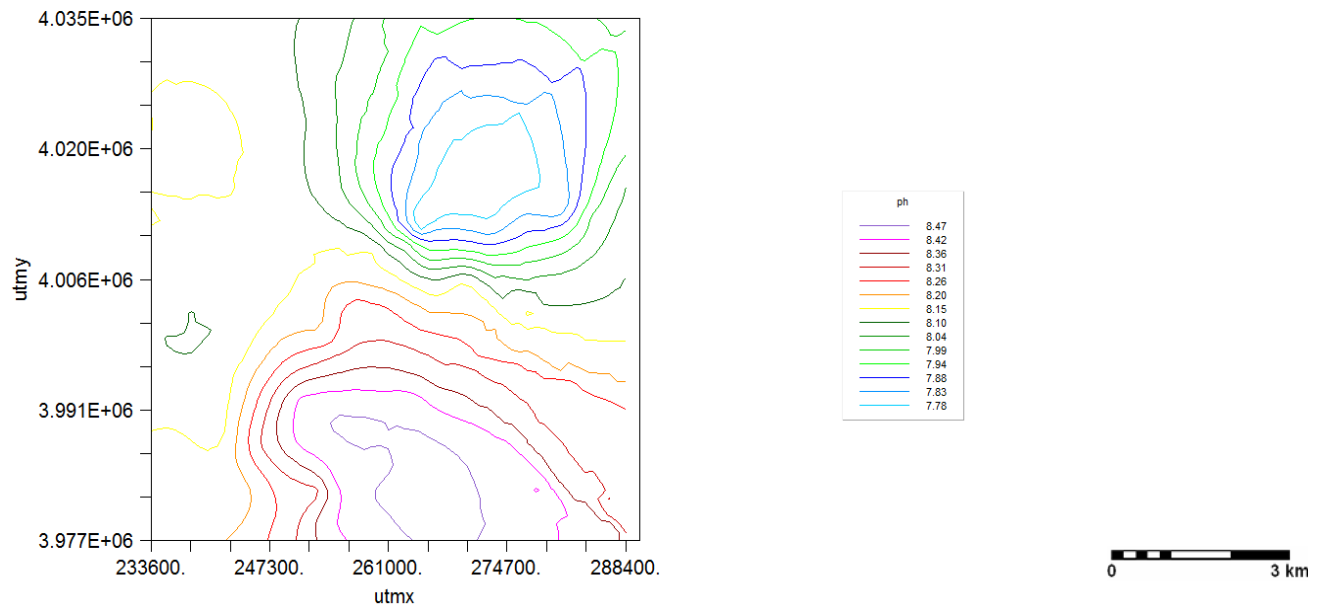


Fig. 3. Average concentration distribution maps of: EC (a), Ca (b), Cat ion (c), Mg (d), Na (e) and pH (f) in Dameghan plain, over 1999-2006

## 7. Discussion and Conclusion

The use of current and traditional methods for investigation of changes of spatial structure of groundwater quality variables are expensive and time-consuming methods. On the other hand classic statistics can not consider spatial changes of variables. Physical and chemical characteristics of water resources change in time and place, even spatial structure of water variables change in various geographic directions. Therefore in this research geostatistical methods are used that consider spatial structure and changes of groundwater quality variables.

The analysis showed that for more groundwater quality variables (e.g. TDS, EC, Cat ion, Na, Ca) kriging technique performed better than WMA-2 technique in characterizing the spatial variability. WMA-2 technique only for some groundwater quality variables like SAR and Mg has better result than kriging to simulate groundwater quality variables.

As seen in the variogram results (Table 1) the most appropriate models fitted to groundwater quality variables are spherical and linear models. However the results of current study show high spatial structure of the variable data but the most appropriate results based on the statistical comparisons showed high capability of kriging technique.

Assessment of effective range of various parameters show that some variables like EC and TDS have short effective range and for their assessment, we should prepare grading with short distance, If we want to calculate sampling distances (grading) for these two variables (EC and TDS) is 2/3 effective range (about 7 km), for Mg, Ca and PH, sampling distance is about 37 km and for SAR, Na and cation, it is about 74 km.

All of physical and chemical soil factors that have been investigated in this research have high value of  $(C/C+C_0)$  parameter, and this issue justifies the use of geostatistical techniques.

This study shows the high capability of geostatistical tools for provision of maps of spatial structure of groundwater quality variables.

The results also confirm the research conducted by Ahmed (2002) and Jager et al.

(1990) that they also concluded geostatistical tools like kriging have high capability for simulating groundwater quality variables.

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