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Geostatistical Based Modelling of Variations of Groundwater Quality During 2006 to 2009 (in Tehran-Karaj Plain)

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ABSTRACT

Preparation of timely maps for changing the qualitative parameters of ground waters is an important pace in the efficient management and exploitation of these resources. Adoption and precision of suitable zoning methods and also mapping of changes in properties of these resources depend upon situations and existence of data and information in the studying area. The current research was aimed to evaluate the geostatistics methods in preparation of map of qualitative characteristics, situation of groundwaters of Tehran-Karaj plain during 2006 to 2009, and zoning of them for drinking purposes. Thus, secret methods of geostatistics – simple, ordinary, separated, universal kriging and co-kriging (using supplementary variant) for the purpose of spatial estimation of the total variants of dissolved solids, electric conduct, nitrate's and sodium's ion were used. The results of the evaluation of Interpolation methods indicate relative advantage of co-kriging method and using a supplementary variant. Therefore, the Interpolation of variants was performed according to RMSE indicator. According to the results, the most density of the variants under the experiment was found in the eastern and the southern regions, which is extended to the north-west of the plain during 1997 to 2000 era. Afterwards, zoning of the plain was done according to drinking water standards, which was categorized into three levels of desirable, admissible, and undesirable, due to the variants. *(Abstract)*
KEYWORDS*:* quality parameters of groundwater, drinking-water standards, spatial modeling, geo-statistics, RMSE

I. INTRODUCTION

The increasing growth of population and the constant promotion of hygienic standards poses policy-making, scheduling investing on providing and owning a vaster volume of clean water as one of the major concerns of the country. On the one hand, limitations on water and water-sources having admissible quality; and on the other hand, the increasing contamination of the accessible water-sources by contaminators from industries, home and urban sewage and also agricultural sewage, make prevention of water-sources from getting contaminated, and promoting the present qualities and using lower-quality sources of water as inevitable (Habibi and Masoumi, 2006).

The change in the quality of groundwater, and the water-sources getting salty, are nowadays critical dangers in the way of development of agriculture in the country, particularly in dry lands. The quality of ground-water is changing continually, the same as surface water. But the changes are much slower than surface water (Mahdavi, 1998).

Providing on-time tables from the changes in characteristics of groundwater can be a great step toward the correct utilization of water-sources.

Furthermore, tables of the changes in chemical characteristics of groundwater, can have worthwhile role in the process of decision-making, usage-management from ground-water (Shabani, 2007).

There are different methods for studying and zoning the changes in the characteristics of groundwater that each one of them, due to the area's condition and availability of statistics and information have different precisions. Some of the methods of interpolation for studying and preparing the tables of the changes in quality of grounwater are kriging geostatistics and cokriging and soecific methods like Inverse Distance Weights, Radial Basis Functions, Global Polynomial Interpolation, and Local Polynomial Interpolation. Selection of a proper method for zoning and preparing a table of the changes in quality characteristics of groundwater are of fundamental steps in management of water-sources of the region.

In recent years, many researchers, using geostatistic methods, have tried to prepare quality tables of groundwater. Maleki Genadishi et al. (1999), besides estimation of some quality parameters available in groundwater in Zarand plain by using kriging method, have also done zoning on the available parameters and have classified grounwater in Zarand plain as well. Ahmed (2002) utilized the usage of kriging method in estimating spatial relation of quality variants of water, like all the dissolved solids, and concluded that kriging is of great capability in this regard. Bajjali (2005) simulated the effect of the four artificial sustenance dams on the quality of grounwater, concerning the total dissolved solids in Oman, using the three methods of kriging, , and Global Polynomial Interpolation. The results proved priority of kriging and Inverse Distance Weights in studying quality of groundwater and zoning the tables of the changes in the total dissolved solids in the case study region. Taghizadeh Mehrjerdi et al. (2009) worked on spatial analysis of some quality characteristics of groundwater, like the total dissolved solids, total hardness(TH),

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electric conductivity(EC), Sodium absorption relation(SAR), Chlorine ion(cl^-) and Sulfate(SO42-), using the three methods of Inverse Distance Weights, kriging and cokriging in a case study in Rafsanjan plain. Evaluation of the outcoming results on the RMSE basis proved that cokriging method exceeded the two other methods and finally was selected as the final and proper method for providing the table of the quality characteristics of groundwater in the region. Barcae and Passarella (2008) used disjunctive kriging and simulation methods for providing the table of the danger of changes in Modena plain_Italy. The results proved that the disjunctive kriging method is proper for studying the danger of ruination of the quality of groundwater. Fetouani and Vanclooster (2008), in a study of the quality of groundwater in the agricultural plains of Triffa, in NorthEast of Morracco, utilized the ordinary kriging method for studying a zoning the quality table of groundwater, concerning the volume of Ammonium Nitrates and Bacterial impurities. The outcoming results indicated meaningful changes, as compared to the former studies, and proved that if no preventive strategy is taken, then the development of agricultural lands in the regions would lead to destruction and decline in the quality of groundwater. Sha'bani (2012), in a study evaluated the geostatistic methods in providing tables of the quality of groundwater and zoning them in Neyriz plain_Fars province. The results of the study indicated the priority of geostatistic methods (cokriging and ordinary kriging) in evaluation of groundwater parameters. Mohammadi et al. (2012) also studied the trend of spatial and time changes in the level of groundwater in Kerman plain, utilizing the geostatistic methods over a 10 year period. According to the study, the level of groundwater in most parts of the plain faced decline as a result of increase in usage and continual droughts, and that in the area of Kerman, it has faced increase of waterflow as a result of increase in returning flow and sewage. According to the importance of groundwater resources, especially in dry and semi-dry regions, and the importance of correct management, the present study was done aiming at simulation of spatial changes of some quality characteristics of groundwater, with the emphasis on drinking uses, using geostatistic methods. The quality variants of drinking water evaluated in the present study include: Total Dissolved Solids (TDS), Electric Conduct (EC), Nitrates' Ion Density (NO3-) and Sodium (Na).

II. MATERIALS AND METHODS

A. *Introduction of the case study region*

The region studied is Tehran-Karaj plain, located between Tehran and Alborz provinces. The plain with a extent of around 4410 square kilometers, is located in the Southern skirt of Alborz and in geographical place of 50 degrees, 41 minutes upto 51 degrees and 48 minutes longitude, and 35 degrees and 3 minutes upto 35 degrees, 57 minutes latitude. The average rainfall in the region is 316 millimeters, and the average temperature is 39.4 degrees centigrade. Fig. 1 shows the geographical location of the region studied, and also shows scatter plot of the parts the samples were taken.

B. *Statistic Resources*

To do the present research, quality data of groundwater from deep and semi-deep wells in the scope of Tehran-Karaj plain, for the years 2007 and 2010 (provided by the local water and sewage company of Tehran province), were used. Among the calculated data in 2007, the information from 90 wells and in 2010 the information from 70 wells were recognized proper in terms of accuracy and were analyzed afterwards. Also the study of statistic characteristics, Interpolation, and quality zoning of the data were done in SPSS 17.0, GS+5.3 and ArcGIS 10.0 softwares.

C. *Survey of spatial structure of data*

Statisticians of geostatistics estimate the unknown values, using the known values and variograms. Variogram is a maths model which is used for describing spatial connectivity of a variant. For this purpose, it is necessary to calculate the total of square subtraction of pair spots which are located as *h* distance from the other, and then draw them before *h*. The first equation and Fig. 2 show calculation form and an overall view of a variogram (Marofi et al. 2009).

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

In which $\gamma(h)$ is variogram value in h distance; $Z(x_i + h)$ is the calculated value of the variant in $(x_i + h)$; $Z(x_i)$ is the calculated value of the variant in (x_i); and n is the number of spots for calculation.

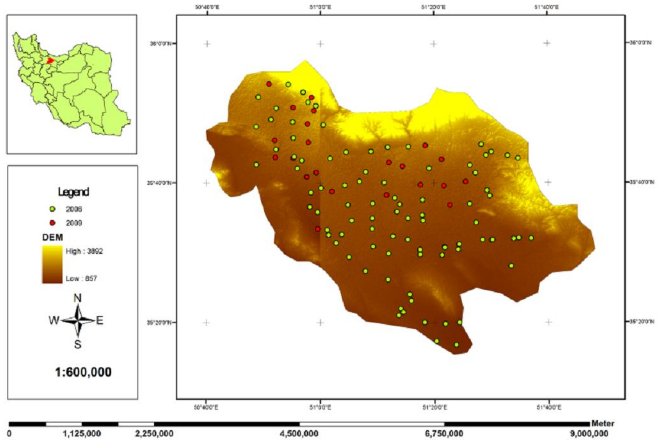

Figure 1. Geographical status of region and scatter plot of testing spots.

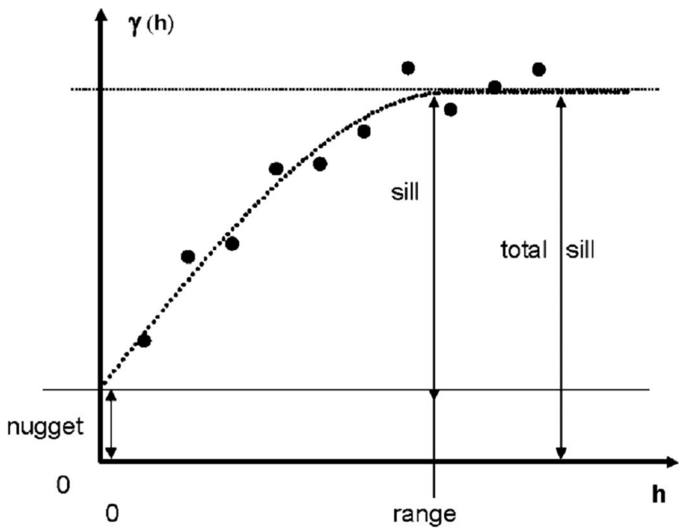

Figure 2. An overall view of Variogram. (*Marofi et al. 2009*)

III. Geostatistic Methods

A. Ordinary kriging

Kriging estimates the values of a variant in non-tested spots as a linear complex of values from the same variant in the surrounding spots and to estimate the unknown spots, it relates some weight to each of the samples (Equation 2).

$$Z_0 = \sum_{i=1}^{n} \lambda_i Z(x_i)$$

In which $Z(x_i)$ is the calculated value of the variant in (x_i); Z_0 is the estimated value of the variant in the spot; λ_i is the dedicated weight to the variant x in I spot; and n is the number of spots that the variant has been calculated in them.

The condition of using this estimator is that the variant has normal distribution (Zehtabyan et al. 2010).

B. Simple Kriging

The estimator in simple kriging is as a weight-holding linear complex; but this average μ which should certainly have the characteristic of 2nd level static, is of much concern in process of estimation.

C. Universal Kriging

It is in such conditions that both categories of changeability (enforced and random), simultaneously be present at the spatial structure of regional variant, in a way that the reactions and the pattern of changeability of the variant could be shown in the following form (Equation 3).

$$Z(x) = \sum_{k=0}^{k} ak.\, fk(x_i) + \varepsilon(x_i)$$

D. Disjunctive Kriging

It is a non-linear estimator and is used in cases that the distribution of variants is complicated, or estimating them with ordinary statistical distributing methods (Normal or Log-normal) would be hard (Habibi Arbatani et al. 2009).

E. Cokriging

As there are multi-variable methods in classic statistics for estimation, in geostatistics also one can estimate using cokriging method based on relation among different variants; the mentioned characteristic can lead to a better precision in estimations and thrift in expenses (Taghizade Mehrjerdi et al. 2009). Cokriging Equation, assuming a supplementary variant and a principal one is as follows:

$$Z^*(x_0) = \sum_{i=1}^{n} \lambda_{1i} Z_1(x_i) + \sum_{j=1}^{m} \lambda_{2j} Z_2(x_j)$$

In which $Z_2(x_i)$ is the supplementary spatial variant; $Z_1(x_j)$ is the principal spatial variant; and $Z^*(x_0)$ is unknown value of variant in x_0.

In sequence of the number of sampling spots of principal and supplementary λ_{1i} and λ_{2j}, m and n are statistical weights dedicated to the principal and supplementary variants.

Choosing a proper method for Interpolation and estimation of a variant depend on the kind of variant and the environmental effective factors and one cannot consider a selected method for a special region as the prior method in general (Istok and Cooper, 1998). Therefore, in the present study the simulation of spatial changes was done using two of the geostatistic methods_kriging (ordinary, simple, universal and disjunctive) and cokriging (along with supplementary variant).

F. Choosing the most proper method and quality zoning for drinking water usage

After drawing variogram and a proper method, the process of Interpolation was dealt with, using the aforementioned methods. For this purpose, one can use different methods, that one of the most proper ones is utilizing the results of Cross Validation (Davis, 1987). First, one of the measuring spots is eliminated, and using the other spots and using Interpolation method for the eliminated spot, statistic estimation is done. In the next step, the spot is replaced on its own place, and another spot is eliminated, and this continues for all the spots, presenting an estimation and a visual value. There are different criteria for evaluating the efficiency of the Interpolation methods. For test of Fitness of Interpolation methods, in the present study, the criterion of Root of Mean Square Error (RMSE) was used, whose equation of calculation of this criterion is as follows (Davis, 1987):

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

□□□

In which $\hat{Z}(x_i)$ is the estimated value in x_i; $Z(x_i)$ is the calculated value in x_i; i is the number of spots; n is the number of the observed spots of the criterion.

Finally the interpolated variants on the basis of national standards, edited by Standard and Industrial Researches Institute, were re-classified for utilizing for drinking purpose, Table 1.

TABLE 1 – DRINKING WATER STANDARDS (INDUSTRIAL RESEARCHES INSTITUTE OF IRAN, 2010)

Variable	Allowed range	Optimal range
TDS (mg/l)	1500	1000
EC (µm/cm)	2000	1500
NO^{3-} (mg/l)	45	0
Na^{+} (mg/l)	250	200

IV. RESULTS

Utilizing geostatistic methods needs surveying the presence of spatial structure through the data, which is surveyed by variographic analysis. Also by the use of variograms, one can recognize the radius correlation of variants, static surveyance, and presence or lack of trend in our data. The analysis could be utilized, provided that the data are normal. Therefore, the utilized data were normalized by taking logarithm from the main data. Also, to Fitting the best model on experimental variogram, lower Residual Sums of Squares (RSS) and stronger space structure was used; the less the $C_0/(C_0+C)$, the better the space structure of the variant would be drawn.(Shi et al. 2007) The results are shown in Tables 2-3.

According to the outcoming results, the best Fitting model was achieved according to the information on 2007 for the total variants of dissolved solids, electric conduct, global sodium ion, and linear model for nitrates ion. Also the best Fitting result was achieved on 2009 for all the global models.

For the space structure of the variants, according to the information of 2003, the total variants of dissolved solids, electric conduct, and sodium ion had stronger space structure (less than 0.25), and nitrates' ion had weak space structure (more than 0.50). The space structure taken from the information on 2009 was also similar to the aforementioned results, and was the progress of space structure of nitrates' ion from weak to average (0.25 to 0.75). Tables 3-4 also show the results taken from variogram of the data on 2007 and 2009, which is necessary for calculations of cokriging method.

TABLE 2 – RESULTS OF VARIOGRAM ANALYSIS OF 2007 DATA

Variable	Mean	Standard devotion	Skewness	Model	Nugget (C0)	Sill (C0+C)	Radius of influence	C0/(C0+C)	R2	RSS
TDS (mg/l)	1051.33	1053.84	2.50	Spherical	0.135	1.016	66400	0.133	0.992	0.005
EC (µm/cm)	1615.52	1581.60	2.56	Spherical	0.129	1.021	74000	0.126	0.988	0.005
NO^{3-} (mg/l)	28.05	22.43	1.08	Linear	2.43	2.43	62718.82	1	0.698	4.72
Na^{+} (mg/l)	186.41	228.45	2.72	Spherical	0.15	2.05	60500	0.073	0.971	0.09

TABLE 3 – RESULTS OF VARIOGRAM ANALYSIS OF 2009 DATA

Variable	Mean	Standard deviation	Skewness	Model	Nugget (C0)	Sill (C0+C)	Radius of influence	C0/(C0+C)	R2	RSS
TDS (mg/l)	769.64	587.52	1.32	Spherical	0.13	0.645	43800	0.201	0.908	0.023
EC (µm/cm)	1197.65	879.50	1.36	Spherical	0.12	0.581	43900	0.21	0.911	0.018
NO^{3-} (mg/l)	38.30	28.00	1.10	Spherical	0.328	0.708	41300	0.463	0.881	0.0165
Na^{+} (mg/l)	117.60	107.11	0.96	Spherical	0.24	1.4190	60884	0.170	0.672	0.486

TABLE 4 – RESULTS OF CONTRASTIVE VARIOGRAM ANALYSIS OF 2007

Variable	Supplementary variable	Correlation Coefficient**	Model	Nugget (C0)	Sill (C0+C)	Radius of influence	C0/(C0+C)	R2
TDS (mg/l)	Mg2+ (mg/l)	0.902	Spherical	7.60	171.30	52100	0.045	0.975
EC (µm/cm)	Mg2+ (mg/l)	0.904	Gaussian	5.90	112.80	95500	0.052	0.993
NO^{3-} (mg/l)	Mg2+ (mg/l)	0.730	Exponential	0.10	36.64	32700	0.003	0.873
Na^{+} (mg/l)	EC (µm/cm)	0.856	Spherical	180	3470	16000	0.051	0.974

**The data are of meaningful relation on 99% scale

ABLE 4 – RESULTS OF CONTRASTIVE VARIOGRAM ANALYSIS OF 2009

Variable	Supplementary variable	Correlation Coefficient**	Model	Nugget (C0)	Sill (C0+C)	Radius of influence	C0/(C0+C)	R2
TDS (mg/l)	EC (µm/cm)	0.999	Exponential	48000	701900	18500	0.069	0.878
EC (µm/cm)	TDS (mg/l)	0.999	Spherical	97	494	48100	0.20	0.910
NO3- (mg/l)	K+ (mg/l)	0.660	Spherical	0.083	0.9930	85500	0.084	0.950
Na+ (mg/l)	TDS (mg/l)	0.864	Spherical	88	663.10	43800	0.133	0.832

**The data are of meaningful relation on 99% scale

In cokriging method, after the formation of correlation matrix for prospecting quality of water, an agent was used as a supplementary variant which had the most correlation percent with the variant. Thus, to evaluate the total variants of dissolved solids, electric conduct 7 nitrates' ion, Magnesium ion on 0.902, 0.904 and 0.730 scale and sodium ion from electric conduct variants of 0.856 in 2007 were used. For evaluating the above mentioned variants in 2009 also supplementary variants of electric conduct (for the total dissolved solids with 0.999 correlation), Potassium ion density (for nitrates with 0.660 correlation), and total dissolved solids (for sodium with 0.864 correlation) were used. The proper models for this method are also Spherical model for total dissolved solids, Gaussian for EC, Exponential for nitrate, and Spherical for sodium in 2006, exponential for total dissolved solids, Spherical model for electric conduct, nitrates & sodium in 2009. The results show that the correlation through the variants becomes stronger by using supplementary variant on average scale on all the items except for the dissolved solids which did not have great change (2.5% decrease). For selecting the best method of interpolation among the geostatistic methods used, RMSE was used (Table 4).

A comparison on the results showed that relatively cokriging method has lower errors in comparison to the other kriging methods and increases precision. Of course, this trend is different for the nitrates' ion variant. In this case, the best results were for 2007 and 2009 for simple kriging and disjunctive kriging. Finally, interpolation of variants using the most proper method and distribution maps, changes, and standard zoning was done in geographical information center(on national standards of drinking water). Figures 3-6 show the spatial characteristics of variants through 2007-2009.

TABLE 4 – COMPARISON OF RMSE VALUES TAKEN FROM GEOSTATISTIC METHODS:2007-2009

Estimation method	**Ordinary kriging**		**Simple Kriging**		**Universal Kriging**		**Disjunctive Kriging**		**CoKriging**	
	2006	***2009***	***2006***	***2009***	***2006***	***2009***	***2006***	***2009***	***2006***	***2009***
TDS (mg/l)	58.2	45.49	81.4	33.61	75.8	44.59	77.0	39.44	27.6	39.33
EC (µm/cm)	71.13	67.1	59.11	65.67	59.11	67.6	63.25	65.7	57.10	52.6
NO3- (mg/l)	10.97	0.65	8.20	0.67	10.97	0.63	8.22	0.59	8.34	0.63
Na+ (mg/l)	6.17	0.339	4.76	0.370	8.78	0.370	8.74	0.367	4.58	0.254

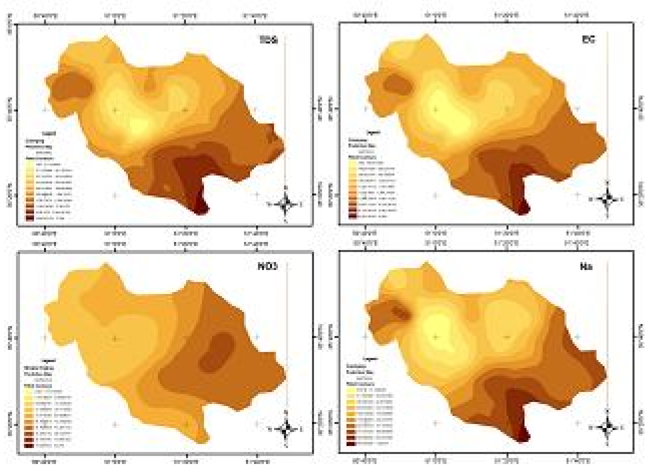

Figure 3. Quality spatial changes – 2006

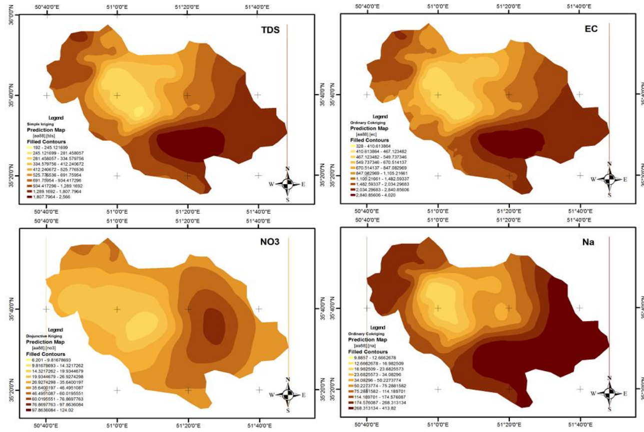

Figure 4. Quality spatial changes – 2009

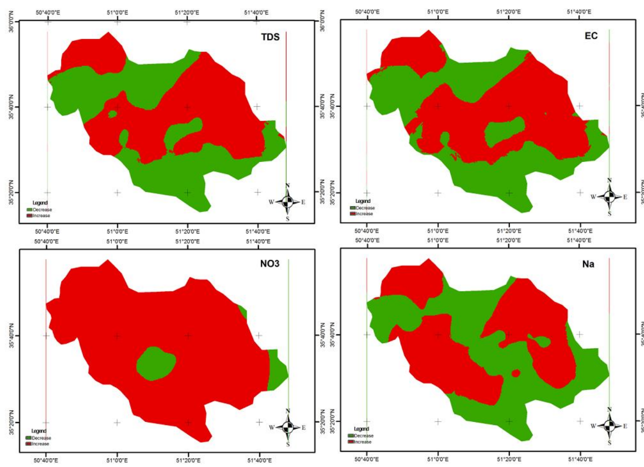

Figure 5. Quality spatial changes – 2006-2009

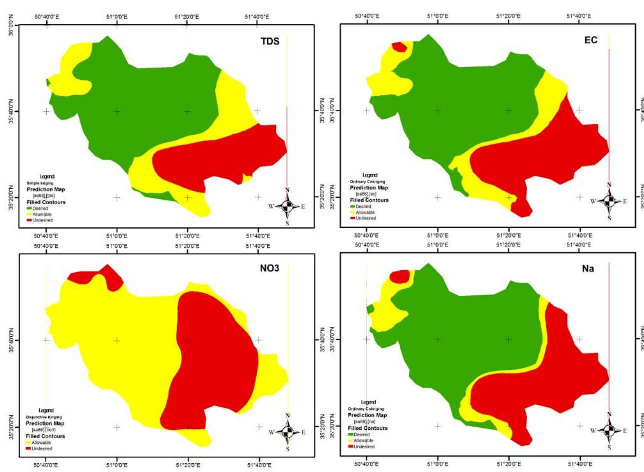

Figure 6. Zoning chart of quality variants based on standards of 'Institute of Standards and Industrial Research of Iran' - 2009

V. CONCLUSIONS

Providing on time charts on the changes of quality parameters of groundwater, is a crusial step toward proper management and Utilization of these resources. Selection and accuracy of proper methods for zoning and providing the charts of the changes in characteristics of these resources depends on conditions and availability of statistics and data of that region. The purpose of the present study was the evaluation of geostatistic methods in providing charts of quality characteristics, surveying the condition of groundwater resources of Tehran-Karaj plain through 2007-2010, and zoning them for drinking water purposes.

According to the outcoming results, most of the surveying variants had high Skewness. which can be because of the few number of samples. Therefore, logarythms were used to normalize the data. After drawing variograms and Fitting of proper sample on them, the related agents were extracted. The strength in space structure of the variants in all cases, except for Nitrates' ion were recognized as proper. This shows sspatial coalition and high precision in the fitted models, which plays a great role in increasing the estimations. To estimate the quality variants of groundwater, secret geostatistic methods like simple kriging, ordinary, disjunctive, universal and cokriging were used. The results from evaluation of interpolative methods on the RMSE basis, proved relative prominence of cokriging method and using supplementary variants. Comparing the results of the present study to that of other researchers, those of Taghizadeh Mehrjerdi et al. (2009) and Sha'bani (2012) could be mentioned who both emphasise the priority of cokriging method over other methods of geostatistics. Other researches emphasizing the priority of kriging methods over the rest of methods are Maleki Gonadishi et al. (2008), Ahmed (2002), Bajjali (2005) (with IDW method)

Barcae and Passarella (2008) (Disjunctive Kriging), Fetouani and Vanclooster (2008) (Simple Kriging). As cokriging method is proper for modt parameters of groudwater, therefoer, it proves that most parameters of groudwater have meaningful relation together(Habibiarbatani et al. 2009). Due to the principles of geostatistics, the variant which has a proper spatial correlation and a lower estimated variance, needs less samples for its estimation, and thus has lower expence for its samples(Zehtabyan et al. 2010).

According to the charts given in figures 3-5, it can be observed that the trend of changes in quality agents of groundwater are relatively similar. Also, totally, the most density of the variants studied, are for the eastern and southeast of the plain, which has extended to the northwest of the plain due to the spatial changes through 2007-2010. Of cource, the trend of these changes could be justified, concerning natural inequalities, and the region's slope.

Besides the effect of natural inequalities, the low quality in eastern and south east regions, and decrease in quality toward north west of the plain could be due to the agricultural lands, over-utilization of groundwater resources, and development of industries around Tehran and also the expand in Alborz province.

In this regard, the best possible suggestion to the region's managers, could be using strategic planning to reach the sustainable development in the region.

On the other hand, on the basis of utilization of drinking water, in this study, the researcher made zoning the plain on drinking water standards.

The results of this zoning about the variant of total dissolves solids (54% proper, 24% admissible, 22% inadmissible), electric conduct (54% proper, 17% admissible, 29% inadmissible) and Nitrates' ion(60% proper, 40% inadmissible), and sodium(58% proper, 10% admissible, 32% inadmissible) are shown in Figure 6. The present zoning can be used as a guide to locate zones proper for extracting drinking water, concerning the other quality parameters of water in the studied region.

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