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A spatial variation study of groundwater quality parameters in the Gonabad Plain using deterministic and geostatistical models

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ABSTRACT

Groundwater is one of the major sources of water supply in arid and semi-arid regions. Thus, in order to protect groundwater quality, data on spatial and temporal distribution of groundwater are important. One way to protect groundwater quality is through the investigation of spatial distribution data. Geostatistical methods are one of the most advanced techniques for the interpolation of groundwater quality. Therefore, in this study by geographic information system ArcGIS and GS^+, deterministic interpolation methods such as Inverse Distance Weighting (IDW), Global Polynomial Interpolation (GPI), and Local Polynomial Interpolation (LPI), with power ranging from 1 to 5, as well as geostatistical interpolation methods such as OK, SK, and UK, with exponential and rational Quadratic models, were used for studying the spatial distribution of quality parameters such as Cl, EC, TDS, and anion. The data were related to 44 exploitation wells in the Gonabad Plain in the Razavi Khorasan Province in the year 2013–14; after normalization, the best model parameters of the fitness semivariogram were selected based on the nugget effect to Sill. Then, based on cross-validation criteria such as MRE, RMSE, and R, the best interpolation method was selected. The results showed that the IDW method, with the powers of 3 and 4, had the lowest error and the most correlation compared to the GPI, LPI, OK, SK, and UK methods. Finally, the zoning maps and spatial distribution for the studied parameters were prepared based on the best interpolation method.

Keywords: Interpolation; Geostatistics; Groundwater quality; Cross-validation; GIS

1. Introduction

Groundwater is one of the most important natural supplies in arid and semi-arid regions where access to surface water is difficult. On the other hand, the rapid population growth in these areas and the improper use of groundwater supply can cause salinity, and a reduction of water quality [1,2]. By increasing the water crisis,the quality of all water supplies is as significantly important as its quantity, especially in groundwater. Therefore, groundwater quality assessment for its sustainable use is considerable, alike other water resources [3–5]. Many factors influence groundwater quality,including precipitation, soil characteristics, zone topography, basin geological structure, geological processes, groundwater recharge, and human activities on land [6]. Thus, Total dissolved solids (TDS) concentrations and the main anions of groundwater are the parameters that assist in the investigation of groundwater quality in terms of drinking water sources. In addition, the main anions of groundwater can be used for water supply management [7]. Tisero and Voudourisk studied the chemical composition of groundwater in shallow aquifers in the Western and the semi-arid area of Iran, and indicated that salinity was the

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most important factor behind the reduction of the quality of groundwater in that area [8]. The evaluation of groundwater quality in a region needs many water samples in the studied area; this is both time-consuming and has high costs (in terms of field and laboratory operations). One of the ways to deal with this problem involves sampling from a limited number of locations that indicate the entire region, and then, the application of these results on the entire region by geostatistical methods [9]. Geostatistical interpolation methods create a continuous surface with the help of measured points and the polygon method, which can predict the desired values in places lacking data [10]. Many studies used geostatistical interpolation methods to estimate the groundwater level, the temperature data, and the soil and mineral concentration [11–13]. A number of these studies have shown that the kriging method has a better performance than IDW [14]. Certain other studies, however, revealed that kriging has a lower accuracy than other interpolation methods such as IDW [15,16]. Shamsudduha conducted a study to assess the most appropriate prediction method for estimating arsenic concentrations in shallow aquifers in Bangladesh by using several spatial interpolation methods and indicated that Ordinary Kriging (OK) has a better performance for estimating arsenic concentrations based on unbiased analysis, validation, and mean prediction error [17]. Taghizadeh et al. used cokriging and IDW methods to predict the spatial distribution of water quality parameters such as TDS, TH, EC, SAR, CL-, and SO_4^{2-} in the Yazd–Ardakan Plain, and has concluded that the IDW method has a lower performance than kriging and cokriging owing to low value root mean square error (RMSE) [18]. Ahmadi and Sedghamiz carried out a study in the Darab Plain in the south of Iran to spatially and temporally analyze groundwater level fluctuations by using Ordinary Kriging (OK) and UK methods. The results showed that the temporal and spatial variations of the groundwater level are very impalpable: three and six percent, respectively [19]. Sunet al. conducted a study to interpolate the spatial and temporal distribution of deep groundwater in the north of China by using several spatial interpolation methods such asIDW, RBF, OK, SK, and UK. The performance of these methods was evaluated by validation test methods such as correlation coefficient (R) and root-mean-square error (RMSE). They concluded that SK,with the lowest RMSE and the highest R^2, is the best method for the spatial distribution of groundwater [20]. In another study, Xie et al. used three different interpolation methods, IDW, OK, and RBF, for the spatial distribution of heavy metals on soil and evaluated the performance of these methods based on RMSE. The results showed that the OK and the RBF methods were more efficient in the estimation of unsampled points on heavy metals [12]. Hooshm and et al. applied kriging and cokriging methods for estimating SAR and Cl on agricultural land and revealed that cokriging has a better performance than kriging [21].

Moghaddam et al. carried out a study in the Mashhad-Plain to evaluate the temporal and spatial variations of water quality parameters by using the methods of Boolean Logic, IDW, and kriging. Based on RMSE, the results showed that kriging and IDW are the best methods for TDS, SAR, Na, EC and SO_4^{-2}, TH, and Cl, respectively [22]. Noori et al. used four interpolation methods for the spatial analysis of groundwater levels at different climatic periods. The performance of these interpolation methods were evaluated by using validation test methods (RMSE, MAE, and R^2). The results of this study revealed that cokriging methods have a better performance than other methods [23].

Geostatistics assume that there is a spatial correlation (Interval-Directional) between measured samples and the samples are not independent from each other [24]. Finally, it can be concluded that the spatial correlation assessment of groundwater quality parameters is one of the most important tools for the analysis of groundwater in arid and semi-arid areas. The kriging method, as one of the most prestigious geostatistical methods, is able to survey and estimate the spatial distribution of the groundwater quality parameters and the aquifer level [25]. The aim of this study is the evaluation of spatial correlation and the estimation of the spatial distribution of the parameters, Cl, EC, TDS, and anions, in the Gonabad Plain using GIS and geostatistical interpolation methods in the year 2013–14.

2. Materials and methods

2.1. Study area

The city of Gonabad is located in the Razavi Khorasan Province. This area lies between the latitudes 37°6′and 38°50′ N and the longitudes 61°8′ and 72°5′ E, covering an area of approximately 5,902 m^2 (Fig. 1). The elevation of this area is 1,105 m above sea level. The climate is generally cool and dry, with warm summers. The minimum and maximum temperatures are −8.4 and 38.7°C, respectively. In addition, the average temperature of the Province is 17.6°C.

This study used data from 44 exploitation wells in the Gonabad Plain in the Razavi Khorasan Province in the year 2013–14. The reason to select this year for this study included increasing the accuracy and the validity of the existing data in order to promote feelers and technology progress in recent years, which reduce the error of collected data and restore them. The position of the study area and the wells is shown in Figs. 1 and 2.

2.2. Interpolation methods

Interpolation methods are classified into two main groups: deterministic and geostatistical. Deterministic methods apply based on the level of measured points and the greatest similarity (such as IDW) or smoothing degree (such as RBF). Geostatistical methods use the statistical properties of measured points and random processes with spatial correlation to estimate the unmeasured value [10].

2.3. Deterministic interpolation methods

2.3.1. Inverse distance weighting (IDW)

IDW uses a simple algorithm based on distance: by increasing distance, the effect of parameters should be reduced to level. In addition, this method uses from surrounding measured value to predict values at unmeasured locations. The closest measured values have the greatest influence. In IDW, the prediction of the values for unmeasured location are determined using Eq. (1):

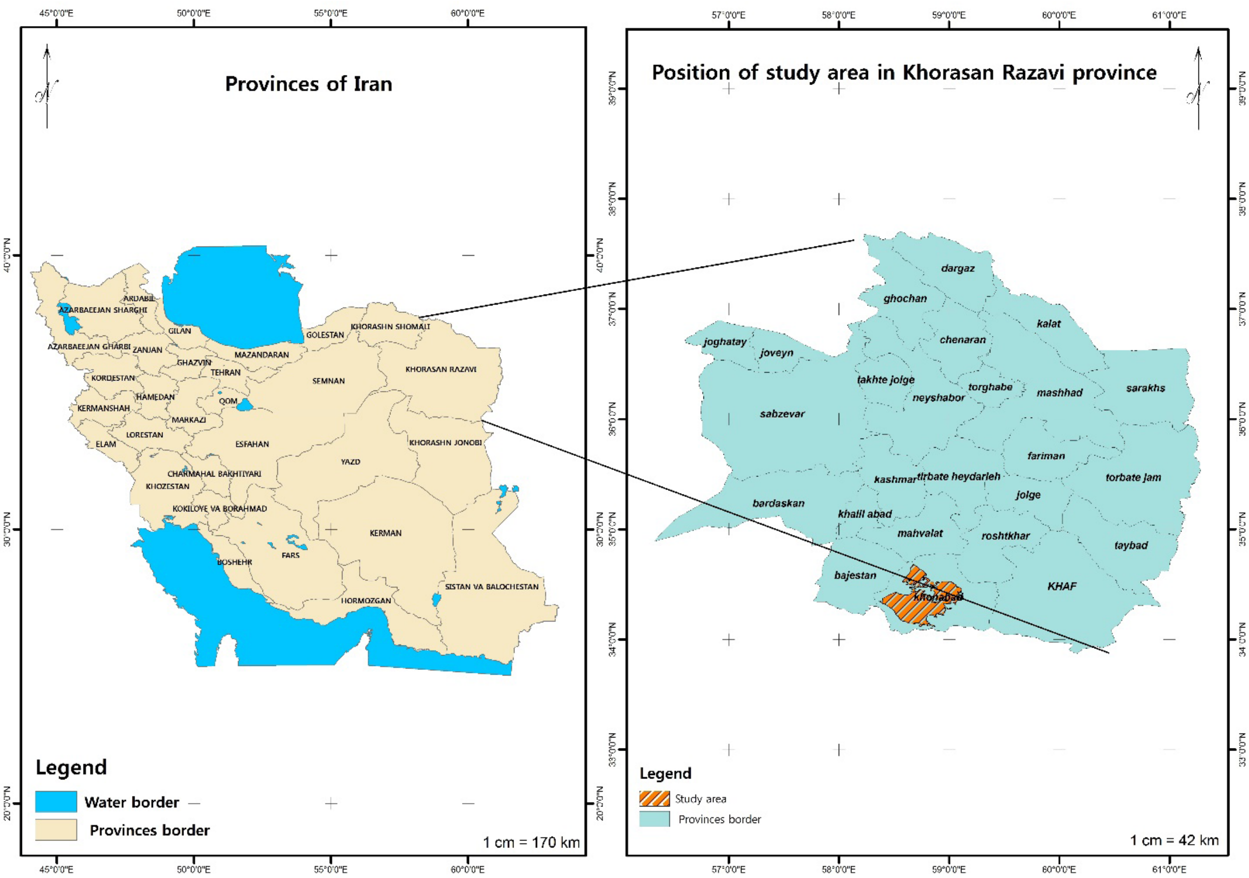

Fig. 1. Location of the study area.

$$z = \frac{\sum_{N}^{i=1} \frac{z_i}{d_i^m}}{\sum_{N}^{i=1} \frac{1}{d_i^m}} \tag{1}$$

where z is the estimated value, z_i is the measured value at the point, d_i is the distance between z and z_i, and m refers to the power weights. Them value ranges from 1–5 and N is the total number of such points that are used in the interpolation [10].

2.4. Global polynomial interpolation (GPI)

GPI is a fitter of the flat surface by mathematical formula eat input points. In this method, in contrast to IDW, surrounding measured values to predict values at unmeasured locations are not used and surface variations are gradually employed. In this method, only a polynomial is fitted for all the data [26].

2.5. Local polynomial interpolation (LPI)

This method uses polynomial formulae for interpolating like IDW. In this method, however, in contrast to IDW, many polynomials are fitted for limited data at a known location, a neighborhood [26].

2.6. Geostatistical interpolation methods

2.6.1. Kriging

Kriging is a geostatistical method like IDW interpolation; it uses a linear combination of weights at known points to estimate the value at unknown points. Kriging uses a semivariogram, a measure of spatial correlation between two points in such a way that weights change according to the spatial arrangement of samples. In contrast to other estimation procedures, kriging provides a measure of the error or uncertainty in the estimated surface [27]. Several forms of kriging interpolation exist, including OK, SK, and UK.

2.7. Ordinary kriging (OK)

OK has a greater application among different kriging methods. Ordinary kriging provides optimal estimations of known values in unsampled locations by using structure semivariogram characteristics and primary value. OK is calculated using Eq. (2):

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

where $Z^*(x_0)$ is the estimated value at x_0, λ_i is the known weight Z at x_i, and n is the number of points of nearby estimated points [28].

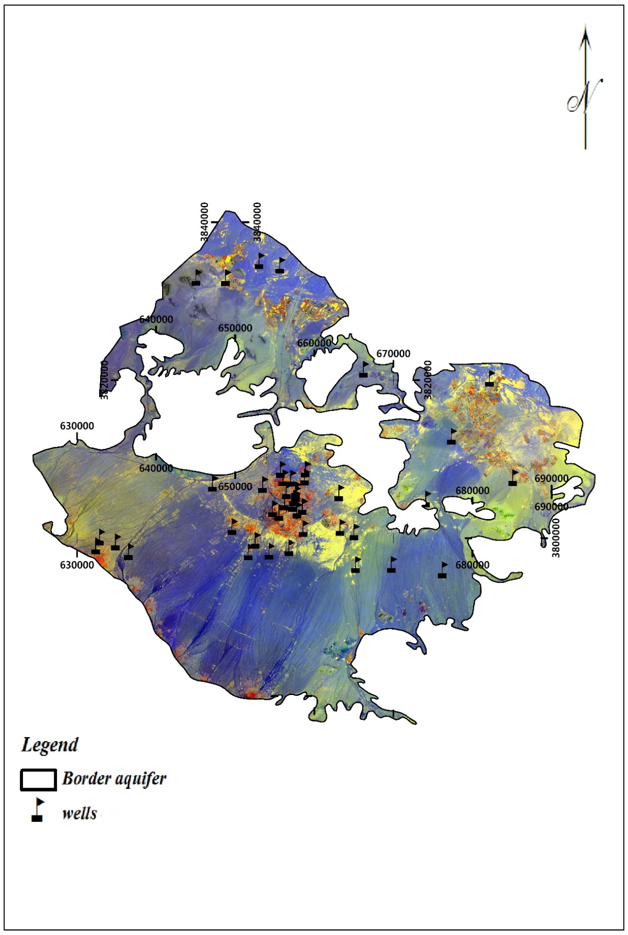

Fig. 2. Location of the wells.

2.8. Simple kriging (SK)

This method assumes that the trend component is a constant and known mean. Owing to the constant and known mean, SK is more efficient than the OK method; in most cases, however, the selection of the mean is difficult [28].

2.9. Universal kriging (UK)

This method is much like ordinary kriging, except that instead of fitting just a local mean in the neighborhood of the estimation point, it fits a linear or higher-order trend in the coordinates of the data points [10].

2.10. Semivariogram analysis

The semivariogram is the most common tool to investigate spatial correlation in geostatistics. The semivariogram shows dissimilarity between properties when the distance increases between samples. Experimental semivariograms are calculated using Eq. (3):

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} \left[z(x_i) - z(x_i + h) \right]^2 \tag{3}$$

where $\gamma(h)$ is the experimental semivariogram, $N(h)$ is the number of observation pairs for x_i, zx_i is the value of variable at location x_i, and $z(x_i + h)$ is the value of the variable at $(x_i + h)$.

The value of the semivariogram at $h = 0$ is called the Nugget effect. The semivariogram value increases to a significant distance with an increase in h, and then, reaches a constant value, which is called sill $(C + C_0)$.

The range of influence (A_0) is the distance between samples which, after the distance, ensure that the variable values do not affect each other [28]. This range determines a confine that can be used to estimate the unknown value by using the existing data. Certainly, the greater range of influence indicates wider spatial correlation [29]. The ratio of $(C_0/C+C_0)$ is used in spatial correlation classification of groundwater quality parameters. It is an indicator of spatial structure power in variables. If the ratio is less than 0.25, the variable has a strong spatial correlation (dependence); if the ratio is between 0.25 and 0.75, the variables show moderate spatial correlation; otherwise, the variables represent poor (weak) spatial correlation [19,30].

2.11. Cross validation

To select the best interpolation method the mean relative error (MRE), the root mean square error (RMSE), and correlation (R) based on Eqs. (4)–(6) were used.

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left[z^*(x_i) - z(x_i) \right]^2} \tag{4}$$

$$MRE = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{z^*(x_i) - z(x_i)}{z(x_i)} \right| \tag{5}$$

$$R = \frac{\sum_{i=1}^{n} \left[z(x_i) - \overline{z(x_l)} \right] \left[z^*(x_i) - \overline{z*(x_l)} \right]}{\sqrt{\sum_{i=1}^{n} \left[z(x_i) - \overline{z(x_l)} \right]^2 \sum_{i=1}^{n} \left[z^*(x_i) - \overline{z*(x_l)} \right]^2}} \tag{6}$$

In this equations, $z(x_i)$ is the observed value at x_i, $z^*(x_i)$ is the estimated value at x_i, $\overline{z(x_l)}$ is the mean observed value at x_i, $\overline{z(x_l)}$ is the mean estimated value at x_i, and n is the number of observed variables. The best values of *RMSE* and *MRE* are 0 and for *R*, it is 1 [12].

3. Results and discussion

The best results of geostatistical and definitive interpolation methods are obtained if the data is normally distributed [31]. The statistical analysis results of the quality groundwater parameters in studied wells are provided in Table 1. As observable, the skewness coefficient of all parameters before normalization is out of range (1 and –1); indicating the data is not normal. For this purpose, the data should first be checked for normality distribution by using the runs-test and SPSS in terms of accuracy and homogeneity. The data were log-transformed prior to the calculation of semi variance and normalization.

Normal Q-Q plots of the quality parameters of Cl,EC,TDS, and anions after applying log-transformation

Table 1
Descriptive statistics of groundwater quality parameters measured in the study area

Parameters	Minimum	Maximum	Mean	Median	Variance	Kurtosis	Skewness
Cl	0.44	133	29.82	20.58	31.37	5.43	71.9
Cl*	–0.82	4.89	2.83	3.02	1.26	4.45	–1.03
EC	341.6	19600	5443.3	4512.5	4775.5	4.83	1.57
EC*	5.83	9.88	8.22	8.41	0.96	3.35	–0.60
TDS	215.21	12348	3429.3	2842.9	3008.6	4.83	1.57
TDS*	5.37	9.42	7.76	7.95	0.96	3.35	–0.60
Anion	3.76	196	55.74	46.83	47.55	4.77	1.54
Anion*	1.32	5.28	3.66	3.85	0.94	0.30	–0.61

*Logarithm transformation

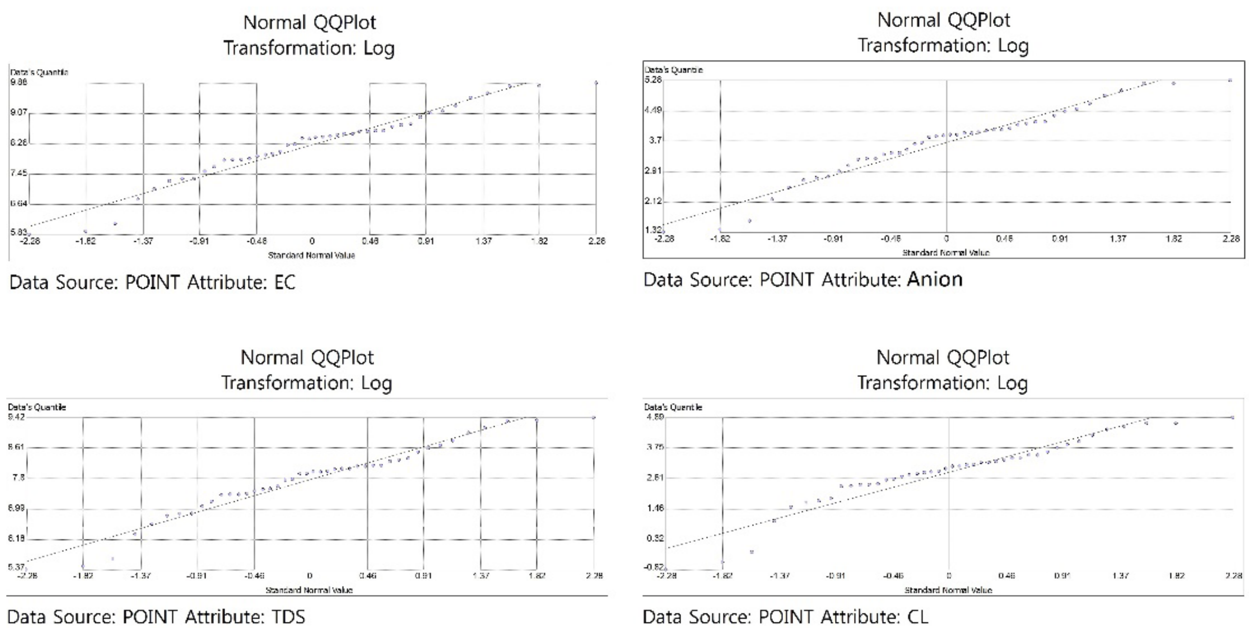

Fig. 3. Normal Q-Q plots of groundwater quality parameters.

is provided in Fig. 3. In a normal Q-Q plot, if the spots are around a straight line, it indicates that the data are normal [31]. The result of this plot shows that the logarithmic conversion causes the normalization of all groundwater quality parameters.

Table 2 shows the best-fitted semivariogram model of groundwater quality parameters. According to the table, the nugget–sill ratio ($C_0/C + C_0$) for the parameters Cl, EC, and TDS range from 0.25 to 0.75, which shows moderate spatial correlation in the fitted model. This ratio is, however, lower than 0.25 for the anion and indicates a strong spatial correlation in the desired model.

In this study, after the validation and homogeneity of data, and the selection of the best fitting semivariogram model, ArcGIS, GS+, and deterministic interpolation methods (IDW, LPI, GPI) with powers ranging from 1 to 5, geostatistical interpolation models (OK, SK, UK),with exponential and rational quadratic models, were used to identify the most suitable interpolation method, the spatial distribution of groundwater quality parameters, and zoning maps (Table 3).

According to the results of Table 3, the IDW method with 3 power weight has the lowest error and the highest correlation for Cl. In addition, the GPI and the LPI methods are located in the second and third places, respectively. When these methods were compared together, it was observed that all the geostatistical interpolation methods yielded relatively close results due to the equality of RMSE and R measures. The SK method and the rational quadratic equation, however, yielded poorer results due to a higher MRE value. The value of RMSE for EC is very high in all the interpolation methods, but the value of this parameter in IDW is lower than the other methods.

The IDW method, in terms of the MRE error measure, is located in second place after OK and UK, with exponential and rational quadratic models,but based on R = 0.82, it has a better performance than other methods. Results show a strong correlation between the measured (observed) and

Table 2
Summary of the best-fitted semivariograms models for groundwater quality parameters

Parameters	Best-fitted model	(C_0) Nugget (L·meq)	($C + C_0$) Sill (L·meq)	$C_0/C + C_0$	Spatial correlations
Cl	IDW	0.236	0.400	0.590	Moderate
EC	IDW	0.085	0.303	0.282	Moderate
TDS	IDW	0.083	0.300	0.278	Moderate
Anion	IDW	0.032	0.351	0.090	Strong

Table 3
The results of interpolation methods for groundwater quality parameters in the Gonabad Plain

Parameters	Methods	Model-Power	RMSE	MRE	R
Cl	IDW	Exponential-power = 3	19.80	0.35	0.77
	GPI	Exponential-power = 2	21.51	8.20	0.73
	LPI	Exponential-power = 1	22.55	0.51	0.71
	OK	Exponential	24.70	0.27	0.72
	SK	Rational quadratic	24.40	0.57	0.71
	UK	Exponential	24.70	0.27	0.72
EC	IDW	Exponential-power = 3	2708.49	0.28	0.82
	GPI	Exponential-power = 2	3177.93	0.58	0.74
	LPI	Exponential-power = 1	3227.40	0.47	0.75
	OK	Exponential	2949.18	0.22	0.80
	SK	Rational quadratic	3588.08	0.45	0.77
	UK	Exponential	2949.18	0.22	0.80
TDS	IDW	Exponential-power = 3	1706.35	0.28	0.82
	GPI	Exponential-power = 2	2002.09	0.58	0.74
	LPI	Exponential-power = 1	2033.26	0.47	0.75
	OK	Exponential	1857.98	0.22	0.80
	SK	Rational quadratic	2260.49	0.45	0.77
	UK	Exponential	1857.98	0.22	0.80
Anion	IDW	Exponential-power = 3	28.48	0.30	0.80
	GPI	Exponential-power = 2	31.89	1.68	0.74
	LPI	Exponential-power = 1	32.30	0.41	0.75
	OK	Exponential	30.43	0.25	0.79
	SK	Rational quadratic	36.07	0.44	0.74
	UK	Exponential	30.43	0.25	0.79

(predicted) estimated values of this parameter. The results of the TDS and the EC interpolation methods were quite similar to each other. In IDW, the value of MRE with 3 powers was higher than the OK and the UK methods with exponential and rational quadratic models, with the rate of 0.6. The correlation coefficient R and RMSE error rate was high and low, respectively, indicating that the IDW method had a better performance based on these measures.

The best results for anions, unlike previous parameters, were obtained by the IDW method with 4 power weight, RMSE = 28.48. The OK and the UK methods, with exponential and rational quadratic models, were located in second place.

Finally, it can be concluded that for all the groundwater quality parameters of the Gonabad Plain, the IDW method with 3 power weight and 4, in terms of RMSE and R measures, has a better performance than other deterministic interpolation methods such as GPI, LPI, and geostatistical methods (OK, UK, and SK). In terms of the MRE error measure, however, the OK and the UK methods were more successful than the deterministic interpolation methods.

For IDW, GPI, and LPI with 1 to 5 power weights, it should be noted that just powers with the best results are provided in Table 3. Zoning maps and the spatial distribution of studied parameters based on the best selective interpolation method of Table 3 are presented in Fig. 3.

The permissible limit of Cl in terms of agriculture is 4–10 meq/l according to Fig. 4(a). The Cl concentration is higher than the guideline values in the north and the northeast of the plain. As a result, this area is not suitable for agriculture [32].

The EC concentration increases by moving from the south to the north of the Plain (Fig. 4(b)). The EC value in

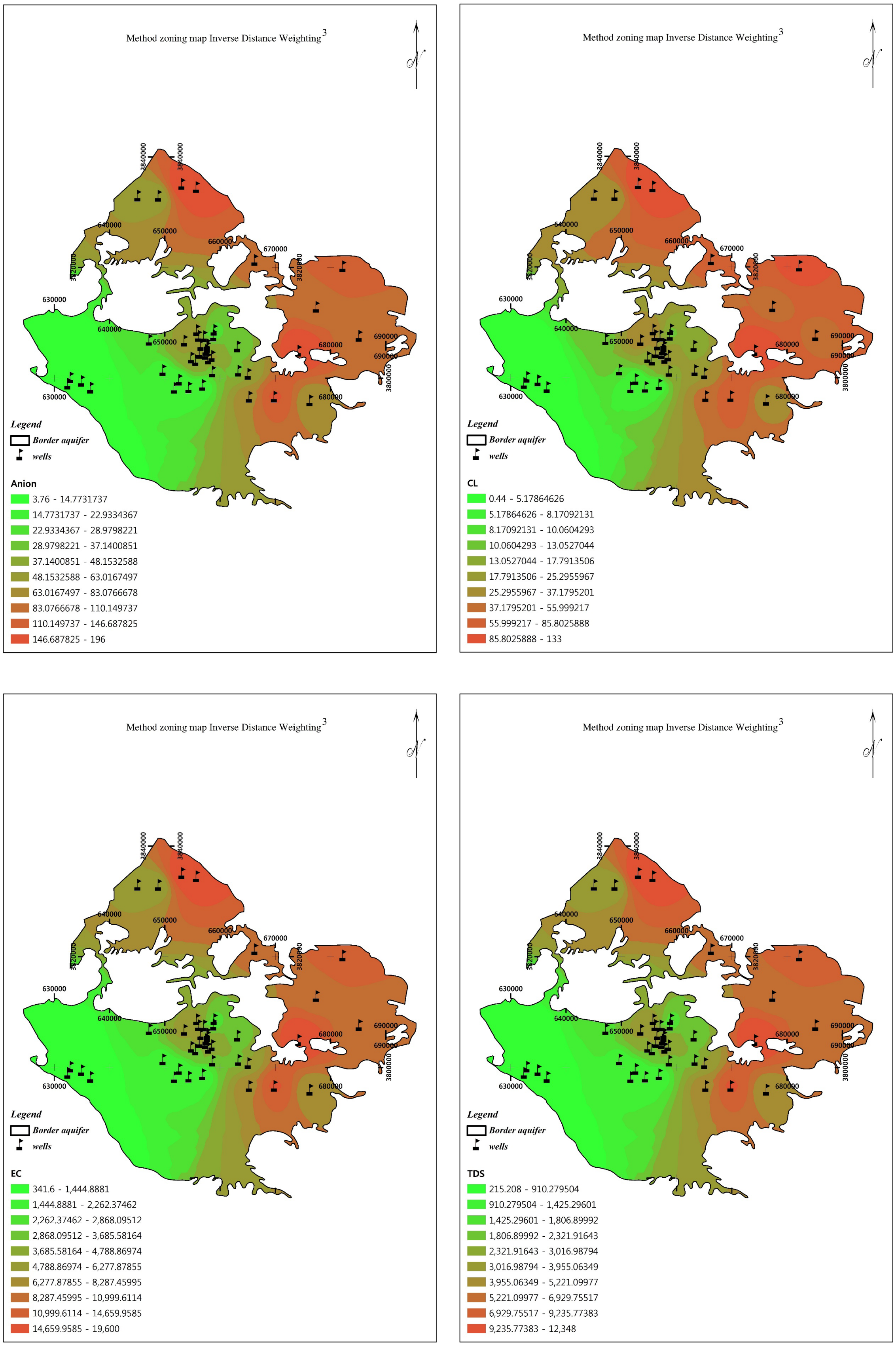

Fig. 4. The zoning map of groundwater quality parameters in the Gonabad Plain a) Cl, b) EC, c) TDS, and d) Anion.

the north and the central parts of the Plain are higher than the guideline values (3000 mg/l); in the southeast parts, it is lower than the permissible limit (1000 mg/l) [32]. Increasing the value of EC in the northern parts of the Plain could be due to the presence of salt and gypsum.

Fig. 4(c) shows the increasing trend of TDS concentration from the south to the north of the Plain. TDS is one of the quality drinking water indicators and its high concentration in the plain may be due to natural runoff, sewage effluent discharge, hazardous waste disposal, soil characteristics, livestock waste, and industrial wastewater. The maximum permissible and desirable limit of TDS in drinking water is 1000 mg/l [33]; only small parts of the southern portion of the plain were in a desirable condition in terms of this parameter. The variations of anion concentration in the plain are seen as increasing from the south to the north, similar to other parameters.

4. Conclusion

This study explored the spatial variation of groundwater quality parameters in the Gonabad Plain using deterministic and geostatistical models in the year 2013–14. For this purpose, after the data of the statistical analysis of the studied wells was determined, log transformation was used for normalizing the data. Then, in order to select the best the fitting semivariogram model, the model's spatial correlation, based on analysis the nugget–sill ratio, was investigated. The results showed that there is a moderate spatial correlation between all the parameters,except anions. Thereafter, in order to select the best interpolation method and zoning map of the of groundwater quality parameters, deterministic interpolation and geostatistical methods were used based on the correlation coefficient and error measures.

The results showed that the IDW method, with powers of 3 and 4, has a lower error and a higher correlation than the five following methods: LPO,OK,SK, and UK. In addition, among the different types of kriging methods, OK and UK provided similar results and were more successful than the SK method.

Finally, zoning maps and the spatial distribution of Cl, EC, TDS, and anions were prepared;in all cases, this represented increases of concentrations from the south to the north of the Plain. By providing spatial distribution maps of water quality parameters, it is possible for operators and decision-makers in the field of water resources management to select the best points for the extraction healthy water in terms of drinking and agricultural standards with the knowledge of the aquifer quality in all parts of plain that are not measurable in terms of their technical and economical aspects. Also, they can identify human and natural pollutant sources of aquifers and proceed relevant approaches to control them.

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