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Research paper

Assessment of Optimum Interpolation Method to Estimate Groundwater Chemical Data

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A R T I C l E I N F O

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A B S T R A C T

Nowadays, the interpolation methods have become an important technology on the groundwater research. Many geographic information system software based on different interpolator tools have been developed and used widely such as ArcGIS, MapInfo and ArcView. This study was conducted to evaluate interpolation tools for the prediction of HCO3, Cl, SO4, Ca and Na distribution in groundwater of northern regions of Khuzestan province. Inverse distance weighted, kriging, radial basis functions, local and global polynomial interpolation were five interpolation methods that used for this subject. 98 deep wells was selected and chemical analysis data was collected in summer 2008. Predicted values of contaminants were compared to observed data by RMSE, MAE (Mean Absolute Error) and MSDR (Mean Squared Standardized Deviation Ratio) indexes to select the optimum interpolator technique. The results show that the kriging method has the highest interpolation accuracy among five interpolation methods for mapping Ca, SO4 and HCO3 by RMSE equal to 0.56, 0.9 and 0.6 respectively. Also, RBF and IDW Methods have acceptable estimations for Cl and Na ions.

Introduction

Groundwater is one of the most important sources of drinking water in the world, especially in sparsely populated areas. Due to human activities, many pollutants from agricultural, industrial and urban wastewater sources enter the groundwater and cause microbial and chemical pollution. The distribution of pollutants at spatial coordinates has developed a zoning tool for analyzing such data. Replacement of spatial variables instead of random variables and the expansion of GIS in relation to spatial statistics have introduced the use of interpolation methods in the preparation and analysis of zoning maps. This technology is also used in estimating anonymous data in cases where sampling is difficult or the available information is not sufficient and accurate (Morio et al., 2010; Bardossy, 2011). The appropriate statistical method in estimating a variable depends on the type of variable and the factors affecting it and the selected method in one region can be generalized to other regions (Safari, 2002).

Application of interpolation techniques in various fields such as estimating soil hydraulic conductivity (Hosseini et al., 1993), determining soil moisture curve (Voltz and Goulard, 1994), evapotranspiration (Mahdian et al., 2001), temperature (Abdullahi and Rahimian , 2007) and the water table (Tabatabaei and Ghazali, 2011) have been investigated.

Therefore, the quality of water resources has been considered by health and environmental experts and various studies have been conducted in this field (Gurunadha Rao and Gupta, 2000;

Tabatabaei et al., 2010; Latif et al., 2005). Numerous studies have been conducted on the use of GIS in zoning and groundwater risk assessment (Ducci, 1999; Nas and Berktay, 2006; Istok and Pautman, 1996).

On the other hand, the increasing expansion of industry and urban life increases wastewater. In areas that do not use a sewage treatment system, sewage contaminants are transferred to groundwater sources and the movement of water causes the spread of salts. The increase in electrical conductivity and concentration of sodium, chlorine, sulfate and nitrate ions in groundwater is mostly due to human activities, such as intensive agricultural operations (application of chemical fertilizers), drinking and industry (Jalili, 2007).

Tabatabaei et al. (2009) Using kriging method under PMWIN software, they studied the risk-taking of Shahrekord aquifer to urban and agricultural pollution sources. The concentration zoning of chlorine, sodium, nitrate, calcium, sulfate, and bicarbonate ions is plotted by the method in the cells defined for the variable-size simulator model at the inner boundaries of the plain. The results identify specific points of the aquifer as contaminant feed sources and indicate the direction of solute movement in groundwater.

Taghizadeh Mehrjerdi et al., (2008) evaluated spatial interpolation methods to determine the groundwater quality parameters of Rafsanjan plain. He used inverse weight distance, kriging methods to investigate the total solute, salinity, adsorption ratio of sodium and sodium ions, chlorine and sulfate in 65 well water samples. The results showed that kriging methods are superior to IDW method for estimating water quality.

Hooshmand and Mohammadi, (2007) studied the trend of spring salinity changes in groundwater in northern Khuzestan between 2000 and 2005 using GIS. He considered the IDW method as the most appropriate method for salinity changes in groundwater in northern Khuzestan. (2008) Fetouani et al., Used kriging method to investigate groundwater contamination with nitrate under the influence of agricultural lands. Zehtabian et al. (2007) by studying the quality characteristics of Garmsar groundwater introduced the kriging method among the geostatistical methods and the radial function method among the more accurate methods.

This study was performed to evaluate 5 interpolation techniques of distance weight weighing, general polynomials, local polynomials, radial basis functions and kriging to investigate the spatial distribution of bicarbonate, chlorine, sulfate, calcium and sodium in groundwater.

Material and Methods

The study area is Dezful area located in the north of Khuzestan province, at 32˚ 01' to 32 ˚ 33' latitude and 42˚ 10' to 42 ˚ 45' longitude that is shown in Fig. 1. Land use in the region is mainly agricultural and residential areas, and the concentration of chemical elements in groundwater is also affected by the return water from these two parts.

The collected data included the results of chemical analysis in 98 deep wells in the summer of 2018 in which the importance of bicarbonate, chlorine, sulfate, calcium and sodium ions was investigated. The statistical characteristics of the observational data are given in Table 1.

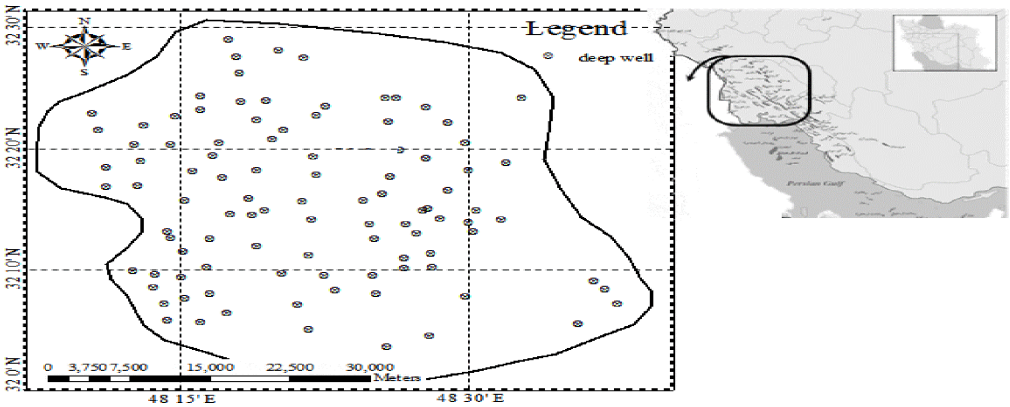

Fig. 1. Location of area in Khuzestan province and Iran

Table 1. Statistical parameters of groundwater quality data

Parameters		Number	Mean (meq/lit)	Standard deviation	Maximum	Minimum
Bicarbonate	HCO3	98	4.1	1	7.2	2.48
Chlorine	Cl	98	4.3	5.3	26	0.35
Sulfate	SO4	98	5.6	10.1	59	0.05
Calcium	Ca	98	4.7	4.7	27	1.48
Sodium	Na	98	5.3	6.3	29	0.27

Interpolation methods

The interpolation techniques used in this research using ArcGIS9.3 software are:

Inverse Distance Weighted Method (IDW)

In this model, the IWD method is used for spatial interpolation of chemical parameters. One of the disadvantages of this method is to consider only the distance of points regardless of the position and arrangement of points for weighting. The weight factor is calculated from the following equation:

$$z^*(x_i) = \frac{\sum_{i=1}^{n}\left(\frac{z(x_i)}{D_i^{\alpha}}\right)}{\sum_{i=1}^{n}\left(\frac{1}{D_i^{\alpha}}\right)} \quad (1)$$

$z^*(x_i)$ = Estimated value, $z(x_i)$ = Measured value,: D_i = Sample distance i to unknown point, and a = Weighting power

Kriging

The harmonic average weight method is used to distribute the variables and is defined as follows:

$$z^*(x_i) = \sum_{i=1}^{n} \lambda_i z(x_i) \quad (2)$$

λ_i = the weight of the sample i.

This method is based on semi-variable analysis and its main purpose is to establish the structure of variable variability relative to spatial distance. Kriging, as an inexperienced estimator, predicts only one variable. The condition of being unbiased is also applied in other estimation methods such as polynomial and inverse distance method, but the feature of kriging is that while being unbiased, the variance of estimation is also minimal. In other words, in the kriging method, along with each estimate, the amount of error is also presented, in which case it is possible to specify the parts where there is a lot of error. In addition, the best sampling points can be suggested using the estimated variance because the method has the ability to determine the reduction of the estimated variance for an additional sample before sampling (Golmohammadi et al., 2008).

Radial basis functions (RBF)

This method was introduced in 1964 as potential functions and today is one of the interpolation methods in which the level of estimation exceeds the observed values. In this method, which is considered as a state of artificial neural network, there are values higher than the maximum observed values or less than the minimum observed values at the estimated level (Aizerman et al., 1964; Bashkirov et al., 1964; Lin and Chen, 2004).

Global Polynomial Method (GPI)

The GPI method is an interpolation technique that fits based on a polynomial function. In this method, all points in the interpolation are used to estimate the unknown value. Therefore, by changing any of the data in the interpolation, the unknown value changes. In this method, calculations are performed very quickly and easily to find the desired value. This method does not provide acceptable results when the data is large and varied.

Local Polynomial Method (LPI)

This method is similar to the GPI method, except that it uses points in a specific neighborhood to determine the unknown value. Therefore, the change in the input data depends on the fact that the changed point is in the vicinity of the unknown value. This method is also able to intercept changes at short distances and creates less error in calculations than the GPI method.

10 wells were selected from 98 sampled with suitable selection. In each computational step, a point is removed from the observation data and its value is estimated by the above interpolation methods. This operation was repeated for 10 selected wells, 5 interpolation methods and 5 measured ions

Mutual evaluation method was used to select the best forecasting method. The RMSE value between the estimated and measured data for selecting the best interpolation method is defined as follows (Eldeiry and Garcia, 2011).

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(\varphi_{cal} - \varphi_{obs})_i^2}{n}} \quad (3)$$

In addition, the Mean Absolute Error (MAE), which indicates the degree of bias, and the Mean Squared Standardized Deviation Ratio (MSDR), which determine the degree of accuracy, are calculated separately to select and validate the optimal method. These indicators show the accuracy of the estimation higher as they approach zero.

$$MAE = \frac{\sum_{i=1}^{n}|\varphi_{cal} - \varphi_{obs}|}{n} \quad (4)$$

$$MSDR = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{\phi_{cal}-\phi_{obs}}{\sigma}\right)^2 \quad (5)$$

φ_{cal} = estimated values, φ_{obs} = observed values, σ = standard deviation and *n* number of test points.

Results and Discussion

The results obtained from the calculations of evaluation indicators are analyzed separately for each of the ions in the form of graphs and tables. To further explain the distribution of ions and the accuracy of estimating the selected method, zoning maps are drawn in each section along with the actual values of each point.

Bicarbonate

Fig. 2 shows the coefficient of determination between the estimated and observed values as well as the estimation error by the RMSE index for the five interpolation methods. The coefficient of determination is very small in all cases, which alone can not indicate the applicability of any of the methods. The main comparison criterion in selecting the best tool will be the RMSE index, which is shown on the left side of Fig. 2. The value of the estimation error is less than one in all methods. Although the general polynomial (GPI) method has the lowest error rate, all methods for bicarbonate zoning will give the desired result.

One of the reasons for the large decrease in the coefficient of determination and the low RMSE is the limited range of bicarbonate changes between 2.5 to 7.2 meq/lit (Table 1). Repeating the experiment in areas with a wide range of bicarbonate concentrations may lead to other results. The methods are compared by MAE and MSDR and the results are presented in Table 2. These indicators have evaluated kriging and general estimator as the most appropriate interpolation methods, respectively. The bicarbonate concentration zoning in the study area is also shown in Fig. 2. According to the irregular distribution pattern, the concentration is seen only in the cases indicated by the circle, and there is regular expansion in the rest of the points without much change.

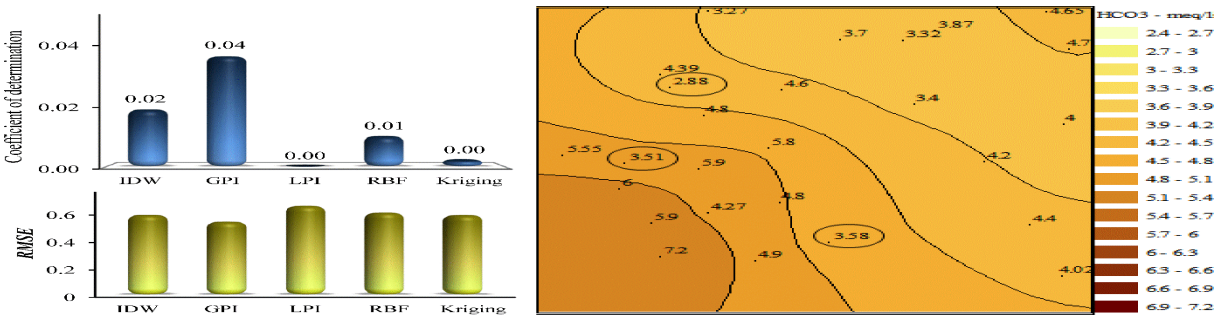

Fig. 2. Distribution of bicarbonate in the study area (the values indicated in the map are the actual amounts)

Chlorine

Kriging methods, inverse distance weighting and radial basis functions have the highest correlation between observational and computational values (Fig. 3). According to the figure, the lowest error index was obtained for the method of radial basis functions, which is the most suitable method for spatial analysis of chlorine concentration (RMSE = 1.3). MAE and MSDR indices also confirm the efficiency of this method (Table 2). Chlorine concentration zoning in the study area is plotted to study the distribution process and compare the accuracy of the calculations with the actual values to the right of Fig. 3. Chlorine concentration, unlike bicarbonate, has a wider range of numbers that are well estimated by the interpolation method (numbers inside the figure are values measured at each point).

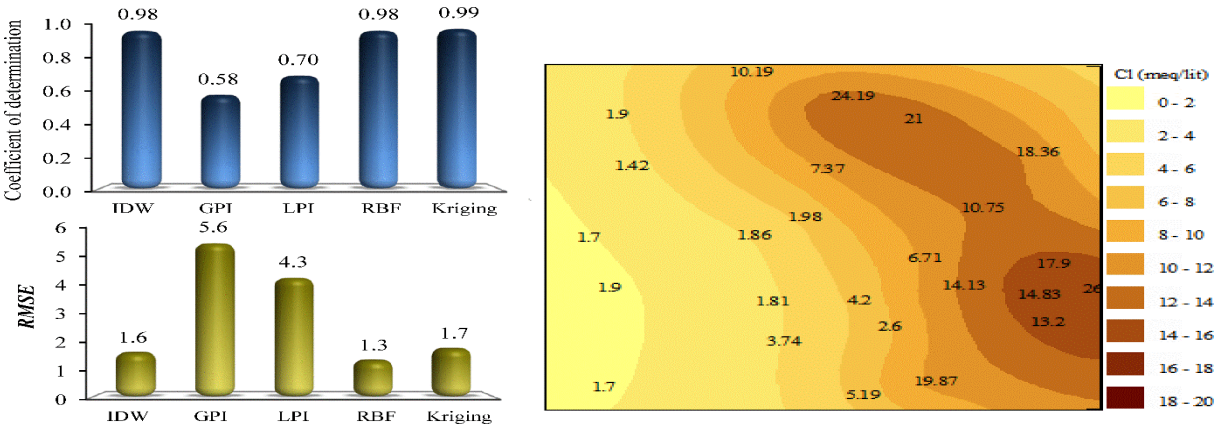

Fig. 3. Distribution of chlorine in the study area (the values indicated in the map are the actual amounts)

Sulfate

The best interpolation tool for the accurate description of sulfate distribution in groundwater for the study area was Kriging method. This result was obtained based on the coefficient of determination 0.89 and with the root mean squared error equal to 0.9 (Fig. 4). Peters et al., (2004) in a similar study introduced the kriging method as the most appropriate method to study the movement of sulfate in groundwater. The lowest values of MAE and MSDR evaluation indices are also related to kriging method.

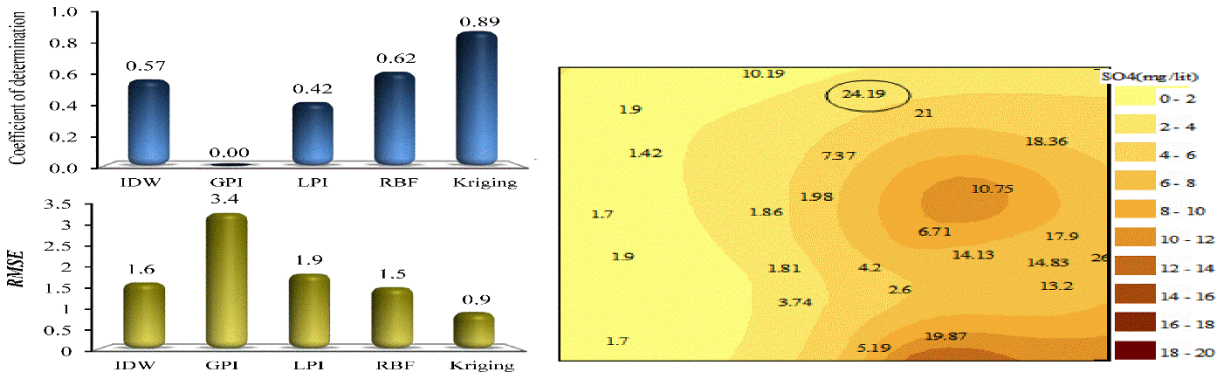

Fig. 4. Distribution of sulfate in the study area (the values indicated in the map are the actual amounts)

According to the zoning map, there is only one point of sudden change outside the integrated interpolation system. This is probably due to the disposal of domestic wastewater in the residential area and as a result of rising sulfate concentration points and has not been properly identified by the map. Sources of sulfate contamination in groundwater are clearly visible in the interpolation map.

Calcium

Kriging and IDW methods with small differences in relation to each other are the best methods for estimating the groundwater data (Fig. 5). Other methods have had acceptable results with RMSE less than 2. The coefficient of determination obtained from the comparison of the results is much lower than that of sulfate and chlorine, which is probably due to the presence of outdated data or sudden changes in the measured amounts of calcium. In the calcium distribution pattern shown in Fig. 5, several points with an irregular trend are identified as a circle pattern. Selected estimators are distinguished by color cells by the means of mean absolute error and standard error variance in Table 2, in both cases the kriging technique is the first priority of calcium ions. Tabatabaei et al. (2009) also used this method to zoning the concentration of calcium in groundwater.

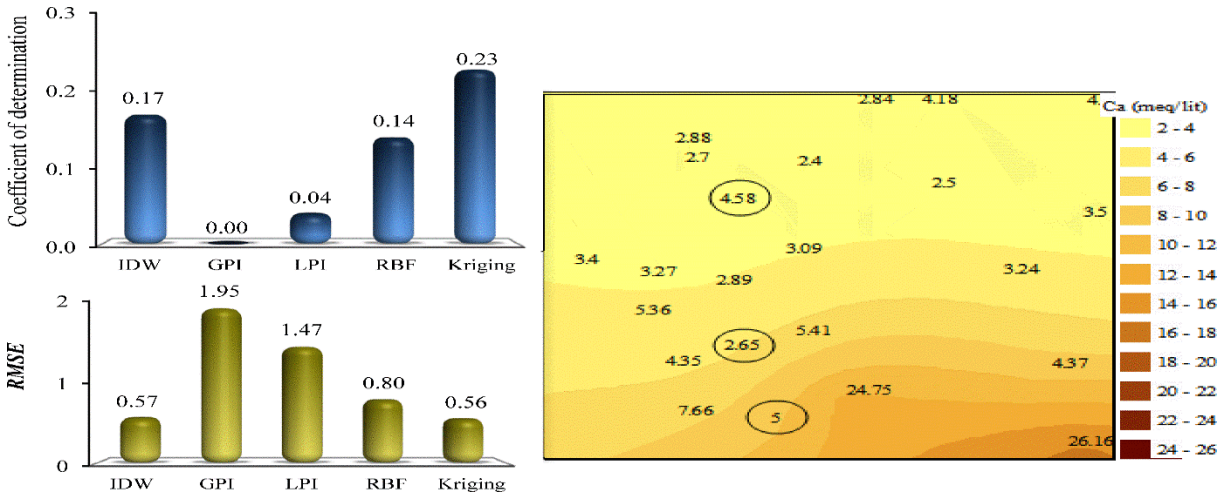

Fig. 5. Distribution of calcium in the study area (the values indicated in the map are the actual amounts)

Sodium

The best coefficient of determination in this study were obtained for the correlation between observational and computational data of sodium ions (Fig. 6). The methods of radial basis functions, kriging and distance weighting are the best choices in choosing the interpolation method, respectively, whose RMSE index has the lowest values in the chart. Among these, based on MAE index, Kriging method and MSDR index, radial basis functions method will give the best results (Table 2). As expected, the highest error rate was observed in the

general polynomial estimator (GPI).

The sodium zoning pattern in Fig. 6 shows a well-defined distribution with a range of 1 to 25 meq/lit. The source of sodium injection into groundwater is given in the figure using a map of sodium concentration. Sodium is dispersed in different directions along with groundwater movement and diffusion processes. Around the marked point, the concentration gradient is high and the distance from the source decreases and stabilizes the sodium concentration.

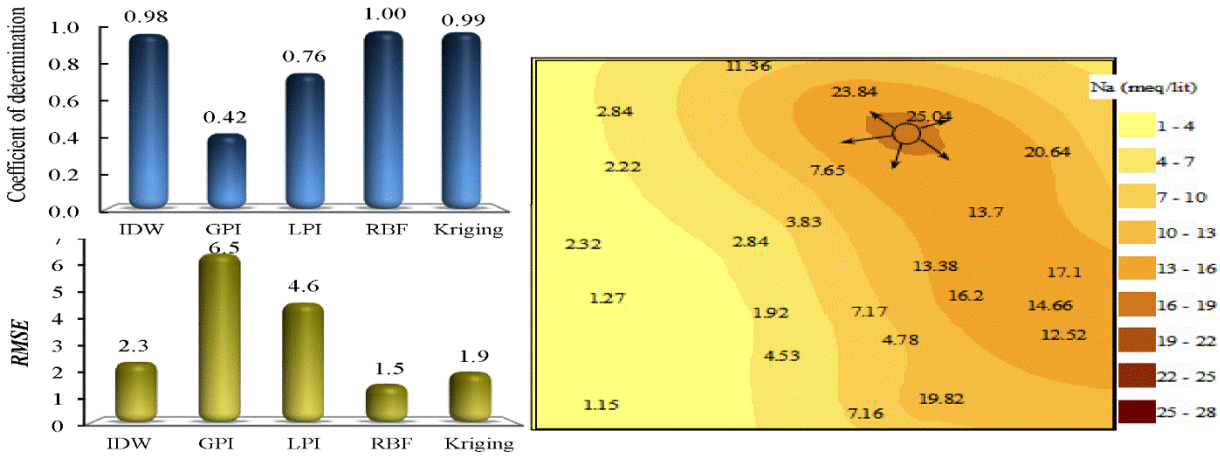

Fig. 6. Distribution of sodium in the study area (the values indicated in the map are the actual amounts)

Table. 2. Comparison between the interpolation methods using MAE and MSDR

Parameters	MAE					MSDR				
	Ca	SO4	Cl	HCO3	Na	Ca	SO4	Cl	HCO3	Na
IDW	0.51	1.49	1.01	0.52	1.5	2.2	0.44	0.04	1.43	0.08
GPI	1.8	2.97	3.81	0.48	4.4	26	1.85	0.56	1.2	0.63
LPI	1.19	1.51	2.43	0.55	2.2	14.7	0.57	0.33	1.78	0.32
RBF	0.64	1.26	0.85	0.52	1.0	4.35	0.38	0.03	1.53	0.03
Kriging	0.47	0.71	0.94	0.47	0.9	2.11	0.13	0.05	1.43	0.05

Conclusion

In this study, groundwater quality is considered as the goal of various interpolation methods for zoning in the aquifer. The results show that the prediction of spatial distribution of calcium and sulfate concentrations by kriging method has been the most accurate. The previous studies confirmed this results. The method of radial basis functions for monovalent ions of chlorine and sodium had the lowest error index and the method of Kriging and IDW had very little difference with the selected method. Due to the lack of large changes in bicarbonate in the groundwater of the study area, all methods for zoning of this parameter are acceptable. In most cases, the general polynomial estimator (GPI) has the highest error due to the use of general observation data in estimating unknown points.

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