

Application of Geostatistical Methods for Mapping Groundwater Quality in Azarbayjan Province, Iran

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Abstract: Soil, surface waters/sediments and shallow unprotected groundwater aquifers are interrelated compartments of the environment that are particularly easy to compromise, sensitive to short- and long-term pollution and directly affect sustainability of ecosystems and human health. A prerequisite of ecosystem management decisions is monitoring of soil and waters that geostatistics methods are one of the most advanced techniques for monitoring of them. At present research, we compare efficiency of three interpolation techniques included IDW, kriging and cokriging for predicting of some groundwater quality indices such as: Na⁺, TH, EC, SAR, Cl⁻, Ca²⁺, Mg²⁺ and SO₄²⁻. Data were taken from 625 wells in Azarbayjan Province, Iran. After normalization of data, variogram was computed. Suitable model for fitness on experimental variogram was selected based on less RMSE value. Then the best method for interpolation was selected, using cross-validation and RMSE. Results showed that for all groundwater quality indices, cokriging performed better than other methods to simulate groundwater quality indices. Finally, using cokriging method, maps of Groundwater quality were prepared in GIS environment.

Key words: Groundwater quality • IDW • Kriging • Cokriging • Azarbayjan

INTRODUCTION

Water resources planning and management provide decision-tools for: (a) allocation of adequate water to the consumers at appropriate time and place, (b) protection from excessive water (e.g. floodwater) and (c) maintenance of acceptable water quality [1]. The increase in water demand with population growth is applying more stress on available water resources and calls for an efficient and acceptable management of the resources [2]. Groundwater quality mapping over extensive areas is the first step in water resources planning [3]. One of tools for mapping of groundwater quality is geostatistical methods.

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 [4].

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 homogene 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 [5,6]. In recent years, many scientists have evaluated accuracy of different spatial interpolation methods for prediction of soil and water quality parameters. Amini *et al.* [7] applied kriging and co-kriging techniques for predicting Cl⁻ concentration of soil in Roudash, Isfahan which showed that kriging method provides more accurate and low cost results. Jager *et al.* [8] also used geostatistical tools like kriging to simulate groundwater quality variables and who added result kriging is better than other geostatistical tools for simulating groundwater quality variables. Misaghi and Mohammadi [9] estimated groundwater table by using geostatistics methods. Nazari *et al.* [10], used geostatistics method to study spatial variability of groundwater quality in Balarood plain. Their results showed that spherical model is the best model for fitting an experimental variogram of EC, Cl and SO₄ variables. Istock and Cooper [11] used kriging method to estimate heavy metals concentration in groundwater and concluded that it the mentioned method is the best estimator for spatial prediction of lead. Dagostino *et al.* [12] studied spatial and temporal variability of groundwater nitrate, using kriging and cokriging methods. Their results show that cokriging method has higher accuracy than kriging in estimating of nitrate concentration. Rizzo and Mouser [13] used geostatistics for analyzing groundwater quality. They used microbial data as an auxiliary variable in cokriging method. Their results show that cokriging method has suitable accuracy to estimate groundwater quality. Ahmad [14] found that kriging method has a high accuracy in estimating of total dissolved salts (TDS) in groundwater. Gaus *et al.* [15] studied groundwater pollution in Bangladesh. They used disjunctive kriging method to estimate arsenic concentration and to prepare risk map. Their results show that 35 milion people are exposed to high concentration of arsenic (50ppm). Finke *et al.* [16] used simple kriging to estimate water surface changes in Netherlands and introduced it as a suitable method for mapping of water surface. Barca and Passarella [17] used Disjunctive kriging and simulation methods to make nitrate risk map in 10, 50(mg/l) thresholds, in Modena plain of Italy. Their results showed that Disjunctive kriging method is the suitable method to study deterioration level of Groundwater. Because of various results reported by above mentioned researchers, it is obvious that suitable method of interpolation to estimate one variable depends on variable type and regional factors, thus any selected method for specific region cannot be generalized to others.

The present study was therefore, carried out with objectives to evaluate accuracy of different interpolation methods, kriging, cokriging and IDW, for prediction of some groundwater quality parameters in Azarbayejan Province of Iran.

MATERIALS AND METHODS

Study Area: The study area is located in north Western of Iran. Groundwater resources in this province are very important sources of water for agricultural and urban activities. Azarbayejan is one of the main locations in Iran with view of agriculture. So knowledge of condition of groundwater quality is very vital. The location of study area and distribution of 625 domestic wells is shown in Fig. 1.

Reaserch Method: 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.

Spatial Prediction Methods

Kriging: The presence of a spatial structure where observations close to each other are more alike than those that are far apart (spatial autocorrelation) is a prerequisite to the application of geostatistics [18,19]. The experimental variogram measures the average degree of dissimilarity between unsampled values and a nearby data value [20] and thus can depict autocorrelation at various distances. The value of the experimental variogram for a separation distance of h (referred to as the lag) is half the average squared difference between the value at z(xi) and the value at z(xi + h) [21,19] used:

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

Where n (h) is the number of data pairs within a given class of distance and direction. If the values at z (xi) and z (xi + h) are auto correlated the result of Eq. (1) will be small, relative to an uncorrelated pair of points. From analysis of the experimental variogram, a suitable model (e.g. spherical, exponential) is then fitted, usually by weighted least squares and the parameters (e.g. range, nugget and sill) are then used in the kriging procedure.

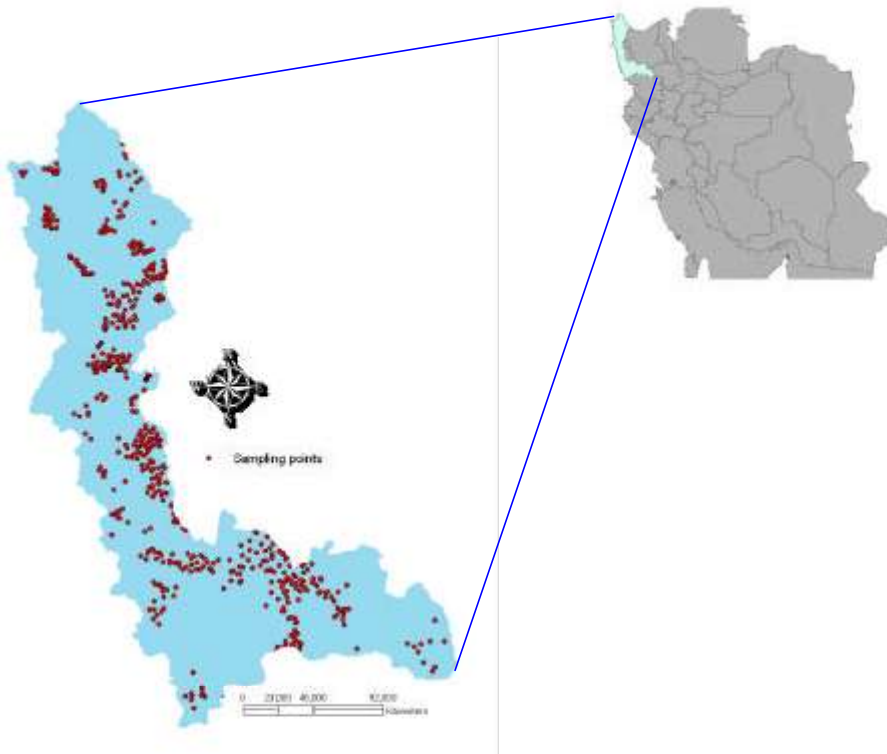


Fig. 1: Situation of studied area and sampling wells distribution

IDW: In interpolation with IDW method, a weight is attributed to the point to be measured. The amount of this weight is dependent on the distance of the point to another unknown point. These weights are controlled on the bases of power of ten. With increase of power of ten, the effect of the points that are farther diminishes. Lesser power distributes the weights more uniformly between neighboring points. We should keep in mind that in this method the distance between the points count, so the points of equal distance have equal weights [22]. In this method the weight factor is calculated with the use of the following formula:

$$\lambda_i = \frac{D_i^{-\alpha}}{\sum_{i=1}^n D_i^{-\alpha}} \quad (2)$$

λ_i = the weight of point, D_i = The distance between point i and the unknown point, α = The power ten of weight

Cokriging: The “co-regionalization” (expressed as correlation) between two variables, i.e. the variable of interest, groundwater quality in this case and another easily obtained and inexpensive variable, can be exploited

to advantage for estimation purposes by the co-kriging technique. In this sense, the advantages of co-kriging are realized through reductions in costs or sampling effort. The crosssemivariogram is used to quantify cross-spatial auto-covariance between the original variable and the covariate [23]. The cross-semivariance is computed through the equation:

$$\lambda_{uv}h = \frac{1}{2} E[\{z_u(x) - z_u(x+h)\}\{z_v(x) - z_v(x+h)\}] \quad (3)$$

Where: $\gamma_{uv}(h)$ is cross-semivariance between u,v variable, $Z_u(x)$ is primary variable and $Z_v(x)$ is secondary variable.

Comparison Between the Different Methods: Finally, we use the RMSE to evaluate model performances in cross-validation mode. The smallest RMSE indicate the most accurate predictions. The RMSE was derived according to Eqs. (4).

$$R.M.S.E = \sqrt{\frac{1}{N} \sum_{i=1}^N (Z(xi) - Z^*(xi))^2} \quad (4)$$

$Z(xi)$ is observed value at point xi , $Z^*(xi)$ is predicted value at point xi , N is number of samples.

RESULTS AND DISCUSSION

A statistical summary of the groundwater quality properties is presented in Table. 1. Based on skewness and histogram, data were normalized using logarithmic method Fig. 2.

Table 1: Results of statistical analysis on Groundwater quality

GWQI	Min	Max	Mean	Std	Kurtosis	Skewness
TH(mg/l)	80	3450	435.132	352.619	15.31	3.25
TH(mg/l)**	4.38	8.15	5.876	0.588	0.81	0.72
SAR	0.08	30.17	2.211	3.269	21.97	3.91
SAR**	-2.53	3.41	0.106	1.166	-0.44	0.18
Na ⁺ (mg/l)	0.1	84	5.252	8.969	22.41	3.99
Na ⁺ (mg/l)**	-2.3	4.43	0.742	1.354	-0.56	0.22
Ca ²⁺ (mg/l)	0.2	35.5	4.102	3.551	17.9	3.52
Ca ²⁺ (mg/l)**	-1.61	3.57	1.182	0.648	1.34	0.26
Mg ²⁺ (mg/l)	0.2	44.5	4.608	4.447	16.37	3.22
Mg ²⁺ (mg/l)**	-1.61	3.8	1.212	0.783	0.55	0.06
SO ₄ ²⁻ (mg/l)	0.1	125	3.976	7.714	103.28	8.04
SO ₄ ²⁻ (mg/l)**	-2.3	4.83	0.649	1.133	0.21	0.4
Cl ⁻ (mg/l)	0.1	90	4.438	10.015	25.95	4.61
Cl ⁻ (mg/l)**	-2.32	4.5	0.409	1.303	0.32	0.84
EC (µs/cm)	63	21120	1322.584	1601.274	43.3	5.02
EC**(µs/cm)	4.14	9.96	6.822	0.782	0.55	0.71

**Using logarithm to normalize data

Table 2: Selection of the most suitable model for evaluation on experimental variogram according to RMSE

GWQI	Models		
	Spherical	Exponential	Gaussian
TH	287.4	269.7	299.6
SAR	2.512	2.584	2.719
Na ⁺	6.745	6.935	7.137
Ca ²⁺	3.587	3.551	3.644
Mg ²⁺	3.046	3.174	3.224
SO ₄ ²⁻	6.743	6.851	6.97
Cl ⁻	6.728	6.872	7.15
EC	1277	1304	1341

Table 4: Correlation matrix of groundwater quality

	TH	SAR	K ⁺	Na ⁺	Mg ²⁺	Ca ²⁺	SO ₄ ²⁻	Cl ⁻	HCO ₃ ⁻	pH	EC
TH	1										
SAR	0.391	1									
K ⁺	0.498	0.485	1								
Na ⁺	0.629	0.912	0.576	1							
Mg ²⁺	0.905	0.438	0.501	0.647	1						
Ca ²⁺	0.847	0.227	0.359	0.437	0.542	1					
SO ₄ ²⁻	0.598	0.432	0.300	0.535	0.611	0.420	1				
Cl ⁻	0.691	0.687	0.532	0.859	0.632	0.578	0.362	1			
HCO ₃ ⁻	0.429	0.238	0.353	0.260	0.459	0.277	0.175	0.048	1		
pH	-0.191	0.133	-0.051	0.040	-0.031	-0.340	0.062	-0.049	-0.291	1	
EC	0.775	0.653	0.519	0.804	0.760	0.585	0.529	0.758	0.359	-0.075	1

After data normalizing, experimental variogram was computed. The best model for fitting on experimental variogram was selected based on less RMSE value. Table 2. These variograms are shown in Fig. 3.

Also, Table 3 illustrates parameters of groundwater quality variograms. The ratio of nugget variance to sill expressed in percentages can be regarded as a criterion for classifying the spatial dependence of ground water quality parameters. If this ratio is less than 25%, then the variable has strong spatial dependence; if the ratio is between 25 and 75%, the variable has moderate spatial dependence; and greater than 75%, the variables shows only weak spatial dependence [24]. All parameters of ground water quality have moderate spatial structure except Ca²⁺. Also effective range of most parameters is close together with the range of 41.78 to 73.81 Km.

In cokriging method, after conducting of correlation matrix, a parameter which has the highest correlation coefficient with primary variable was selected as an auxiliary variable (Table 4). Consequently, Mg²⁺, Na⁺, SAR, TH, TH, Mg²⁺, Na⁺ and Na⁺ variables were selected as auxiliary variables for estimation of TH, SAR, Na⁺, Ca²⁺, Mg²⁺, SO₄²⁻, Cl⁻ and EC, respectively. Cross variograms are presented in Fig. 4. The best model for fitting on cross

Table 3: Best-fitted variogram models of ground water quality and their parameters

GWQI	Model	(C _o)	(C _o +C)	(Km)	(C _o /C _o +C)%
		Nugget	Sill	Range effect	
TH	Exponential	0.114	0.253	55.52	45
SAR	Spherical	0.355	1.102	67.91	32
Na ⁺	Spherical	0.466	1.551	73.81	30
Ca ²⁺	Exponential	0.214	0.249	41.78	86
Mg ²⁺	Spherical	0.22	0.414	61.02	53
SO ₄ ²⁻	Spherical	0.357	1.061	71.12	34
Cl ⁻	Spherical	0.431	1.506	56.22	29
EC	Spherical	0.206	0.456	63.57	45

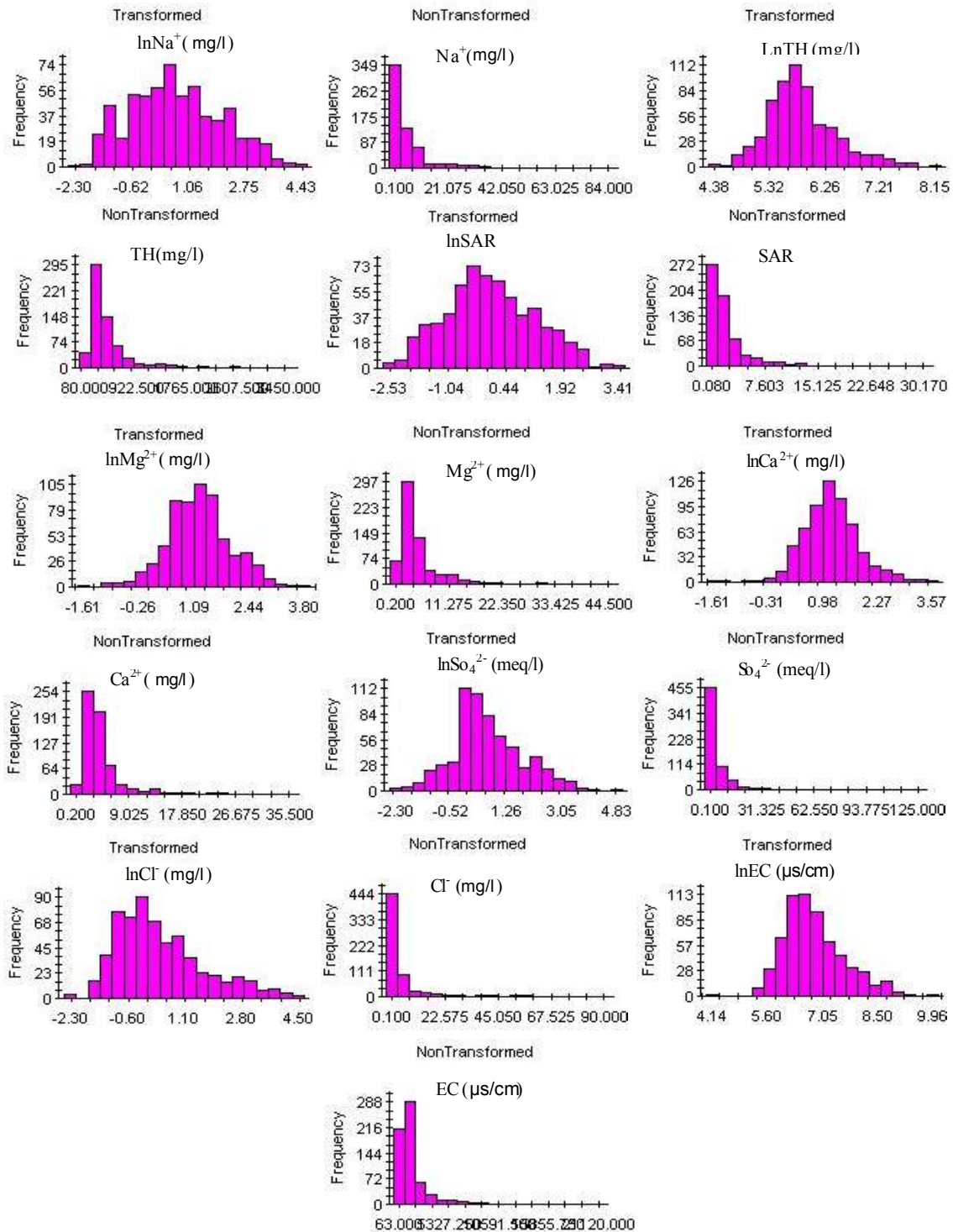


Fig. 2: Histograms of water quality indices (after and before transformation)

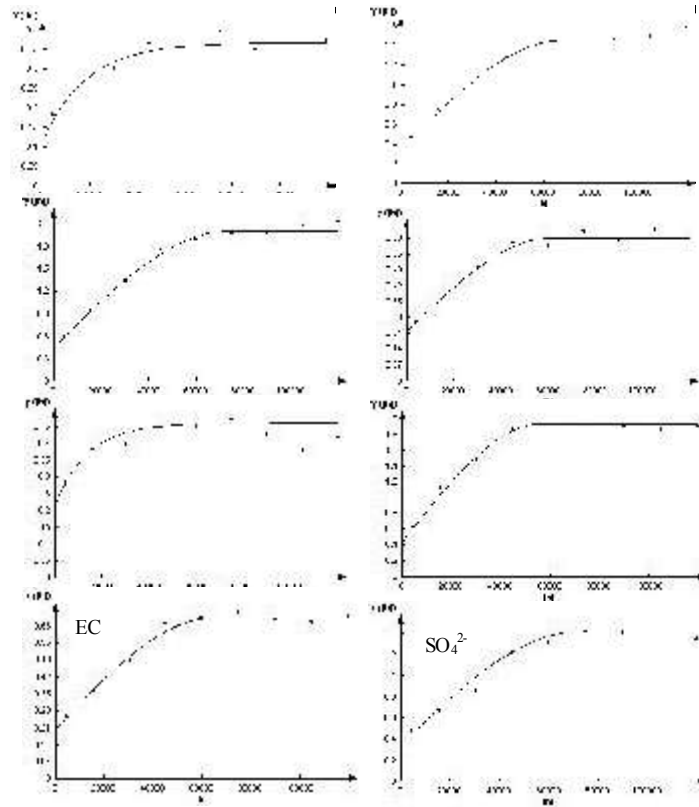


Fig. 3: Variograms related to groundwater quality

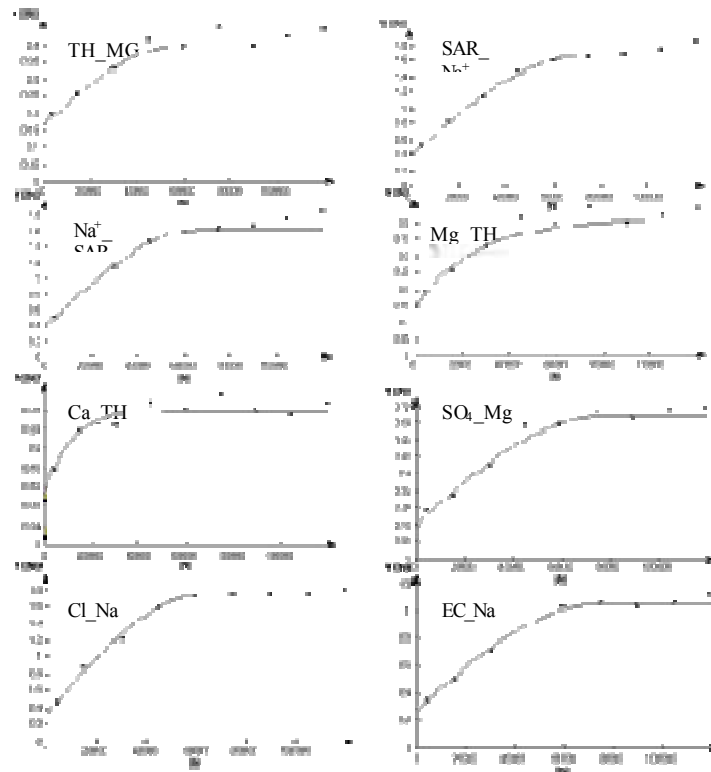


Fig. 4: Cross variogram of groundwater quality

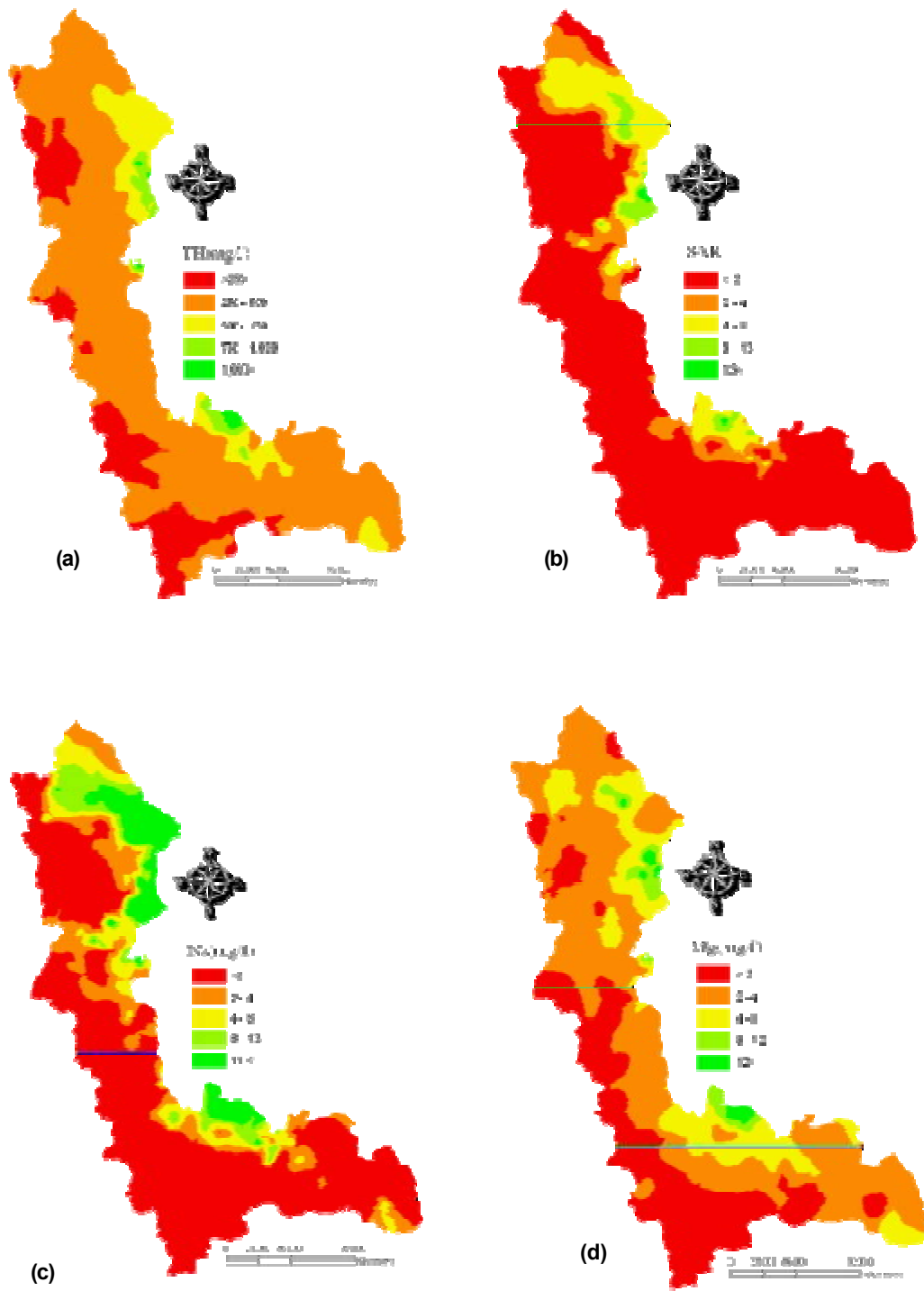


Fig. 5: Groundwater quality maps

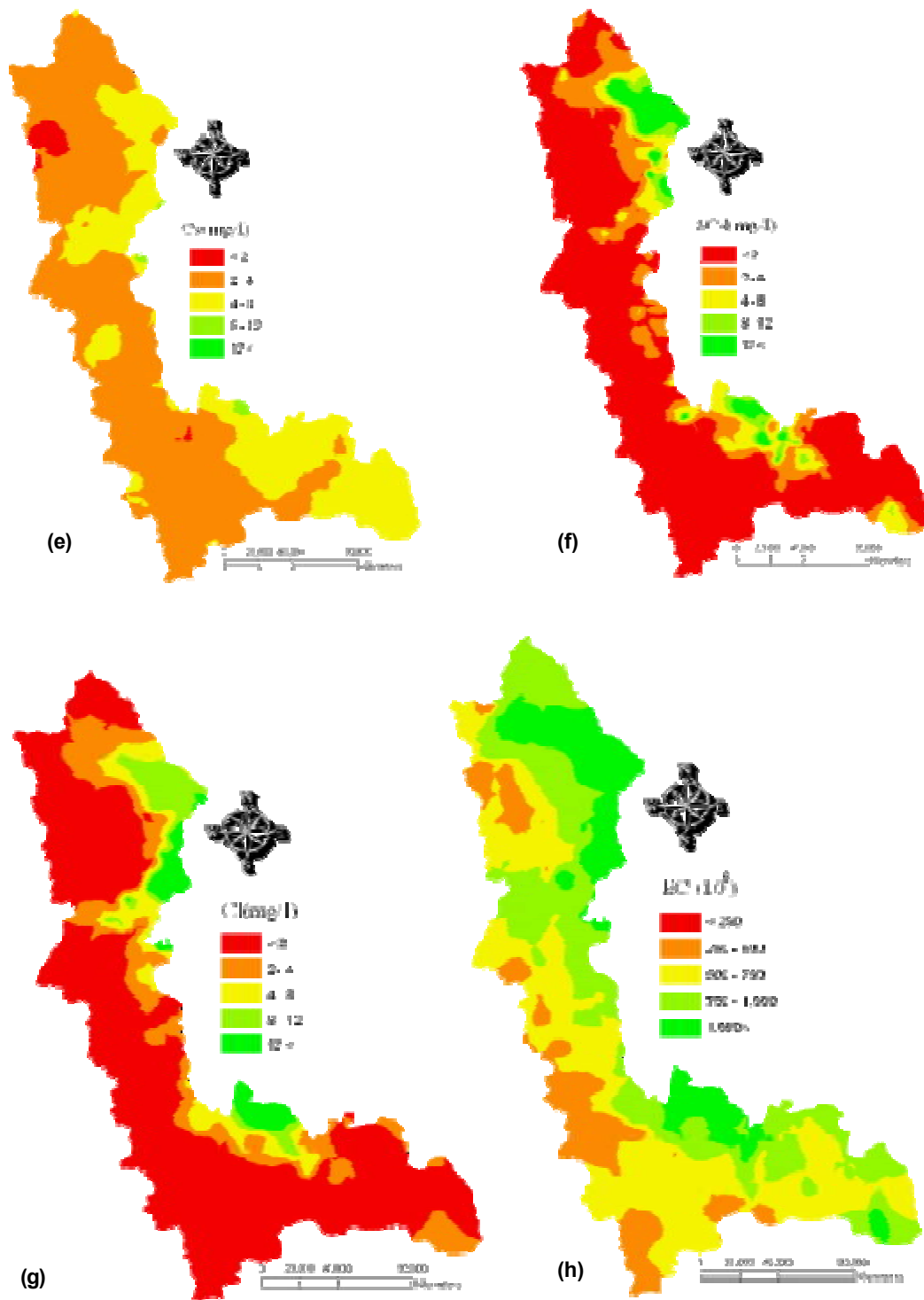


Fig. 5: Groundwater quality maps

Table 5: Selection of the most suitable model for evaluation on cross-variogram according to RMSE

GWQI	Models		
	Spherical	Exponential	Guassian
TH_ Mg ²⁺	228.8	308.4	302.2
SAR_ Na ⁺	2.476	2.564	2.699
Na ⁺ _ SAR	6.588	6.805	7.053
Ca ²⁺ _ TH	3.131	2.987	3.279
Mg ²⁺ _ TH	3.565	3.199	3.704
SO ₄ ²⁻ _ Mg ²⁺	6.703	6.803	6.956
Cl ⁻ _ Na ⁺	4.482	6.273	7.141
EC_ Na ⁺	1048	1235	1329

Table 6: Best-fitted cross-variogram models of ground water quality and their parameters

GWQI	Model	Nugget (C ₀)	Sill (C ₀ +C)	Range effect(Km)	(C ₀ /C ₀ +C)%
TH_ Mg ²⁺	Spherical	0.166	0.232	56.22	71
SAR_ Na ⁺	Spherical	0.406	1.257	70.87	32
Na ⁺ _ SAR	Spherical	0.394	1.24	66.12	32
Ca ²⁺ _ TH	Exponential	0.104	0.177	31.74	59
Mg ²⁺ _ TH	Exponential	0.146	0.269	76.97	54
SO ₄ ²⁻ _ Mg ²⁺	Spherical	0.163	0.506	74.76	32
Cl ⁻ _ Na ⁺	Spherical	0.323	1.415	61.07	23
EC_ Na ⁺	Spherical	0.285	0.765	72.22	37

Table 7: Selecting the best interpolation method according to RMSE

GWQI	Cokriging	Kriging	IDW		
			Exp 1	Exp 2	Exp 3
TH	228.8	269.7	277.6	275.5	281.4
SAR	2.476	2.512	2.484	2.545	2.651
Na ⁺	6.588	6.745	6.76	7.01	7.281
Ca ²⁺	2.987	3.046	3.085	3.082	3.141
Mg ²⁺	3.199	3.551	3.416	3.413	3.505
SO ₄ ²⁻	6.703	6.743	7.262	8.167	8.503
Cl ⁻	4.482	6.728	6.98	6.866	6.99
EC	1048	1277	1328	1368	1436

variogram was selected according to less RMSE (Table 5). Also table. 6. Showed parameters of the best model fitted on cross-variogram. All parameters of ground water quality have moderate spatial structure except Cl-Na.

For determination of the most suitable method, among Kriging, cokriging and IDW, RMSE was used. Results showed that geostatistic methods had more considerable accuracy than IDW method for all parameters. Furthermore, cokriging method increased prediction accuracy and had less RMSE which is in line with the work done by Rizzo and Mouser [13],

Nazari *et al.* [10], Ahmad [14], Barca and Passarella [17]. They confirmed cokriging has higher accuracy than other methods (Table 7). Finally, maps of groundwater quality were prepared by cokring in GIS environment.

CONCLUSION

Results showed that the majority of studied parameters had high skewness, due to insufficient number of samples and unsuitable distribution. However, data were normalized using logarithmic method. Also results showed that effective range of most qualitative parameters of groundwater are closed to each another indicating their high correlation. Spatial structure models were moderate in most of the studied water parameters.

This study has attempted to predict the spatial distribution and uncertainty of some groundwater quality indices in the North Western of Iran, Azarbayjan Province, using three interpolation techniques (kriging, cokriging and IDW). The analysis showed that for all groundwater quality indices cokriging performed better than kriging and IDW techniques in characterizing the spatial variability.

Generally, results showed that deterioration of ground water quality in Azarbayjan Province is not very serious problem but discharging water from aquifer more than its potential can devastate ground water quality in near future.

Groundwater pollution hazard assessments should prompt municipal authorities or environmental regulators to take both preventive actions to avoid future pollution and corrective actions to control the pollution threat posed by existing and past activities.

It is suggested that in the future studies, other methods especially indicator and disjunctive kriging is used in order to prepare risk maps.

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