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EVALUATION OF SPATIAL INTERPOLATION TECHNIQUES FOR MAPPING GROUNDWATER NITRATES CONCENTRATIONS - CASE STUDY OF AIN ELBEL-SIDI MAKHLOUF SYNCLINE IN THE DJELFA REGION (ALGERIA)

ÉVALUATION DES TECHNIQUES D'INTERPOLATION SPATIALE POUR LA CARTOGRAPHIE DES CONCENTRATIONS DES NITRATES DES EAUX SOUTERRAINES - ÉTUDE DE CAS DU SYNCLINAL AIN ELBEL-SIDI MAKHLOUF DANS LA RÉGION DE DJELFA (ALGÉRIE)

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ABSTRACT

The presence of nitrate is one of the factors limiting the quality of groundwater resources, particularly in arid and semi-arid regions. Geostatistical methods have been used widely as a convenient tool to make a decision on the management of the behavior of hydrochemical parameters in groundwater. The purpose of this study is to evaluate the accuracy of several spatial interpolation methods, comparing inverse distance weighting (IDW), simple kriging, ordinary kriging, and universal kriging methods using nitrate concentration data from 305 groundwater wells in the synclinal of Ain el bel-Sidi Makhlouf (Algeria). To select the best interpolation method, errors of predicted values were determined by Mean Error (ME) and Root Mean Square Standardized Error (RMSS). The results make clear that Kriging methods performed better, showing greater consistency in the generated surfaces, fewer interpolation errors, and lower biases. However, universal kriging was determined to be the optimal method, striking a balance between accuracy and simplicity and gives a good spatial distribution of the nitrate contents in the syncline of Ain el bel and Sidi Makhlouf.

Keywords: Geostatistics, Groundwater; Nitrate concentration, Spatial interpolation methods, Ain el bel Sidi Makhlouf syncline

RESUME

La présence de nitrate est l'un des facteurs limitant la qualité des ressources en eaux souterraines, en particulier dans les régions arides et semi-arides. Les méthodes géostatistiques ont été largement utilisées comme un outil pratique pour prendre une décision sur la gestion du comportement des paramètres hydro chimiques dans les eaux souterraines. Le but de cette étude est d'évaluer la précision de plusieurs méthodes d'interpolation spatiale, en comparant la pondération à distance inverse (IDW), le krigeage simple, le krigeage ordinaire et les méthodes de krigeage universelles en utilisant les données de concentration de nitrate de 305 puits d'eau souterraine dans le synclinal d'Ain el bel- Sidi Makhlouf (Algérie). Pour sélectionner la meilleure méthode d'interpolation, les erreurs des valeurs prédites ont été déterminées par l'erreur moyenne (ME) et l'erreur standardisée quadratique moyenne (RMSS). Les résultats montrent clairement que les méthodes de krigeage ont été plus performantes, montrant une plus grande cohérence dans les surfaces générées, moins d'erreurs d'interpolation et moins de biais. Cependant, le krigeage universel a été déterminé comme étant la méthode optimale, établissant un équilibre entre précision et simplicité et donnant une bonne répartition spatiale des teneurs en nitrates dans le synclinal d'Ain el bel et de Sidi Makhlouf.

Mots clés : Géostatistique, Eaux souterraines, Concentration de nitrate, Méthodes d'interpolation spatiale, Synclinal Ain el bel Sidi Makhlouf

INTRODUCTION

Assessment of groundwater quality of a region is of paramount importance to plan for proper groundwater development. Increased groundwater demand for agricultural production, industrialization and urbanization necessitates regular monitoring of its quality. The deterioration of groundwater quality affects its usage for drinking, agriculture and industrial activities (Kahoul et al., 2014). The causes for the deterioration of groundwater quality may be natural or anthropogenic or both. After the identification of contamination sources, it is often difficult to adopt a management option to overcome the poor groundwater quality. Hence, it is essential to monitor the quality of groundwater regularly to sustainably manage the groundwater resource.

Several studies have dealt with nitrate impact on the groundwater quality degradation over different parts of Algeria. Zamiche et al. (2018) evaluated the degree of contamination by nitrates of Mitidja aquifer located in Northern Algeria using a statistical approach and the Water Quality Index (WQI) to estimate the impact on the quality of the aquifer. Their results show that the aquifer is strongly contaminated by nitrates with an average of 71.58 mg/l. Likewise, the principal component analysis technique indicated that intensive agricultural production and irrigation practices responsible for groundwater pollution and water quality degradation. In a previous study, Nasri et al. (2018) also evaluated the physicochemical quality of groundwater in the region of Timiaouine in southern Algeria. They showed that the groundwater in this area is not suitable for consumption as drinking water. Based on the recommendations of WHO (2011) and the Algerian reference limits of 50 mg/l nitrate, about 93% of wells have a nitrate concentration above the recommended limit. Furthermore, their results make clear that groundwater pollution from the Timiaouine aquifer due to the intensification of livestock, camelin farming, and septic tanks. In southern Hodna, an arid region of Algeria, Abdesselam et al. (2012) studied nitrate contamination of groundwaters and its increase from 1967 to 2008, using the archive data of 113 wells sampled in the whole agricultural area. The study points at general contamination of aquifers from the anthropic origin, as the population increased and irrigation agriculture developed with large use of nitrogen fertilizers and organic amendments, contamination extended spatially and vertically to deep aquifer

Today, efforts have been made to identify the predicting systems for water quality assessing as the best way to prevent pollution and investigate the quality of groundwater (Fallahzadeh et al., 2016). GIS (Geographic Information System) is considered one of the most powerful technologies in this field to identify, analyze, interpret and make inferences about data (Childs, 2004; Benslimane et al., 2015; Kerboub et al., 2016; Mangoua et al., 2019). Its capabilities for spatial interpolation have improved through integrating advanced methods as well as linking GIS to a system designed for modeling, analyzing, and visualizing a continuous field (Mitas and Mitasova, 1999). This system gathers data from a determined geographic location in order to store, collect and analyze data which is a great step to make a huge source of spatial and descriptive data accessible in a short time (Anselin and Getis, 1992). Numerous studies have shown that GIS used as explored spatial analyzes, interpolation and mapping all over the world. Also, in science and health services, it can provide users and authorities with useful information (Sahoo and Jha 2014; Merwade, 2009). It is demonstrated that Kriging and IDW are efficient for spatial interpolation of nitrate concentrations in flat areas water resources (Anselin and Getis, 1992; Curtarelli et al. 2015). Uyan and Cay (2010) showed that Universal kriging, a type of geostatistical technique, can be applied to distribute the groundwater nitrate concentration data. In statistics, mainly in geostatistics, it is a powerful method of interpolation. The basic idea of Kriging is to predict the value of a function at a given point by computing a weighted average of the known values neighboring the function. Mathematically, the method is closely related to regression analysis. Semi-variogram plays a central role in the analysis of geostatistical data using the kriging method (Okobiah et al., 2013; Koziel and Bandler, 2012). It is showed that the kriging method was the most suitable technique for mapping the bathymetry of the Yucatan submerged platform (Merwade et al., 2009). Inverse Distance Weight (IDW) is based on the extent of similarity of cells used in order to determine the depth and spatial variability of groundwater quality in areas that are not flat (Childs, 2004; Naoum and Tsanis, 2004). Azpurua and Ramos (2010) showed that it is most likely to produce the best estimation in interpolation. Natural Neighbor is based on a discrete set of spatial points. The value of an interpolation point is estimated using weighted values of the closest surrounding points in a triangulation (Bannister and Kennelly, 2016). One of the important keys in the interpolation method is error determination. There are a lot of ways to determine the interpolation errors such as the Mean Bias Error and Root Mean Square Error.

The purpose of this paper is to evaluate the distribution of nitrate concentration with geostatistical methods such as the IDW method, Ordinary Kriging (OK), Universal Kriging (UK), and Simple Kriging (SK) in the synclinal of Ain el bel-Sidi Makhlouf (Algeria).

STUDY AREA DESCRIPTION

The Ain El Bel syncline from the Djelfa region (Figure 1) is located in the central part of northern Algeria between longitudes 2°57′ and 3°20′ E and latitudes 34°07′ and 34°28′ N, and covers approximately an area of 647 km^2. The water tables of Ain El Bel syncline represent an important source for drinking water, agricultural and industrial purposes due to the scarcity of surface water.

The syncline extends over 48 km along an axis North East - South West and for 18 km along a perpendicular axis. It is bordered in the northeast by Zakar and Djebel Tafara, and in the northwest by Djebel Djellal Rharbi. In the southwest by Djebel Zergua and west by Tadmit (Pouget, 1977). The entire depression is drained by the Oued Tadmit crossing Zerga Jebel before joining Oued Messaad to the east, and El Oued Bel ending in the town of Ain El Bel, which is a basic level of water flows (Basseto and Guillemot, 1971). The plain has a semi-arid climate type characterized by dry and hot summer and wet and cool winter seasons, with a mean annual rainfall of 329 mm, and a mean annual temperature of 14.32°C.

In this study, various bibliographical documents were consulted and exploited to establish a sufficient synthesis of knowledge. Further, a number of trips were arranged to ANRH (National Agency of Hydraulic Resources) along with repeated field surveys for the study. A sampling campaign was performed during March 2009 with 305 groundwater samples (Figure 2) have been collected from the synclinal of Ain el bel-Sidi Makhlouf by the ANRH. A statistical summary related to nitrate concentration data is displayed in Table 1.

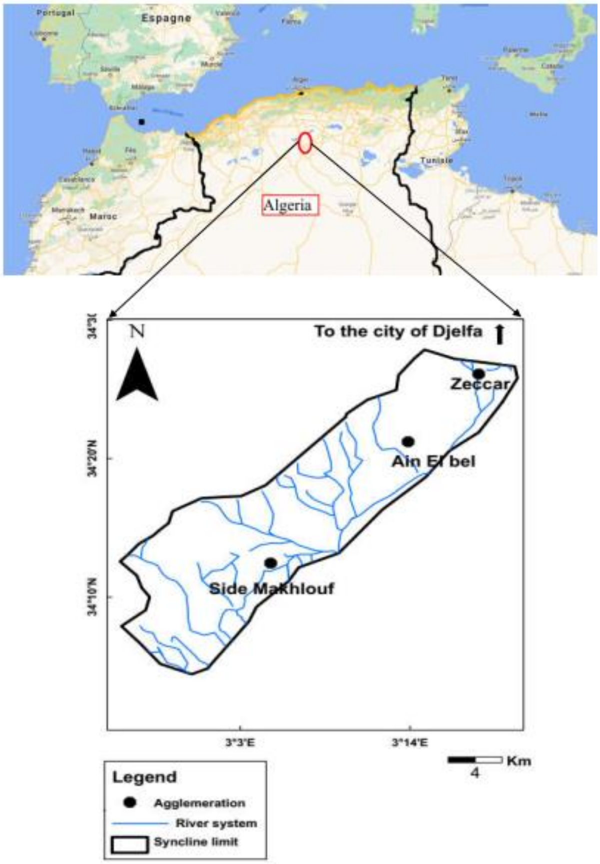

Figure 1: Geographical situation of the Syncline Ain EL Bel-Sidi Makhlouf

Table 1: Basic statistics of the raw nitrate data from 305 wells

Parameter	Min	Max	Mean	Samples	Std. Dev	Skewness	Kurtosis
Nitrates (mg/l)	0	162	32.83	305	32.30	1.57	5.25

Chemical analyses of water samples were carried out in the laboratory of the ANRH of Djelfa. Cations (Ca^+, Mg^+, Na^+, K^+) were analyzed by atomic absorption spectrometry, anions (Cl^-, HCO_3^-, and NO_3^-) by high-performance ionic liquid chromatography (HPILC). Bicarbonates (HCO_3^-) were determined by the acid-base titration method. A statistical summary of groundwater hydrochemical parameters is presented in Table 2.

Table 2: Statistical summary of physico-chemical parameters calculated on the 305 sample size obtained from the study area

Parameters	Symbol	Average	Standard Deviation	Coefficient of Variation
Sodium	Na	191.87	129.96	0.66
Magnesium	Mg	127.83	104.57	0.81
Calcium	Ca	113.96	85.11	0.74
Potassium	K	5.60	5.31	0.95
Chlorure	Cl	252.32	169.03	0.67
Bicarbonate	HCO3	228.24	127.83	0.56

In reviewing Table 2, we can see that the sodium analysis of the water samples at the whole points studied varied from 10 to 500 mg/l, while the chloride contents vary between 15 and 750 mg/l, which poses a health hazard because the levels exceed the standard limit value recommended by WHO. Furthermore, the nitrate concentrations in the water analyzed varied between 4 mg/l and 150 mg/l, all these concentrations are lower than the WHO guideline value except for a few wells, which exceed 50 mg/l located in the north of the syncline.

Figure 2 shows the spatial distribution of inventory data from 305 groundwater wells. Nitrate concentration measurements taken at wells were summarized for the march 2009 period. The summary values are related to a map location (usually by adding the X and Y coordinates of a well) to create a new set of points holding the summarized time series. To automate this process, we used the Make Time Series Statistics tool available as part of the AHGW tools. The tool inputs include a set of well features and related nitrate concentration measurements stored in a table. The output from this tool is a set of point features with an attribute representing the calculated statistic (e.g. average nitrate concentration).

Analysis of the nitrate contents shows a high variability with a coefficient of variation (98%) and the average of the values does not exceed the standards of the World Health Organization (50 mg/l).

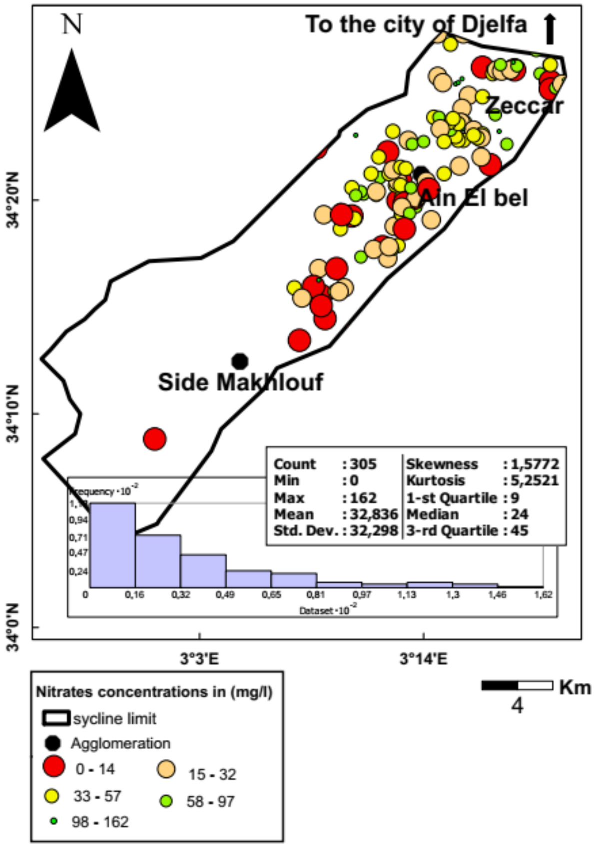

Figure 2: Spatial distribution of inventory data

METHODS

Interpolation techniques can be grouped into 2 main categories: deterministic and geostatistical. Deterministic interpolation techniques create surfaces from measured points, based on either the extent of similarity (e.g. IDW). A deterministic interpolation can either force the resulting surface to pass through the data values or not. An interpolation technique that predicts a value identical to the measured value at a sampled location is known as an exact interpolator. An inexact interpolator predicts a value that is different from the measured value and should be used to avoid sharp peaks or troughs in the output surface.

Geostatistical interpolation techniques (e.g. kriging) utilize the statistical properties of the measured points. Geostatistical techniques quantify the spatial autocorrelation among measured points and account for the spatial configuration of the sample points around the prediction location (Buchanan and Triantafilis, 2009; Rabah et al., 2011). The chart in Figure 3 shows the strategy, which is based on simple assumptions for demonstrate the use of these methods.

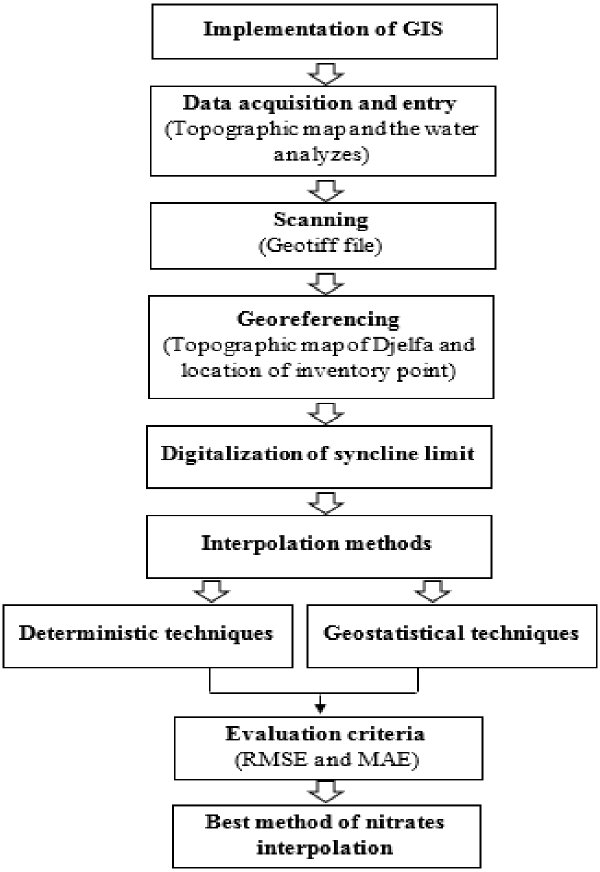

Figure 3: Simplified chart of strategy adopted

All analyses were accomplished by using the Geostatistical Analyst extension in ArcGIS 10.3 using nitrate concentration data from 305 groundwater wells distributed almost regularly on our study site.

Inverse distance weighted

IDW interpolation explicitly implements the assumption that objects that are close to one another are more alike than those that are farther apart. Thus, IDW assumes that each measured point has a local influence that diminishes with distance. To predict a value for any unmeasured location, IDW will use the measured values surrounding the prediction location. Those measured values closest to the prediction location will have the greatest influence on the predicted value (Ashraf et al. 1997; Nalder and Wein, 1998; Johnston et al., 2001).

Kriging

Over the past several decades, kriging has become a fundamental tool in geostatistics (Caruso and Quarta, 1998). Kriging forms weights from surrounding measured values to predict values at unmeasured locations. As with IDW interpolation, the closest measured values usually have the most influence, but kriging weights are more sophisticated. IDW uses a simple algorithm based on distance, whereas kriging weights come from a semivariogram developed from the spatial structure of the data. To create a continuous surface or map of the phenomenon, predictions are made for locations in the study area based on the semivariogram and the spatial arrangement of nearby measured values (Collins and Bolstad, 1996; Johnston et al., 2001). Four different kriging types were used in this study.

Ordinary kriging (OK)

This is the most general and widely used of the kriging methods. It estimates the value of the climatic variable at a given point from the values at surrounding stations and from a variogram model for that variable (Nalder and Wein, 1998; Johnston et al., 2001; Akramkhanov et al., 2011).

Simple kriging (SK)

This uses the average of the entire data set (while ordinary kriging uses a local average, i.e. the average of the scatter points in the kriging subset for a particular interpolation point). As a result, SK may be less accurate than ordinary kriging, but it generally produces a result that is smoother ((Nalder and Wein, 1998).

Universal kriging (UK)

This assumes that there is an overriding trend in the data which can be modeled by a deterministic function, i.e. by a polynomial. This polynomial is subtracted from the original measured points, and the autocorrelation is modeled from the random errors. Once the model is fit to the random errors, before making a prediction, the polynomial is added back to the predictions to give meaningful results (Nalder and Wein, 1998; Johnston et al., 2001).

THE EVALUATION METHOD FOR THE ACCURACY OF SPATIAL INTERPOLATION

Cross validation

The cross-validation method is a statistical analysis method used to verify the accuracy of the interpolation model, the basic idea is to classify the original dataset into the train set and the validation set. The validation set is used to test the model obtained from the training set, which is the indicators to evaluate the accuracy of the model.

Inverse distance interpolation (IDW), OK, SK and UK are applied to establish the best interpolation model, mean relative errors, root-mean-square errors, and absolute errors are the frequently used indexes of cross-validation. The error being the minimum is the evaluation criteria for the best-fit interpolation model (Triki Fourati et al. 2017; Arslan 2012). The computational formulas are as follows:

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

$$MRE = \frac{1}{n}\sum_{i=1}^{n}\left|\left(Z(x_i) - Z^*(x_i)\right)/Z(x_i)\right| \tag{2}$$

$$RMSE = \sqrt{\frac{1}{n}\sum[\,Z(x_i) - Z^*(x_i)]^2} \tag{3}$$

Where *Z(xi)* is the observed value at location *xi, Z*(xi)* is the interpolated value at location *xi,* and *n* is the sample size.

For indicator kriging, prediction performance was evaluated by cross-validation. As well as the average error and the mean squared error, three other criteria were retained for this validation step: Root mean square standardized which should be close to 1, mean standardized which must be close to 0 and the average standard should be as low as possible (Arslan, 2012).

Semivariogram is used to describe the spatial variability of groundwater quality. Assume that the mean of the random function is stable and the value is only related to the distance between samples, semivariogram r(h) may be defined as half the incremental variance of random function Z(x).

$$r(h) = \frac{1}{2}E[Z(x) - Z(x+h)]^2 \tag{4}$$

where *r(h)* is the semivariogram, *Z(x)* is the random function, *h* is the distance between samples.

A spherical model of the tested semivariogram models was fitted to the experimental semivariograms. The spherical model is defined by the following equation:

$$\rho(h) = \begin{cases} 0 & x = 0 \\ H_{0S} + H_s\left(\frac{3h}{2a} - \frac{h^3}{2a^2}\right) & 0 < x \le b \\ H_{0S} + H_s & x > b \end{cases} \tag{5}$$

where H_{0S} is the nugget value arising from random components such as measurement error and physical factors, H_S is the structural variance arising from spatial autocorrelation, $H_{0S} + H_S$ is the sill, and *b* is the distance at which the semivariogram equals 95 % of its sill variance.
Spatial variability characteristics are represented by the nugget to sill radio. The nugget value represents the variability while the sill value represents the overall variability inside the variables. The nugget to sill ratio shall be between 0 and 1. When the nugget effect is <0.25, the considered strongly spatially dependent; the variable is considered moderately spatially dependent as the nugget effect is between 0.25 and 0.75, while the nugget effect is >0.75, the variable is considered weakly spatially dependent (Ghazi et al. 2014).

RESULTS AND DISCUSSION

Inverse distance weighted

Spatial distributions of nitrate concentrations are shown in Fig. 4 using the nitrate concentration data from 305 groundwater wells. Results from this analysis show that the highest values of nitrate concentrations occur in the Zacara region. While the lower values of groundwater nitrate concentrations are located in the southern part of the study area. According to the World Health Organization (WHO) and the European Community (EC), the maximum contaminant level (MCL) of nitrate is given to be 50 mg/L whereas the US Environmental Protection Agency (EPA) allows for only 44.27 mg/L in drinking water. In contrast, the spatial distribution of nitrate concentrations shows that the Zaccar region was greatly exceeded this threshold with the values fluctuated between 50 and 160 mg/L. However, this form of the map obtained reflects the fact that the IDW method depends greatly on the location of the sampled points and is based solely on the neighborhood.

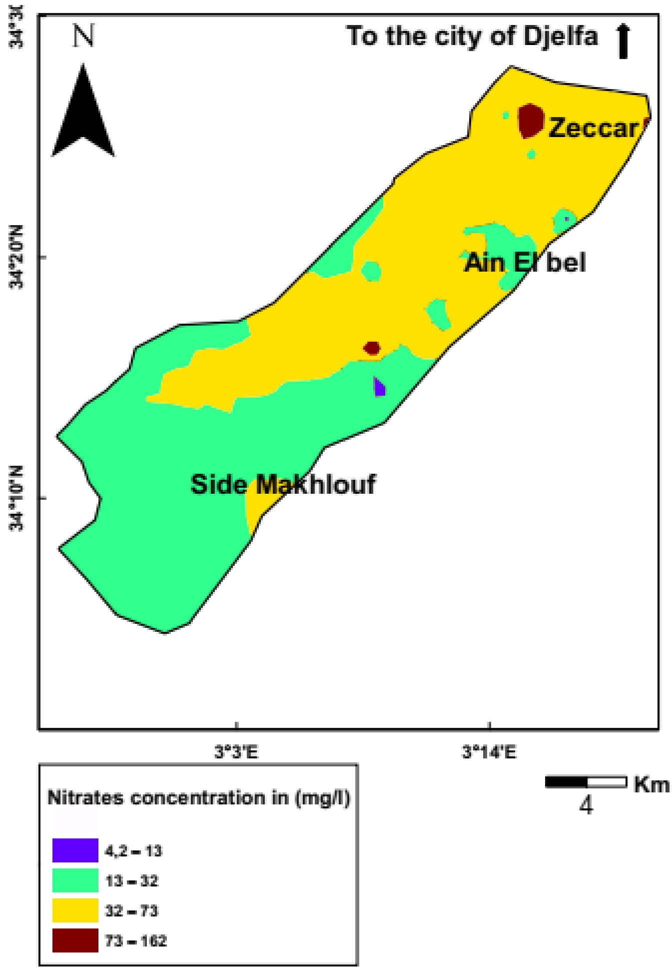

Figure 4: Spatial distribution of nitrate concentration in wells using the inverse distance weighted method

Geostatistical interpolation methods

Kriging, which is part of the geostatistical methods, allows the prediction by homogenizing the statistical characteristics of the real data (Safarbeiranvnd et al., 2018). According to the geostatistical algorithm, the kriging, the weighting rule and therefore the resulting map is directly determined by the spatial behavior of the data of the item to be analyzed. In the context of the geostatistical method of kriging, the natural spatial characteristics of the pollutant are taken into account using a variographic analysis also called structural analysis (Arslan, 2012). This analysis is fundamental for the choice of the interpolation model to apply to the experimental data. The variographic analysis makes it possible to quantify the spatial variability of the pollutant from the values observed at the various point measurement sites and according to the distance between them. The variogram thus illustrates the spatial continuity or correlation of the phenomenon studied (Delhomme, 1978). Figures 5, 6 and 7 show the experimental variograms and the data-fitted variogram model for the three kriging methods (Ordinary: OK; Simple: SK; Universal: UK). The results of the variograms values of the three kriging methods are presented in Table 3.

Table 3: Characteristics of the experimental variogram

Kriging models	Variogram model	Nugget effect	Direction
Ordinary kriging	Exponentiel	0.0327	90
Simple kriging	Exponentiel	0.619	50
Universal kriging	Exponentiel	0.071	90

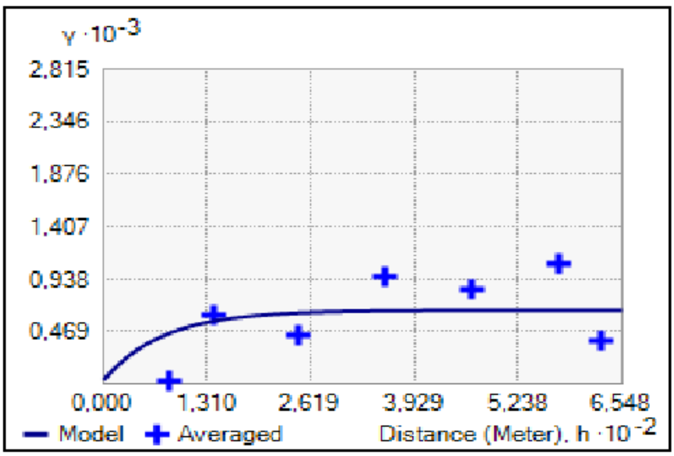

Figure 5: Variogram of ordinary kriging (OK)

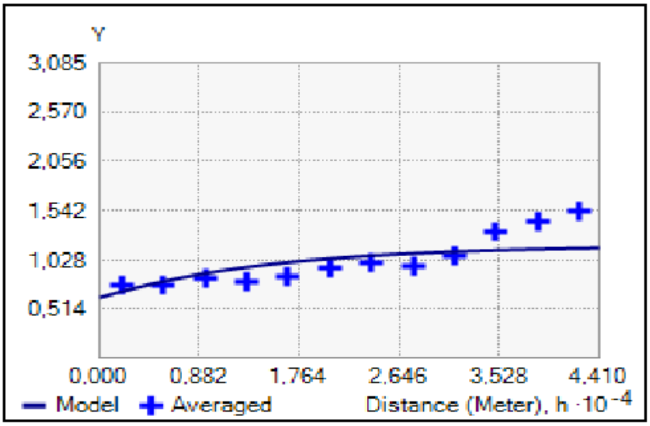

Figure 6: Variogram of simple kriging (SK)

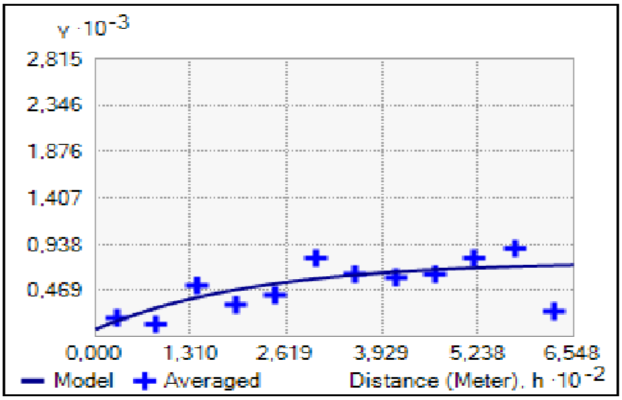

Figure 7: Variogram of universel kriging (UK)

Through the above analysis, we can see that the prediction accuracy of simple kriging and universal kriging show a similarity of the spatial distribution of the groundwater nitrate concentrations of Djelfa (Fig 8 and 9), but with relatively small differences at the southern level of the municipality of Ain el bel. On the other hand, the map resulting from the ordinary kriging method (Fig. 10) shows a different spatial distribution of nitrates and especially the identification of sites that have the nitrate concentration exceeds the threshold limit (50 mg/l).

The highest nitrate concentrations (50-160 mg/l) were always seen in the northern part of the aquifer (near Zeccar village), which can with high probability be related to the leaching of nitrate from agricultural soils and the presence of shale and marl formations which contain either nitrate or ammonium (Heriarivony et al., 2016).

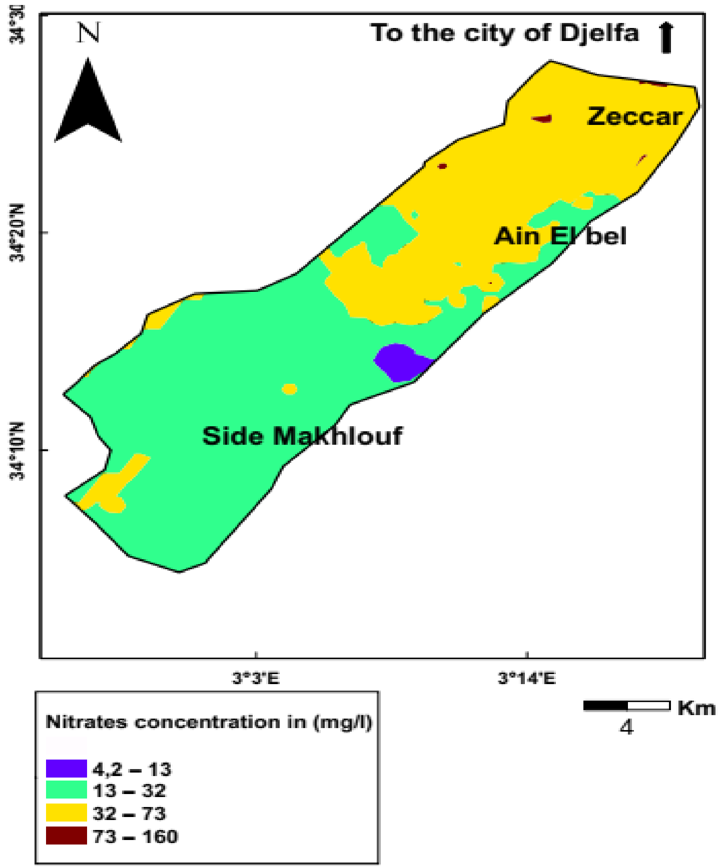

Figure 8: Spatial distribution of nitrate concentration in wells using the ordinary kriging method

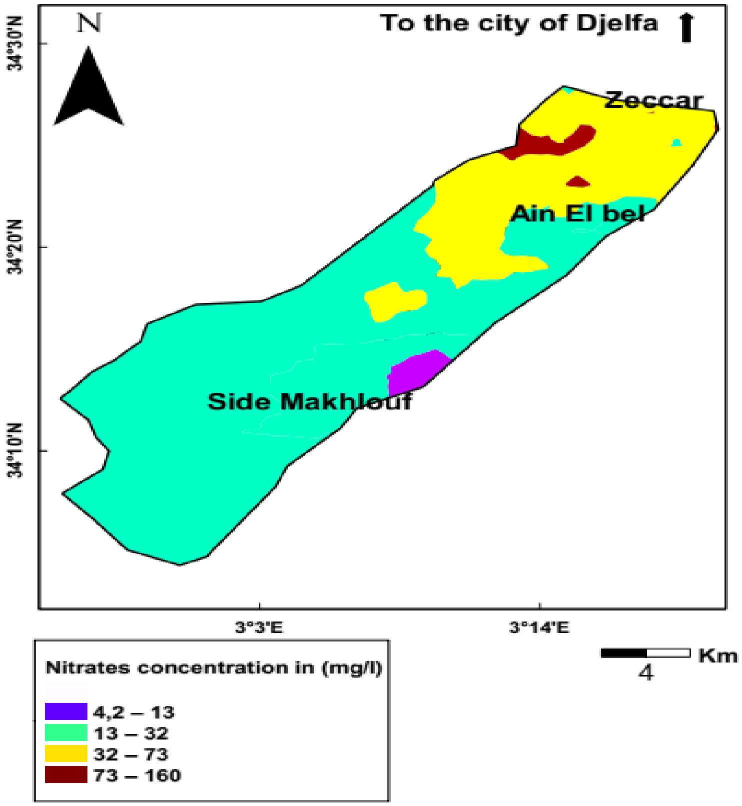

Figure 9: Spatial distribution of nitrate concentration in wells using the Simple kriging method

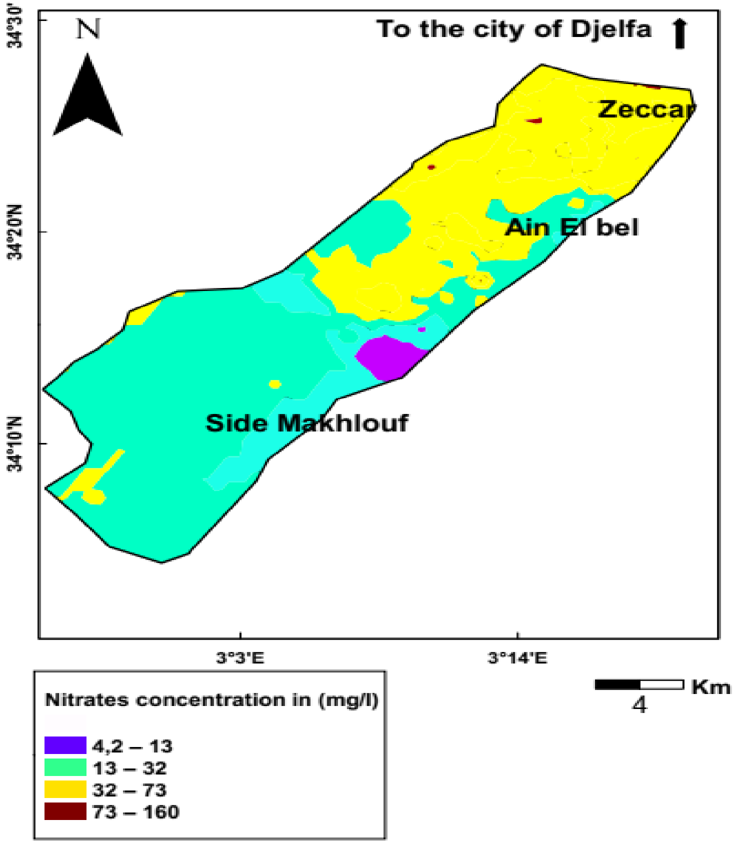

Figure 10: Spatial distribution of nitrate concentration in wells using the Universal kriging method

Evaluating Model Performance

Detailed statistics of the prediction accuracy of interpolation methods are given in Table 4. The performance of four models (IDW, OK, SK, UK) has been compared according to the cross-validation parameters. Generally, all four models performed fairly well. However, the Mean Error (ME) of the universal kriging model is close to 0 and the Root Mean Square Standardized prediction error (RMSS) is close to 1, more than others. This infers that universal kriging is the most precise method and gives a good spatial distribution.

Table 4: The prediction accuracy of interpolation methods

Method (Model)	Mean error (ME)	Root-mean-square standardized error (RMSS)
IDW	0.1	28.77
Ordinary kriging	0.225	1.089
Simple kriging	0.261	0.01
Universal kriging	0.0093	1.058

These findings are consistent with those of previous studies. Indeed, Mousavifazl et al. (2013) conducted a study for evaluated nitrate and sodium in the groundwater of 276 wells in Mashhad (Iran). They used both Kriging and IDW interpolation methods. Their results also indicated that Kriging could be more appropriate based on its root mean square error (RMSE) in comparison to non-geostatistical methods (inverse distance weight and normal distance weight). Likewise, Abdolahiman-sorkhani et al. (2012) also employed spatial interpolation methods including kriging, co-kriging, inverse distance weighting, and radial basis functions to evaluate the spatial distribution of nitrate in 56 wells in Shahrekord, Iran. According to their results, kriging was the most accurate method for modeling nitrate spatial distribution because of its minimum RMSE. The map of nitrate spatial distribution in groundwater was prepared by means of ordinary kriging. In a previous study, Taghizadeh et al. (2009) also evaluated the spatial variation of water quality characteristics using Kriging, co-Kriging and IDW interpolation methods in Rafsanjan, Iran. According to their results, Kriging and co-Kriging methods were more suitable than the IDW method.

In the study conducted by Ohmer et al. (2017), a total of nine deterministic and geostatistical methods were examined for optimal contour mapping of groundwater levels. The comparison was made using statistical criteria. In conclusion, geostatistical methods showed better fitting performance than did deterministic methods.

In general, it is impossible to find a universal method for choosing an interpolation type. The creation of the most reliable picture of spatial variability of an analyzed characteristic should always be preceded by the selection of an interpolation method. In the preliminary selection, the following should be taken into consideration: sample sizes, sampling types, and data distribution. After performing specific interpolations, the best method can be selected on the basis of appropriate quality measures.

CONCLUSIONS

The choice of an interpolation method is very important for spatial analysis of nitrate distribution. The aim of this study was to compare the results of the applied interpolators and finding a method characterized by the highest accuracy of point estimations using nitrate concentrations data from 305 groundwater wells in the synclinal of Ain el bel-Sidi Makhlouf (Algeria). The analyses conducted in this study enabled the creation of the most reliable picture of the variability of nitrate pollution in the study area. The results obtained show that geostatistical interpolation makes it possible to produce nitrate distribution maps that are more realistic than those obtained by conventional interpolation methods. On the other hand, it is important to note that IDW method, which is the most frequently used deterministic method was characterized by the highest values of RMSE and MAE. In addition, the geostatistical approach makes it possible to quantify the uncertainty associated with the map, because kriging takes into account the spatial continuity of the observed data. The results make clear that the universal kriging seems to be more appropriate than IDW for estimating the nitrate content in the groundwater of the Djelfa region. Finally, these findings may help decision-makers of the local authorities to protect groundwater and prevent groundwater pollution over the study area.

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