GEOSTATISTICAL METHODS FOR MAPPING GROUNDWATER NITRATE CONCENTRATIONS

Mevlut UYAN, Tayfun CAY

Abstract

The purpose of this study is to evaluate the spatial changes of groundwater nitrate concentrations by using geostatistical methods based on data from 119 groundwater wells. Geostatistical methods have been used widely as a convenient tool to make decision on the management of behavior of hydrochemical parameters in groundwater. To evaluate the spatial changes nitrate concentrations in groundwater, GIS is used for the application of universal kriging method with cross-validation leading to the estimation of groundwater nitrate concentrations. Nitrate concentrations followed a log-normal distribution and demonstrated a moderate spatial dependence according to the nugget ratio (60%). The experimental variogram of groundwater nitrate concentrations was best-fitted by a spherical model. Cross-validation errors are within an acceptable level. According to spatial distribution map, nitrate pollution in the groundwater occurred most in the center of the city because of nitrate excess from wastewater in industrial production.

Key Words: Geostatistics, Universal kriging, Groundwater nitrate content, Geographic Information System (GIS)

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1. INTRODUCTION

Approximately 1 million people depend on groundwater for their daily water supply in the city of Konya, Turkey as in many areas. Therefore, groundwater is the most important resources used for drinking and utility and irrigation purposes in this region. Most of drinking water sources has been contaminated by microbial or chemical contaminants potentially hazardous to human health (Sylvestre and Rodriguez, 2008) on the part of intensive agriculture, unsewered sanitation in densely populated areas, or from point sources such as irrigation of land by sewage effluents (Suthar, et al., 2009). Nitrate contamination in groundwater is a common problem in many part of the world (Suthar, et al., 2009, Almasri, 2007). Nitrate is naturally occurring ions that are part of the nitrogen cycle. The nitrate ion is the stable form of combined nitrogen for oxygenated systems. Although chemically unreactive, it can be reduced by microbial action (Nas and Berktay, 2006). In the Turkish Standards Institute (TSE), the World Health Organization (WHO) and the European Community (EC), the maximum contaminant level (MCL) of nitrate is given to be 50 mg/L. In the US Environmental Protection Agency (EPA), MCL of nitrate is given to be 44 mg/L in drinking water. TSE and EC describe the guide level (GL) of nitrate as 25 mg/L (TSE, 1997, WHO, 2007, EPA, 2002).

Geostatistics provides a set of statistical tools for analyzing spatial variability and spatial interpolation. These techniques produce not only prediction surfaces but also error or uncertainty surfaces. A semivariogram is used to describe the structure of spatial variability. The semivariogram plays a central role in the analysis of geostatistical data using the kriging method. They take into account the spatial autocorrelation in data to create mathematical models of spatial correlation structures commonly expressed by variograms. Kriging provides the best linear unbiased estimation for spatial interpolation (Gundogdu and Guney, 2007).

A major advantage of geostatistic (kriging) is that it is more flexible than other methods used interpolation and spatial averaging such as inverse distance weighing and deterministic splines, which are used in interpolation and contouring, or thissen polygons. Another advantage of geostatistic is that it provides the means to evaluate the magnitude of the estimation error. The mean square error is a useful rational measure of the reliability of the estimate. It depends only on the variogram and the location of the measurements (Kitanidis, 1996). In this study, prediction performance was evaluated by cross-validation. Stochastic methods enable us to characterise the water table dynamics in terms of risk, which may be valuable in taking strategic decisions on water management according to their expression.

Geostatistical methods may be integrated with GIS software. Hence, spatial changes can be evaluated more easily and quickly. GIS can bring together and investigate several variables for decision and support purposes. Geostatistics is a technique saving time, money and effort and spatialising the characteristics of the area by using the relations between the parameters in parallel with the advances in the computer technology. Today, geostatistics is increasingly used combined with GIS software for modeling of groundwater, soil mapping and respective commercial domains.

The purposes of this paper are (1) to analyse the spatial pattern and mapping nitrate concentration for the observation period; (2) to evaluate distribution of nitrate concentration with geostatistical methods in the Central Anatolian region, Konya at year 2008.

2. MATERIAL AND METHODS

2.1 Theory

Advantage of geostatistics is the use of quantitative measures of spatial correlation, commonly expressed by variograms (Diodato and Ceccarelli, 2005). The semivariogram is a fundamental tool in geostatistics. The empirical semivariogram (γ(h)) is defined as half the average quadratic difference between two observations of a variable separated by a distance vector h (Journel and Huijbregts, 1978). It is calculated according to the following formula:

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

Here, γ(h) means the semivariogram value at the distance, h; N(h) means the total number of the variable pairs separated this distance, and Z(x) means the value of the variable.

Before the geostatistical estimation, a variogram is calculated for classes of distance between sample pairs. The most widely used models are spherical, exponential, Gaussian and pure nugget effect (Isaaks, Srivastava, 1989). The validation and the sufficiency of the developed model variogram can be tested via a technique called cross validation. Cross validation estimation is obtained by leaving one sample out and using the remaining data. This test allows to assess the goodness of fitting of the variogram model, the appropriateness of neighbourhood and type of kriging used. The interpolation values are compared to the real values and then the least square error models are selected for regional estimation (Leuangthong, et al., 2004).

Kriging is a method for linear optimum appropriate interpolation with a minimum mean square error. One of the main advantages of Kriging, although there is no general consensus on its usefulness, is that it presents the possibility of interpolation estimation error of the regionalised variable (ReV) where there are no initial measurements. This feature offers a measure of the estimation precision and reliability of the spatial variable distribution (Theodossiou and Latinopoulos, 2006). The general equation of the kriging method is as follows:

$$Z^*(x_p) = \sum_{i=1}^{n} \lambda_i Z(x_i) \qquad (2)$$

The model parameters (range and sill variance) describe the structure of spatial variation and are used for estimation at unsampled locations using kriging. A nugget variance parameter is common for sample data of a continuous variable.

Measurement error and stochastic variation in data contribute to the nugget, the largest source of variation is commonly due to spatially dependent variation that occurs over distances much smaller than the shortest sampling interval. When the difference between samples in space is at a maximum for the average separation distances, the sill variance is reached and the model is bounded. The lag distance at which the variogram reaches its sill is the range, which indicates the limit of spatial dependence (Chappell, at al., 2003).

In this study, the groundwater nitrate concentrations were collected in April 2008 from 119 observation wells for geostatistical analysis. Calculation of experimental variograms and modeling of spatial variability of groundwater nitrate concentrations are performed using the Geostatistical Analyst integrated into ArcGIS 9.1 software.

2.2 Case Study

The field of the study includes the dwelling areas in the city of Konya, which are within the borders of Konya Metropolitan Municipality. The city of Konya is geographically situated between 36.5º-39.5º north latitudes and 31.5º-34.5º east longitude and it is the largest province of Turkey. It is located nearly in the center of Turkey (Figure 1). The population of the city is approximately 967,000 according to 2007. The average height from the average sea level is about 1,016 m.

Konya province is located in the part of the country with least rainfall, where the continental climate conditions prevail with summers that are hot and arid while winters are cold and snowy. Nitrate concentrations in groundwater are measured by Water Authority of Konya City Municipality.

3. RESULTS AND DISCUSSION

The interpolation methods that are used to generate a surface give the best results if the data is normally distributed. To determine whether or not the groundwater nitrate concentrations followed a normal distribution, two testing methods were used.

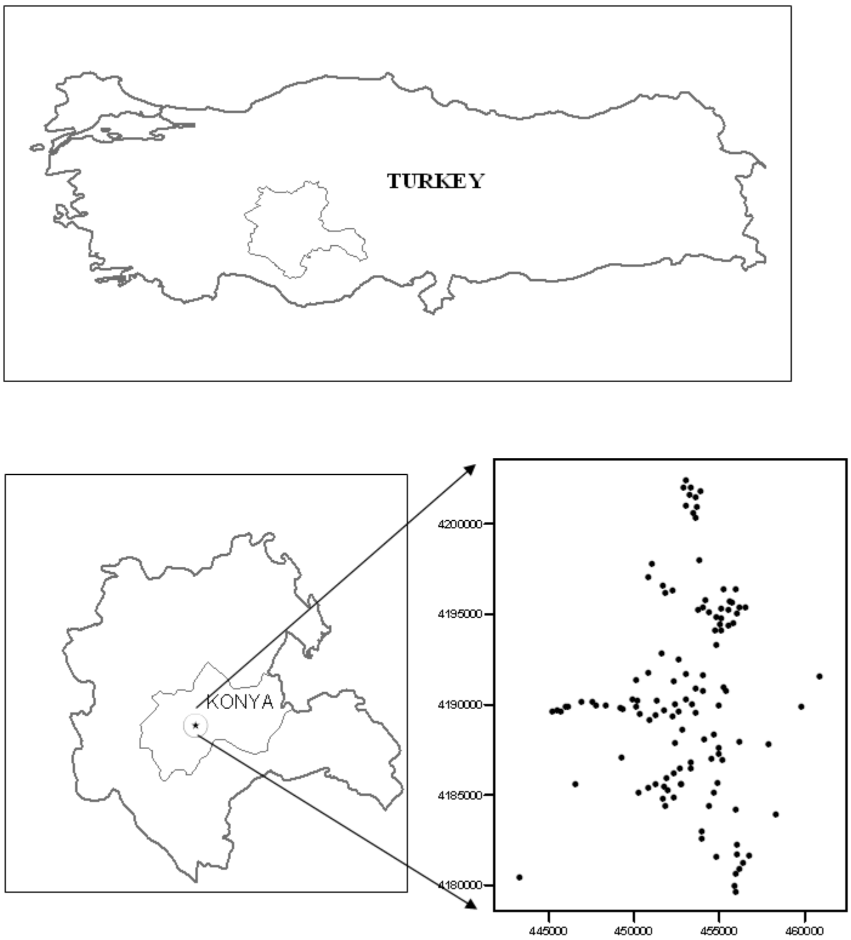

Figure 1. Location map of study area and observation wells

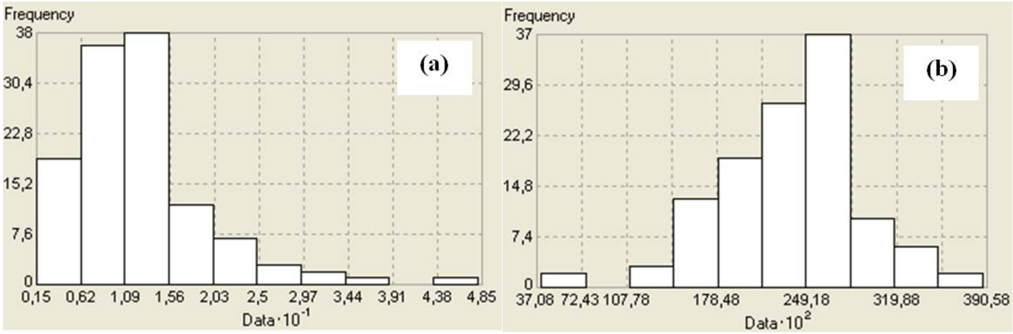

Figure 2. Histograms of groundwater nitrate content data (a) and log-transformed data (b) in Konya

First, histograms of groundwater nitrate concentrations were plotted with a normal distribution curve of both the untransformed and the logarithmically transformed data (Figure 2). This showed that the statistical distribution of the untransformed data for groundwater nitrate concentrations was positively skewed. However the logarithmically transformed data was more normally distributed. Table 2 summarizes basic statistics of the groundwater nitrate concentrations. The skewness values in the first line were obtained without making any transformation on the nitrate concentrations values. If these values are close to zero, this means it matches the normal distribution. In the table, skewness values in the first line are not close to 1. In order to adjust the nitrate concentrations values to the normal distribution, Log-transformation was made and the histogram was formed again. Skewness values for the obtained histogram were listed in the second line in Table 1. Thus, it was concluded that using log transformation, the data match the normal distribution (Gundogdu and Guney, 2007).

Second, a probability-probability (P-P) plot was used. A P-P plot of a variable shows the cumulative proportions against the cumulative proportions of the normal distribution. The probability plot is generally used to determine whether the distribution of a variable matches the normal distribution. If it does, the points cluster around a straight line (Wang, et al., 2009).

In this study, As shown in Figure 3, there was a considerable deviation from the straight line in the untransformed data plots. On the other hand, the log-transformed data were close to the straight lines. So, it can be concluded that the nitrate concentrations found in Konya City generally followed a lognormal distribution on basis of the P-P plot. After this tests, log transformation of the data was made and their semivariograms were calculated.

Table 1. Basic statistics of the raw nitrate data and the log-transformed data

Variable	Count	Min	Max	Mean	StdDev	Skewness	Kurtosis	1-st Quartile	Median	3-rd Quartile
Raw nitrate data	119	1.5	48	12.48	7.18	1.78	7.98	7.7	11.1	14.9
ln(nitrate data)	119	0.41	3.87	2.38	0.56	-0.37	3.94	2.04	2.41	2.7

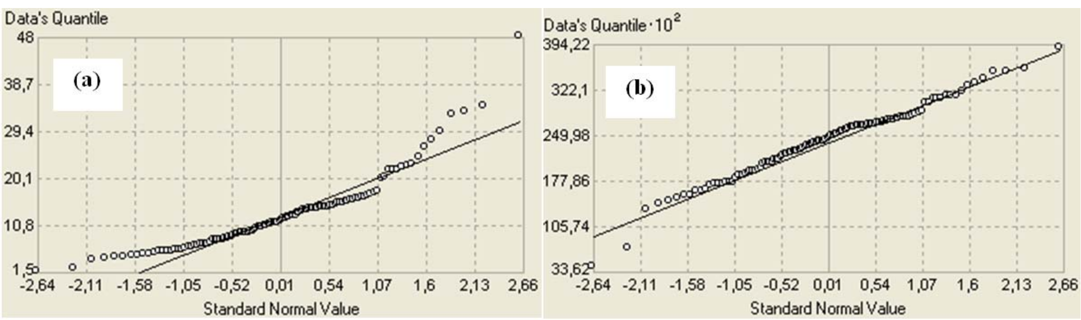

Figure 3. Probability-probability plots of groundwater nitrate concentrations (a) and log-transformed groundwater nitrate concentrations [ln(groundwater nitrate concentrations)] (b)

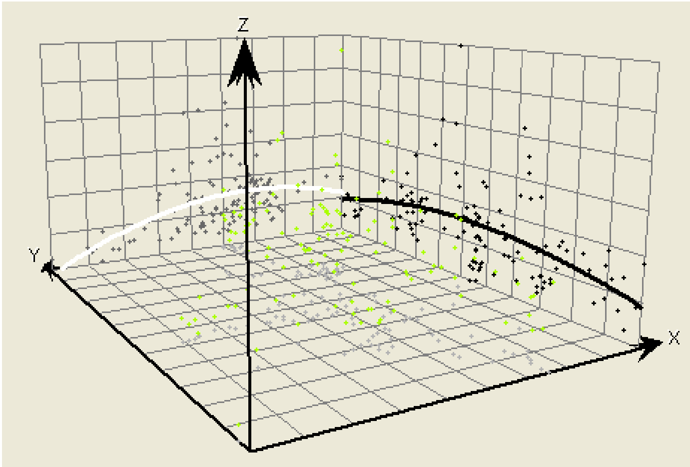

Figure 4. Identifying global trends in our data

The trend analysis can help identify global trends in the input datasets and provides a three dimensional perspective of the data. The points are projected onto the perpendicular planes an east west and a North-south plane. A best-fit line (a polynomial) is drawn through the projected points, which model trends in specific directions. If the line were flat, it would indicate that there would be no trend (Cay and Uyan, 2009). There appears to be a quadratic trend at the white and black lines. That is, we saw that the data exhibited a trend using the ArcGIS Trend Analysis tool in Figure 4. In this study, universal kriging was used. Because universal kriging only used for data if there is a trend.

The performance of five models (Circular, Spherical, Tetraspherical, Exponential, Gaussian) have been compared. According to the cross-validation parameters, generally all five models performed fairly well. As Root Mean Square Standardized prediction error (RMSS) of spherical isotropic model is close to 1, more than others. The model fitted to experimental variogram was spherical as it results from cross-validation. Nugget-sill rate can be used in the classification of the spatial dependency. If the nugget sill rate of a variable is less than 0,25 it can be said that it has a strong spatial dependency and if the rate is between 0,25 and 0,75 it can be said that the variable has moderate dependency. Otherwise, it can be concluded that the variable has a weak dependency (Ahmadi and Sedghamiz, 2007). In this study, the nugget-sill ratio showed moderate dependency with 0.60. The semivariogram model and some geostatistical parameters shown in Table 2 (confidence interval; α = 0.01). Table 3 shows prediction errors of the groundwater nitrate concentrations.

Table 2. Semivariance parameters for the logarithmically transformed groundwater nitrate concentrations

Model	Nugget	Sill	Range	Nugget / Sill	R^2
Spherical	0.12	0.20	2330 m	0.60	0.62

Table 3. Prediction errors of the groundwater nitrate concentrations.

Prediction errors	
Mean	0.01925
Root-Mean-Square	6.046
Average Standard Error	7.864
Mean Standardized	-0.06945
Root-Mean-Square Standardized	1.004

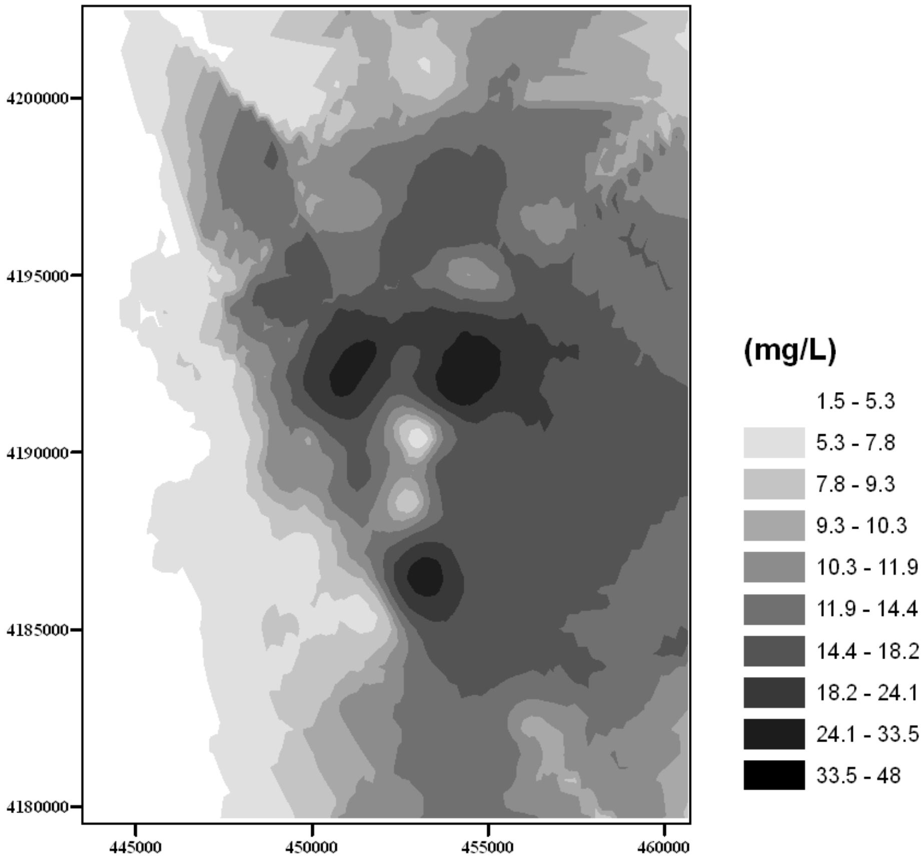

Figure 5. Spatial distribution map of groundwater nitrate concentrations

In the study field universal kriging method is used for the estimation of the groundwater nitrate concentrations. Figure 5 shows the a spatial distribution map of the values of kriged groundwater nitrate concentrations.

From the spatial distribution map of groundwater nitrate concentration, we can see that the highest groundwater nitrate concentrations occur in the center of the city. The lower values of groundwater nitrate concentrations are located at the edge of the city. In contrast with, the values in the study area are below the limit values. There is not observed a dangerous position for health. Mapping groundwater nitrate concentration provides strategically important information in the struggle to control the spread of chemical contaminants.

4. CONCLUSION

This study has attempted to predict the spatial distribution and uncertainty of groundwater nitrate concentration in the city of Konya (Turkey). Universal kriging, a type of geostatistical techniques, is applied to the groundwater nitrate concentrations data for a distribution map. Geostatistics can provide the tools to describe spatial and temporal behavior of hydrochemical parameters. Groundwater nitrate concentrations were lognormally distributed. The spherical model is found to the best model representing the spatial variability of groundwater nitrate concentrations. The average value of the variograms for the spatial analysis was approximately 2.33 km in the Spherical model.

Nitrate pollution in the groundwater occurred most in the center of the city because of nitrate excess from wastewater in industrial production. As a solution, the groundwater quality can be saved from nitrate pollution by filtering the wastewater of industrial institutions. The modeling results indicate that the kriged groundwater nitrate concentrations satisfactorily matched the observed groundwater nitrate concentrations.

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