

Water Resources and Surveying Engineering

Review of the Kriging Technique Applications to Groundwater Quality

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ABSTRACT

Kriging, a geostatistical technique, has been used for many years to evaluate groundwater quality. The best estimation data for unsampled points were determined by using this method depending on measured variables for an area. The groundwater contaminants assessment worldwide was found through many kriging methods. The present paper shows a review of the most known methods of kriging that were used in estimating and mapping the groundwater quality. Indicator kriging, simple kriging, cokriging, ordinary kriging, disjunctive kriging and lognormal kriging are the most used techniques. In addition, the concept of the disjunctive kriging method was explained in this work to be easily understood.

Keywords: Kriging, Groundwater quality, Modeling, Contaminants

مراجعة تطبيقات تقنية Kriging لجودة المياه الجوفية

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الخلاصة

تم استخدام تقنية Kriging ، وهي تقنية إحصائية جغرافية ، للحصول على أفضل بيانات تقدير للنقاط غير المستندة إلى عينات اعتمادًا على المتغيرات المقاسة لمنطقة ما. تم استخدام هذه التقنية لعدة عقود من الزمن لتقييم جودة المياه الجوفية. كما تم استخدام العديد من أنواع kriging لتقييم تركيز ملوثات المياه الجوفية في العديد من البلدان في جميع أنحاء العالم. تقدم هذه الدراسة مراجعة لأكثر طرق kriging شيوعًا : kriging العادية ، و cokriging ، و kriging البسيط ، و kriging المؤشر ، و kriging اللوغاريتمي الطبيعي و kriging المنفصل والتي تم استخدامها لتقدير ورسم خريطة توزيع ملوثات المياه الجوفية.. بالإضافة إلى ذلك ، تم توضيح منهجية طريقة kriging المنفصلة في هذه الدراسة لفهم مفاهيم هذه الطريقة. الكلمات الرئيسية: تقنية Kriging، جودة المياه الجوفية، النمذجة، الملوثات.

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1. INTRODUCTION

Worldwide, groundwater is considered as the main source of drinking water where surface water is almost not available. quality of the groundwater needs to be measured before using it for drinking purposes. For example, the concentrations of the chemical constituents in the water. Such as TH, TDS, S04, NO3, Mg, and Cl. need to be examined. For agricultural use, Sodium percentage (Na %) and Sodium Adsorption Ratio (SAR) are the two most crucial measures of groundwater quality (**Passarella, et al., 2002**).

Early research in water resources planning for widespread areas is groundwater quality mapping. Because of the difficulty of obtaining a large quantity of water quality areas, a discrete sampling program to collect water quality data was used (**Gaugush, 1993**). A Geostatistical technique was developed by using mathematical models to convert the point-data coverage into a map plain surface (**Rivoirard, 1994**). The most important spatial interpolation technique used to find the best linear unbiased estimate of a regionalized variable in a non-sampled location is the Kriging technique (**ESRI, 2001**).

Many types of kriging exist as an estimation method that gives the best unbiased linear estimates of point values or block averages such as (1) Ordinary Kriging. (2) Cokriging (3) Simple Kriging, and (4) Indicator Kriging (**Armstrong, 1998; Hohn, 1999**). However, there are many other kinds of kriging techniques such as universal kriging, probability kriging, regression kriging, and lognormal kriging.

Cooper and Istok, 1988 produced a review of a procedure for applying geostatistics to characterize the spatial distribution of groundwater contaminants. The first step of their first paper explained and discussed the additive and normal distribution (i.e., appropriate transformations and qualifications) of the data. The second step was the estimation of the spatial correlation of the distance. The third step was the structure analysis and fitting the semi-variogram model to the experimental semi-variogram. Only exponential, linear, and spherical models were established and presented as the most widely used models in addition to the nugget model. The fourth step of the (methodology – kriging) was to approximate the minimum error and map the likely values of contaminant concentrations for unmeasured points. The second paper of **Cooper and Istok, 1988** focused on applying the methodology procedure that was presented in their first paper to measure the values of six contaminants of groundwater at the Chem.-Dyne toxic waste site which is located in Hamilton, Ohio. The six contaminants were manganese, zinc, boron, barium, total volatile organic compounds (TVOC), and iron. The rational results given with the applied methodology provides mapping of contaminant distribution in groundwater.

Candela et al., 1988 used two different surveys over time as their source of data to construct a kriging map of chloride distribution in the constricted aquifer in Barcelona, Spain. In their studies, logarithmic chloride concentration histograms were used to show the delivery of the chloride, as a product of seawater intrusion, in addition to the need for data qualification. Their structural analysis presented a spherical semivariogram fitted to the experimental semivariogram. The maximum and average of the standard error were used to verify the effectiveness of the constructed network by kriging estimator. It was noticed that a very low standard error needed a large number of observations.



Gupta et al., 1995 made use of geostatistical methods to analyze groundwater quality for three aquifers located in Bangkok, Thailand. Block kriging was utilized for approximating concentrations of water contaminants and it was found that a serious decline in the quality of water occurred in different areas. In addition, they used kriging standard deviations to verify the acceptability of the existing monitoring network and it was determined that the existing network was not suitable to monitor groundwater quality mainly when the water has critical pollution.

Mrtos et al., 2001 produced maps of groundwater quality using experimental and theoretical variograms and ordinary block-kriging of the detrital aquifer of Spain. It was found that utilizing geostatistical methods was very beneficial to examine the distribution of the variable employing its approximation and successive mapping.

Passarella, et al., 2002 utilized the disjunctive kriging computational utensil to evaluate the hazard of groundwater quality with a spatial distribution of conditional expectations. The variables that were made use of in their methodology were nitrate concentrations which were applied to the aquifer of the Modena plain in the country of Italy. **Passarella, et al., 2002** utilized Maximum Allowable Concentration (MAC) and Guide Value (GV) as the main two verges of disjunctive kriging maps for fit to drink usage of water. The maps which were drawn by disjunctive kriging were found beneficial by giving a good signal of the distribution of the nitrate concentration in groundwater.

Gaus et al., 2003 made use of disjunctive kriging to roughly calculate the concentrations of arsenic in the close to surface (shallow) groundwater in Bangladesh. **Gaus et al.** took advantage of Hermite polynomials to change the data as an alternative to using lognormal kriging for the reason that they believed that the distribution of the data was still distant from ordinary. They determined that the disjunctive kriging procedure provided a direct regional pattern of the arsenic concentrations in groundwater all over most of Bangladesh.

Trinh et al., 2005 utilized regression block kriging (RBK) and ordinary block kriging (OBK) to evaluate N concentrations (NO₃-N) in the Red River Delta, located in North Vietnam. The semivariograms for the statistics of (NO₃-N) accumulation for original explanations and remainders were determined. Additionally, they tailored the variogram representations to the semivariograms, and interpolations for the N concentration were completed. From the results it was discovered that the contrast for regression block kriging was much lower compared to the contrast for ordinary block kriging; accordingly, regression block kriging was more precise than ordinary block kriging in foreseeing N concentrations in shallow (close to the surface) groundwater.

Hossain et al., 1999 inspected the efficiency of the ordinary kriging method for arsenic polluted groundwater supervision in Bangladesh. That is to say: “we measured the precision of the kriging technique in sensing harmless and harmful wells at non-tested sites,” they said. The studies mainly fixated on shallow (close to the surface) wells by overlooking wells deeper than 75m which is the maximum determined depth of the safe to drink water wells in the country of Bangladesh and the statistics of the concentrations of arsenic were acquired from earlier surveys. Furthermore, log-transformation was used to alter statistics for an appropriate univariate dispensation; therefore, for kriging application. It was determined that the kriging technique was cross authenticated only over the wells in which their arsenic concentrations were harmless (unused in the variogram



examination). Recently, modeling is more and more utilized in research to facilitate tasks and save time (Shukur, 2017; Azawi and Sachit, 2018).

Jang et al., 2008 made use of multiple variable indicator kriging to find clean and safe groundwater for irrigation in the Chouhui River alluvial fan in Taiwan. They discovered that the best locations to pump clean and safe groundwater for irrigation were clearly distinguished by using indicator kriging.

Barca and Passarella, 2008 compared the disjunctive kriging and application of using stochastic conditional simulation (Turning Bands Simulation) to the assessment of the spatial risk values of groundwater quality in Modena Plain, Italy. They concluded that disjunctive kriging was more effective than simulation. They justified their conclusion by stating that the characteristics of disjunctive kriging maps were smoother and had shown a more regular spatial behavior with respect to the real phenomenon they described.

Assaff and Saadeh, 2009 made use of geostatistical analysis to assess the groundwater conditions in Upper Litany Basin (ULB) in Lebanon. Spatial distribution of nitrate contamination was interpolated through using the ordinary kriging technique. In their structural analysis, they calculated experimental semivariograms and they fitted an alternative semivariogram (theoretical) model. In addition, Assaff and Saadeh, 2009 determined the Root and Mean Square Standardized Prediction Error (RMSSPE) and the Mean Standardized Prediction Error (MSPE) to find the unbiasedness and the estimation of uncertainty, respectively. Both the RMSPPE and MSPE results were acceptable according to the limits which were set by Cooper and Istok, 1988. In addition, geostatistical results were compared to those from DRASTIC results and they concluded that the limitations in the DRASTIC had shown the distribution of nitrite levels compared to the other method.

Clean water is the most important factor that effects the public health. 80% of human diseases is caused by polluted water based on World Health Organization (WHO) (Mohammed and Abdulrazzaq, 2021).

In conclusion from the work above, groundwater quality was assessed by using different types of kriging technique. The aim of this paper was to present the most common kriging techniques used to estimate and map the distribution of groundwater quality. These techniques are: (1) ordinary kriging (2) cokriging (3) simple kriging (4) lognormal kriging (5) indicator kriging and (6) disjunctive kriging Methodology of the disjunctive kriging technique which is relatively modern to soil and hydrologic sciences is also presented in this paper.

2. METHODOLOGY OF THE DISJUNCTIVE KRIGING TECHNIQUE

The disjunctive kriging, is a nonlinear estimation process and it contains many benefits compared to the linear estimation method. First, an estimate of the conditional probability can be easily obtained. Second, the estimation of interest can usually be achieved more accurately (Alley, 1993). This process consists of four main components: (1) coefficients estimation, (2) raw data (3) local averages and frequency distributions calculation and (4) a semi variograms of normalized data.



3. TRANSFORMATION

The initial data of the groundwater contaminants which are needed for the geostatistical analysis are not always normally distributed or typical. Many problems face data sampling. Some of these problems include clustered wells in some areas, poor well control in others, and poor spatial correlation caused by measurement error or poor sampling, and skewed data distribution with possible outliers (Hohn, 1999). For example, Fig. 1, shows the distribution of the available wells and the groundwater monitoring network in the study location of Bangkok City, Thailand by Gupta, et al., 1995. New locations were identified to avoid cluster of wells and inappropriate locations of monitoring wells were removed.

The following form is commonly used as kriging estimator

$$z^*(x_0) = \sum_{i=0}^n f_i[z(x_i)] \tag{1}$$

f_i is a function that needs to be calculated. In the disjunctive kriging (DK), Hermite polynomials are used to convert the data instead of using lognormal kriging. Hermite polynomials transfers the original variable $z(x_i)$ in a space, S_1 , into a univariate random variable, $y(x_i)$ in space, S_2 (Hohn, 1999). The transform relationship between $z(x_i)$ and $y(x_i)$ can be represented by the following formula using Hermite polynomials with coefficients C_k (Passarella, et al., 2002).

$$\phi[y(x_i)] = \sum_{k=0}^{\infty} C_k H_k[y(x_i)] \tag{2}$$

Where $H_k[y(x_i)]$ is calculated from the following relationships (Hohn,1999).

$$H_0[y(x_i)] = 1$$

$$H_1[y(x_i)] = -y(x_i)$$

$$H_{k+1}[y(x_i)] = y(x_i)H_k[y(x_i)] - kH_{k-1}[y(x_i)]$$

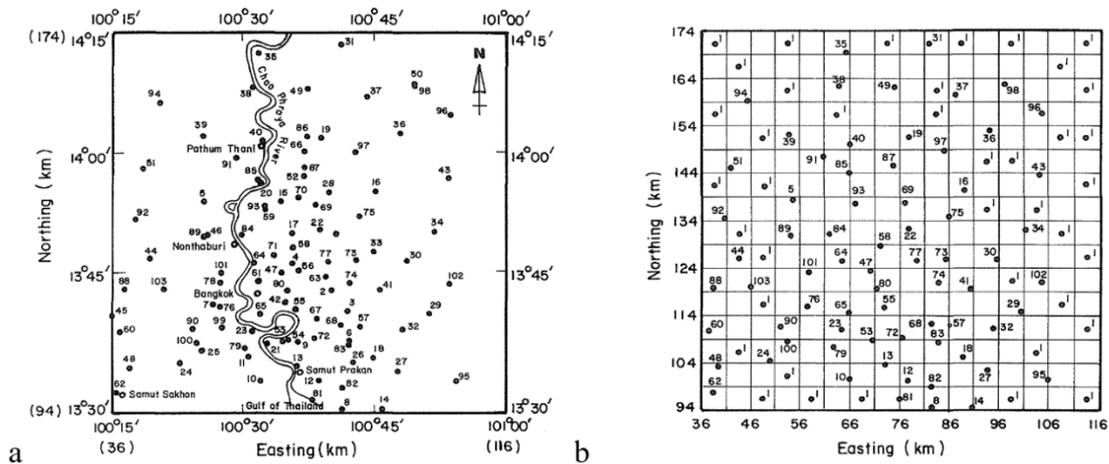


Figure. 1 a & b wells that have been monitored in the study area-city of Bangkok, Gupta et al., 1995.



Fig. 2, shows the differences of the distribution of arsenic concentration in the shallow groundwater in Bangladesh among three histograms by using no transformation, Hermite polynomial transformation and lognormal transformation (**Gaus et al., 1995**) The comparison reveals that much of skewness was removed by the transformation. **Gaus et al. 1995** said “the large proportion of values close to the detection limit makes it impossible to achieve a smoothly increasing curve in the lower part of the scale. The steps in the lower part of the transformed scale are clear in **Fig. 3** The upper range of the transformed scale, however, follows a normal curve well.”

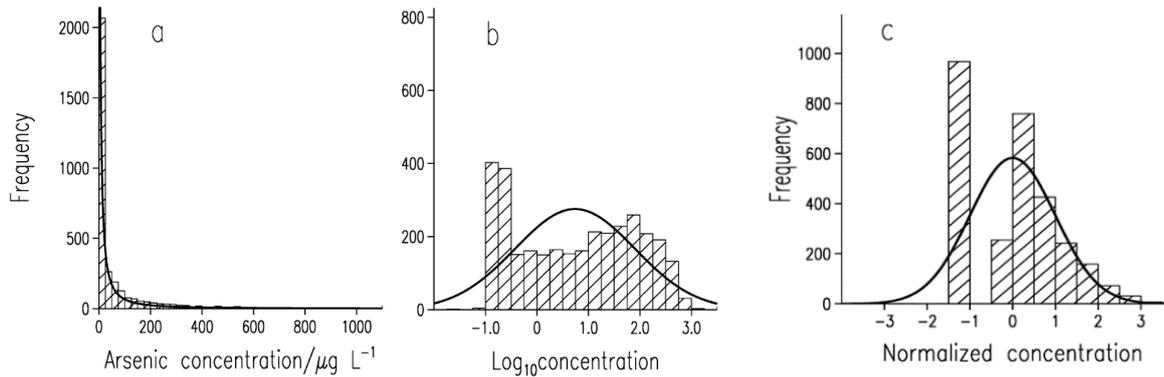


Figure. 2 The concentration of arsenic -Bangladesh (a) no transformation (b) lognormal transformation (c) Hermite polynomial transformation, **Gaus et al., 2003**.

4. DATA TRANSFORMED BY SEMI-VARIOGRAM

The experimental semi-variograms are calculated and drawn with the separation distances (h) after transforming the data according to the equation in section 2, Then theoretical variogram models are applied to the semi- variogram to get the best fitted model. The theoretical models include spherical, linear, Gaussian and exponential model. Covariance with sill of 1 is used in the disjunctive kriging (**Hohn, 1999**). Therefore, the covariance has the following formula:

$$C(h) = C - \gamma(h) = 1 - \gamma(h) \tag{3}$$

Where $\gamma(h)$ = a Spherical, Linear, Gaussian or Exponential model which one is better fitted to the Semi- variogram. Experimental and theoretical variograms have the following formulas:

Experimental Semi- variogram,
$$\gamma^*(h) = \frac{1}{2n} \sum_{i=1}^n [z(x_i) - z(x_i + h)]^2 \tag{4}$$

Spherical Model,
$$\gamma(h) = C \left[\left(\frac{3h}{2a} \right) - \left(\frac{h^3}{2a^3} \right) \right] \text{ for } h \leq a \tag{5}$$

$$\gamma(h) = C \text{ for } h > a$$

Exponential Model,
$$\gamma(h) = C_o + C \left[1 - \exp \left(\frac{-h}{a} \right) \right] \tag{6}$$

Gaussian Model,
$$\gamma(h) = C_o + C \left[1 - \exp \left(\frac{-h^2}{a^2} \right) \right] \tag{7}$$



Where,

- h = the separation distance between wells.
- n = number of pairs at each distance.
- $z(x_i)$ = the transformed variable at well x_i .
- $z(x_i + h)$ = the transformed variable at well x_{i+h} .
- C = a constant called the sill.
- a = the range of the separation distance between wells.
- C_0 = the y intercept with a straight line.

The fitted model as shown in **Fig. 4** is the exponential model to the transformed arsenic concentrations in the shallow groundwater in Bangladesh (**Gaus et al., 2003**).

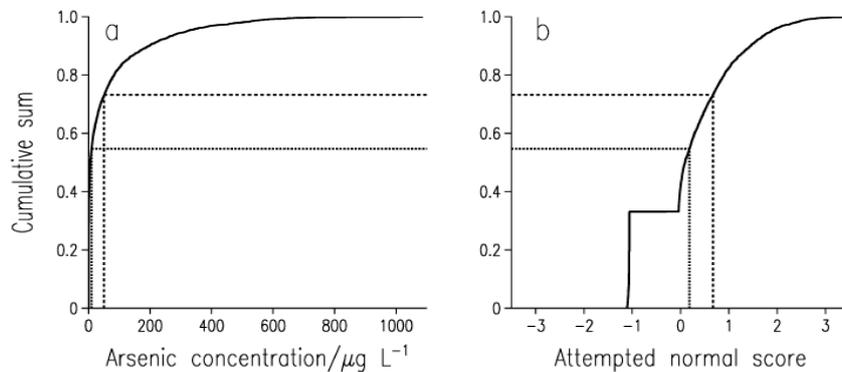


Figure 3 (a) The cumulative arsenic concentration of (b) the transformed concentration with Bangladesh standard marked by dashed lines (**Gaus, et al., 2003**).

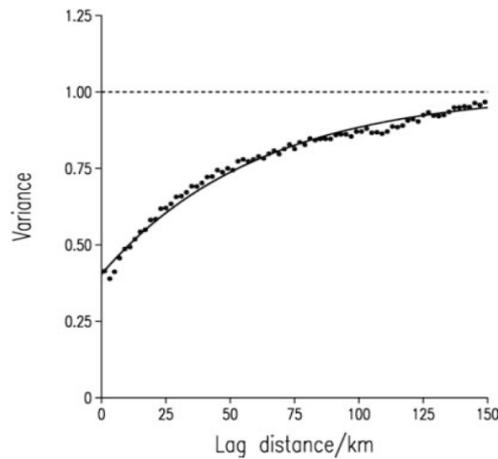


Figure 4 Variogram of transformed arsenic concentration- shallow groundwater - Bangladesh (**Gaus, et al., 2003**).



5. THE ESTIMATION

Similar to other types kriging technique, Disjunctive Kriging is used to achieve the minimum of standard deviation of the normalized variables. By using unknown functions to convert the original data into univariate and bivariate random variables this objective can be accomplished. Coefficients such as C_k , K and n for each value of K are required to be calculated as a second step of disjunctive kriging (Hohn, 1999).

Because $H_0[y(x_i)] = 1$ for ($k = 0$) and $H_1[y(x_i)] = -y(x_i)$ for ($k = 1$), k starts with 2 and for each value of K , n values of linear equations to calculate kriging weights, λ_{ik} , should be solved by using the formula below (Hohn, 1999):

$$\sum_{i=1}^n \lambda_{ik} (\rho_{ij})^k = (\rho_{0j})^k, \quad j = 1, \dots, n \tag{8}$$

For $H_0[y(x_i)] = 1$, the summation of kriging weights, λ_{ik} equal 1 which it means an unbiasedness condition (Hohn, 1999).

Disjunctive kriging is different from the other kriging techniques by providing a conditional probability $P(x_0)$ that is a crucial output to determine whether the correct value of a sample location exceeds a given threshold z_c or not by using the expression below (Passarella, et al.,2002; Hohn, 1999):

$$P(x_0) = 1 - G(y_c) - g(y_c) \sum_{k=1}^K H_{k-1}[y_c H_k[y(x_0)]]/k! \tag{9}$$

Where “ $G(y_c)$ is the Gaussian cumulative distribution function” (Hohn, 1999).

Disjunctive kriging process is different from ordinary kriging because it uses Hermite polynomial to transfer sample data to normalized variables in a selected location. Ordinary kriging which is a linear system that uses a lognormal to obtain normal distribution of the data in a chosen area (Hohn, 1999).

6. RESULTS AND DISCUSSIONS

In summary, the work above shows that most of the kriging techniques have been used in the studies of groundwater quality. The distribution of the groundwater contaminants was shown by using the Lognormal kriging and Block kriging in the aquifer in Spain. The distribution of the nitrate concentrations in the groundwater in Italy was assessed by using and comparing disjunctive kriging with other geostatistical methods. More clear maps for the contaminant’s distribution were given by using the disjunctive kriging method than the stochastic method. In addition, the concentration of the nitrogen in Vietnam was estimated by using the regression block kriging and the ordinary block kriging. The ordinary kriging was less accurate than the regression kriging. On the other hand, in Iran the Cokriging was presented in two studies of the contamination of groundwater. Also, the disjunctive kriging methodology was described in this review. The disjunctive kriging procedure includes four steps that are easily understood and followed. This methodology shows that the disjunctive kriging consists of a crucial step that converts the original data by using coefficients such as K and C_k . Besides, an important output which is the conditional probability is given by the disjunctive kriging.

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