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Optimal Interpolation of the Multivariate Spatial Estimation for Groundwater Balance Data with Boundary Conditions

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Abstract:

This research dealt with estimation of water balance between groundwater levels by spatial interpolation of multivariate using the cokriging technique in unknown locations and at border points. One of the objectives of this research is to arrive at a method for estimating the probability curves for the specific boundary effects of groundwater aquifers, as well as to obtain a smooth approach and method for spatial covariance models, as well as to obtain the spatial relationship between probability, slope, and universal cokriging method to estimate the directional derivatives of a regional spatial variable from scattered measurements of the variable and gradient measurements for groundwater levels. The data used in this research are real data for groundwater levels in the city of Mosul. Unbiased estimation and least variance estimation were used to obtain the estimated values of the spatial observations and obtained good results that support the advantages of the cokriging method. Accuracy becomes clear to us through the smallest errors by applying the basic error criteria in forecasting. The resulting estimate describes spatial associations and illustrates multivariate covariance model analysis. The conclusion gives us the benefit of using the Mathron variation model with the ability to adjust the parameter for second-order fields to determine the groundwater balance, while the gradient is considered an approach to the specific difference between the groundwater levels studied. This paper discusses the use of the universal cokriging, which is a widely used multivariate linear estimator for geostatistics. In the context of spatial random processes, the paper covers the possibility of increasing the spatial resolution of the spatial variable (downscaling), estimating direction derivatives, and spatial interpolation with respect to boundary conditions. All spatial estimators are unbiased and reduce the variance of the estimation error. Multivariate is an effective method for improving the contour maps between the hydraulic head and the rest of the other data under study.

Keywords: Hydrogeology, cokriging, hydraulic head, boundary conditions.

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1. Introduction

The multivariate geostatistical interpolation method is used to create maps of the primary variable using the experimental data of that variable and the experimental data of the auxiliary variables associated with the original data. The spatial random variable is the basic material in geostatistics, as spatial statistics allow us to know the mathematical form of the virogram function that gives a quantitative description of the spatial variation found by Matheron. (KLEIBER and GENTON, 2013). As well as predicting the characteristics of groundwater levels and soil data by kriging, and designing optimal sampling plans (de Fouquet, et al. 2023). Therefore, a good model and appropriate techniques for estimating the virogram parameters are essential, because the method of moments in estimating the regional spatial variable can be misleading and inaccurate, and the commonly used virogram models (spherical, exponential, and Gaussian) lack flexibility (Somayasa, et al. 2021). Common models assume a specific form of the local spatial process; in other words, the virogram has a predetermined behavior near its source. Moreover, due to the many uncertainties inherent in spatial data that make it difficult to estimate all the parameters of the nested model accurately. Since most models assume the same local behavior (Genton and Kleiber, 2015, Chen, and Genton, 2019).

Spatial analyses in earth sciences and GIS (Anderson, et al. 2015), machine learning (De Iaco et al. 2022), medical geology (Zhang et al. 2021), and the Matheron variance process are important and fundamental techniques for estimating geostatistical spatial phenomena. There is little benefit in using nested Kriging models. Instead, in 1999, Stein promoted the use of a class of Matérn models named after the Swedish forest statistician, Bertil Matern.

The Matérn model has great flexibility in modeling spatial variability and can model many regional spatial processes. Thus, it can be used as a general model for soil variability, pollution data, rainfall data, and hydrological data of aquifers. The generalized Matérn model was used for real data, in order to evaluate the value of the Matérn model to describe the spatial variability of groundwater levels in general and then estimate the parameters of the boundary data (Alonso Malaver, et. al, 2015).. We will describe the Matérn model, explain how it fits the spatial data, and illustrate how to apply it. To illustrate the behavior of the Matérn model, we studied random fields along the transects with different smoothing parameters. In addition, we considered the features of the variance functions and the effect of the mass variance. (Freixas, et al. 2017; Wang et al. 2021)

In this paper, we used the comprehensive cokriging method to estimate the directional derivatives of a regional spatial variable from sparse measurements of the variable and the gradient measurements (Nerini D, et al. 2010). In order to estimate the hydrogeological gradient from the head boundary data in groundwater levels (Illman, W. A. 2014), Freixas et al. 2017), an inferred variance or variance ratio from the measurements of the regional variable is required (Xue et al. 2022). The idea of estimating the gradient using natural undulation was extended to global undulation by Pardo-Eguzqueza and Checa-Olmo, 2004) in order to know and interpret the trend in several regional variables, for example, the study of aquifer heads, rainfall with orographic influence, and the trend in geophysical variables related to the geometry of the place. (KLEIBER, W. and PORCU, E., 2015).

2.Kriging with a trend

Kriging with external drift or called universal kriging assume that the mean is not constant, and if the drift (trend) denote as $m(u)$ then the estimator of universal kriging defined as:

$$\hat{z}(u_o) = m(u) + \sum_{l=0}^{L} \gamma_l \, f_l(u) \tag{1}$$

Where $m(u)$ is the mean, L is order of polynomial approximation, and $f_l(u)$ the bases functions, if $L = 0$ then the universal kriging get to ordinary kriging (unknown mean), if $L = 2$ is linear trend. For linear drift $f_0(u) = 1,\ f_1(u) = x,\ f_2(u) = y$ and for quadratic drift also include second -order terms $f_3(u) = x^2,\ f_4(u) = xy, f_5(u) = y^2$

2.1 Unbiasedness

Unbiased estimator defined that expectation of the estimate equal the expectation of the true unknown value:

$E[\hat{z}(u_o)] = E[z(u_o)]$ and $E[\hat{z}(u_o) - z(u_o)] = 0$

The unbiasedness condition is expressed with respect to the trend as well as the mean

$$\sum_{i=1}^{N} w_i \, f_l(u) = f_l(u), for\ all\ l$$

The expected value at each point of all the function must be that predicted by that function.

2.2 Kriging prediction variance

The variance of the estimation is written $var[\hat{z}(u_o) - z(u_o)]$ or $var[\hat{z} - z_o]$and for any weighted average, with weights w_i then $var[\sum_{i=1}^{N} w_i \, z_i - z_o]$

To minimizing this expression, define two vectors of length (n+1)

$v = \begin{pmatrix} \lambda \\ -1 \end{pmatrix}$, $z = \begin{pmatrix} Z \\ z_o \end{pmatrix}$

Then $var[\sum_{i=1}^{N} w_i \, z_i - z_o] = v^T var(z) v = v^T \begin{pmatrix} C & c_o \\ {c_o}^T & c_{oo} \end{pmatrix} v$

$$var\left[\sum_{i=1}^{N} w_i \, z_i - z_o\right] = \lambda^T C \, \lambda - -2\lambda^T \, c_o + c_{oo} \tag{2}$$

Where C is covariance between sample points, c_o covariance of each sample point, and c_{oo} variance at a point (nugget).

2.3 Minimization approach to universal kriging

The objective function to be minimized is the variance; in addition to the unbiasedness constraint on the mean, and on the value of base functions:

$$\sum_{i=1}^{N} w_i \, \gamma(u_i, u_j) + \varphi_o + \sum_{k=1}^{K} \varphi_k \, f_k(u_i) = \gamma(u_o, u_i) \quad , \qquad \forall i \tag{3}$$

$$\sum_{i=1}^{N} w_i = 1 \tag{4}$$

$$\sum_{k=1}^{N} w_i\ f_k\,(u_i) = \ f_k\,(u_o) \quad , \qquad \forall k \tag{5}$$

In a minimization problem, must define an objective function to be minimized, its kriging variance with weights:

$$f(w) = 2\sum_{i=1}^{N} w_i\ \gamma(u_i\,, u_o) - \sum_{i=1}^{N}\sum_{j=1}^{N} w_i\,\alpha_i\ \gamma\big(u_i\,, u_j\big) \tag{6}$$

When all weights setting to zero, add constraint to bound of object function, also need the condition $\sum_{i=1}^{N} w_i\ = 1$ with a Lagrange multiple ϕ:

$$f(w, \phi) = 2\sum_{i=1}^{N} w_i\ \gamma(u_i\,, u_o) - \sum_{i=1}^{N}\sum_{j=1}^{N} w_i\,\alpha_i\ \gamma\big(u_i\,, u_j\big) - 2\ \phi\ [\sum_{i=1}^{N} w_i\ - 1\,] \tag{7}$$

where the condition $[\,\sum_{i=1}^{N} w_i\ - 1] = 0$, then the prediction is unbiased. Minimize by put all N+1, partial derivatives to zero:

$\frac{\partial(w_i\ ,\phi)}{\partial w_i} = 0\ ,\ \ \frac{\partial(w_i\ ,\phi)}{\partial \phi}\ = 0 \quad , \quad \forall i$ (Farag et al. 2020).

2.4 Covariance Models

The function 2γ(h) is calculated for a set of observations in more than one direction (horizontal or vertical). It shows us different values for each direction. If γ(h) does not depend on the direction, then $\gamma(h) = \gamma(|h|)$ is isotropic and is characterized by the uniform quasi-variogram function.

A relationship between covariance, variance, and the semivariogram function:

$\gamma(h) = \sigma(0) - \sigma(h)$ because

$$2\gamma(h) = E[z(u+h) - z(u)]^2 \quad = E[(z(u+h) - \mu) - (z(u) - \mu)]^2$$

$$= E[(z(u+h) - \mu)^2 + (z(u) - \mu)^2 - 2(z(u+h) - \mu)(z(u) - \mu)]$$

$$= E(z(u+h) - \mu)^2 + E(z(u) - \mu)^2 - 2E(z(u+h) - \mu)(z(u) - \mu)$$

And $E(z(u+h) = E(z(u))$

$2\gamma(h) = \sigma^2 + \sigma^2 - 2cov(z(u+h), z(u))$

$2\gamma(h) = 2\sigma^2 - 2c(h)$ then

$$c(h) = c(0) - \gamma(h) \tag{8}$$

(Jovan, et, al. 2019)

3. True derivative approach

The estimation procedure begins with a linear combination of direct measurements of parameters and head data to find out the boundary condition of groundwater levels using a multivariate cokriging system using real spatial data for the equilibrium state of groundwater heights, as well as using covariance functions with their derivatives for analysis of variance to find out the linear estimate of cokriging technique.

$$\hat{z}(u_o) = \sum_{i=1}^{N} w_i \, z(u_i) + \sum_{j=1}^{M} \alpha_j [\, \hat{v}\left(u_j\right) \bullet \nabla \, z\left(u_j\right) \tag{9}$$

Where $\hat{z}(u_o)$ is estimator of location (u_o), i, j dummy variables, N, M number of head and notes of boundaries respectively , $z(\bullet)$is potential at locations (u_i, u_j) , w_i, α_j cokriging weights, and $\hat{v}\ \left(u_j\right)$ vector of unit level.

3.1 Generalized Cauchy covariance function

Cauchy's integral formula is named after the scientist Augustin Louis Cauchy, and this formula is used in complex analysis. The solid function defined on the disk is completely determined by its values on the disk boundaries. Cauchy's formula appears in complex analysis: Complex integration gives good results under disc limits, a result that does not give the same results in real or mathematical analysis.

The generalized Cauchy model is also used in analyzing magnetic gravity and uses geophysical data. The Cauchy model is written as follows:

$$\sigma(h) = \sigma^2 \left(1 + \frac{h^2}{a^2}\right)^{-p} \tag{10}$$

Where p is exponent, a is the range, and h^2 square lag, if $p = \frac{1}{2}$ is gravity field, and $p = \frac{3}{2}$ is magnetic fields using statistical models, while the case $p = 1$ corresponds to the standard Cauchy model. (Neuman, S. P. 2020).

The first directional derivative of equation (10) by direction $\hat{v}$ is:

$$\sigma\hat{v}(h) = \frac{2p\sigma^2 \, h.\hat{v}}{a^2}\left(1 + \frac{h^2}{a^2}\right)^{-p-1} \tag{11}$$

and the second directional derivative by $\hat{l}$ is:

$$\sigma\hat{l}\hat{v}(h) = \frac{2p\sigma^2 \, h.\hat{v}}{a^2}\left(\frac{2(p+1)h.\hat{l}\, h.\hat{v}}{a^2}\left(1 + \frac{h^2}{a^2}\right)^{-p-2} - \left(1 + \frac{h^2}{a^2}\right)^{-p-1} \right) \tag{12}$$

3.2 The MATÉRN Models

Model of Matérn is a true model of geoststistics, and the benefit of uses this model, it is the ability to modify the parameter in an easy and smooth way for second-order fields, as an example of increasing or decreasing at v. To clarify the knowledge of approximate homogeneity, the Matérn model is drawn with the following formula. The Matérn model denoted as: $\mathcal{M}_{v,a}$

$$\mathcal{M}_{v,\ \beta}(h) = \frac{\sigma^2 \, 2^{1-v}}{\Gamma(v)} \ (\frac{h}{\beta})^{v} \, \mathcal{K}_v \left(\frac{h}{\beta}\right) \quad , \qquad v, h > 0 \tag{13}$$

Where $\beta > 0,$ the scale parameter, $v > 0,$ the smooth parameters, σ^2: is Matérn covariance function and if $\sigma^2 > 0$ the variance of gaussian random field.

and $\mathcal{K}_v$ is Bessel function of second kind of order $v = 2\ or\ 9\ or\ 6,$ if $\mathcal{M}_{v,\beta}(0) = 1$, then equation (13) is a correlation function.

If $v = p + \frac{1}{2},\ p\,\epsilon N^+$

if $v = \frac{1}{2}$ (p=0), then $\mathcal{M}_{\frac{1}{2}}(h) = \sigma^2 exp\left(-\frac{h}{\beta}\right)$ gives the absolute exponential function.

if $v = \frac{3}{2}$ (p=1), then $\mathcal{M}_{\frac{3}{2}}(h) = \sigma^2(1 + \frac{\sqrt{3}h}{\beta})\ \exp\left(-\frac{\sqrt{3}h}{\beta}\right)$

if $v = \frac{5}{2}$ (p=2), then $\mathcal{M}_{\frac{5}{2}}(h) = \sigma^2(1 + \frac{\sqrt{5}h}{\beta} + \frac{\sqrt{5}h^2}{3\beta})\ \exp\left(-\frac{\sqrt{5}h}{\beta}\right)$

the Gaussian case gives as $v \to \infty$, then the Matérn converges to the square exponential covariance function $\lim\limits_{v\to\infty} \mathcal{M}\,(h) = \sigma^2 exp\left(-\frac{h^2}{\beta^2}\right)$

and the first and the second derivatives of equation (13) are:

$$\frac{\partial \mathcal{M}_{\frac{1}{2}}(h)}{\partial\beta} = \frac{h\sigma^2}{\beta^2} exp\left(-\frac{h}{\beta}\right) \tag{14}$$

$$\frac{\partial^2 \mathcal{M}_{\frac{1}{2}}(h)}{\partial\beta^2} = \frac{-2h\sigma^2}{\beta^3} exp\left(-\frac{h}{\beta}\right) + \frac{h^2}{\beta^4}\ exp\left(-\frac{h}{\beta}\right) = (\frac{h^2}{\beta^4} - \frac{-2h\sigma^2}{\beta^3}) exp\left(-\frac{h}{\beta}\right)$$

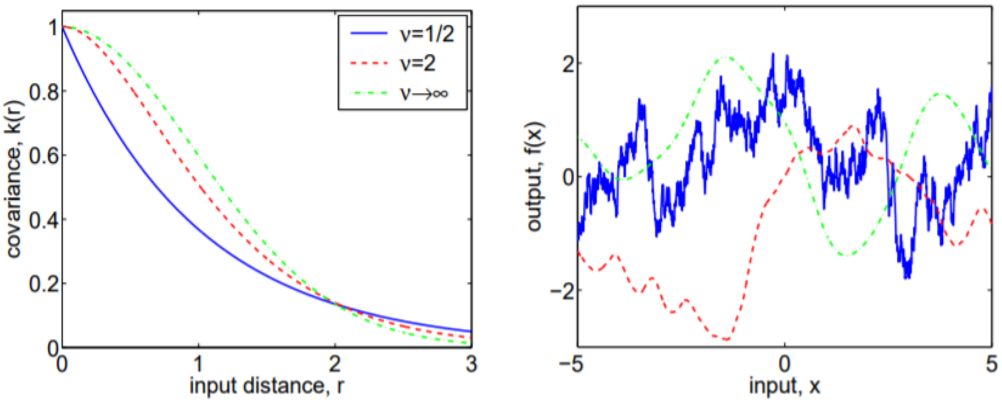
$$\frac{\partial \mathcal{M}_{\frac{3}{2}}(h)}{\partial\beta} = \frac{3\sigma^2 h^2}{\beta^3}\ \exp\left(-\frac{\sqrt{3}h}{\beta}\right) \tag{15}$$

$$\frac{\partial^2 \mathcal{M}_{\frac{3}{2}}(h)}{\partial\beta^2} = \frac{3h^2\sigma^2 \exp\left(-\frac{\sqrt{3}h}{\beta}\right) .(\sqrt{3}h - 3\beta)}{\beta^5}$$

$$\frac{\partial \mathcal{M}_{\frac{5}{2}}(h)}{\partial\beta} = \frac{5h^2\sigma^2 \exp\left(-\frac{\sqrt{5}h}{\beta}\right) .(\frac{\sqrt{5}h}{\beta} + 1)}{3\beta^3} \tag{16}$$

(Panneconcke, L, 2020)

The most common models of variation functions are the Matern model and the generalized Cauchy model, which gives more points in the mathematical formulas. The Matern variation function is a generalization of the Gauss function, and because it has an absolute exponential kernel, it gives us different results, and it is better able to capture physical processes because of its limited variation of parametric derivatives and its convergent behavior in terms of terms.



(a) (b)

Figure (1): (a) Matérn variance function, (b) output of function

In Figure (1): The property of the results is related according to the Matérn variance function ν=1/2, ν=1/2. When this result is passed through a gradually decreasing curve, the new result is the Matérn variance function ν=3/2ν=3/2. In general, a series of nn low-pass filters on a white Gaussian noise has the effect of correlating it according to the Matérn function ν=(2n−1)/2ν=(2n−1)/2. In physics systems, we often find the effects of the Matérn variance function according to exponential decay due to one or more independent physical mechanisms, which lead to Matérn variance functions. (Ramon, et al. 2020).

In mathematics, Cauchy's integral formula (named after Augustin Louis Cauchy) is a central formula in complex analysis. It expresses the fact that "a solid function defined on a disk is completely determined by its values on the disk's boundary" and gives integral formulas for all derivatives of the solid function. Cauchy's formula shows that in complex analysis "differentiation is equivalent to integration", a result that does not hold in real mathematical analysis.

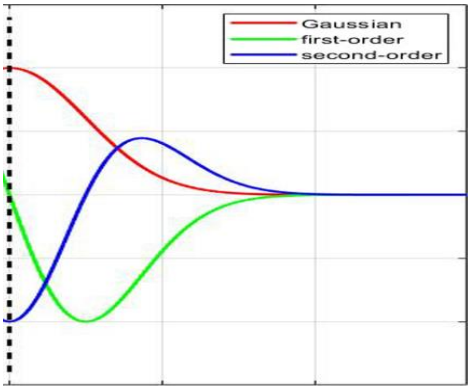
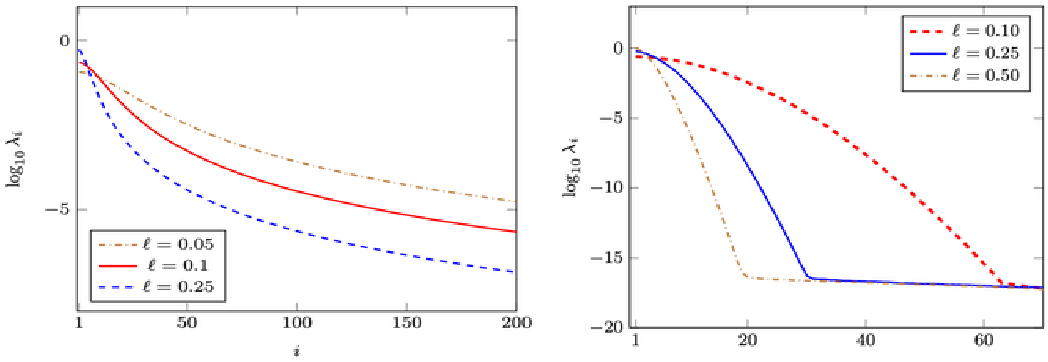


Figure (2): The first-order and second-order derivatives of Gaussian

Figure (2) shows the first- and second-order derivatives of the Gaussian function after normalization. The first-order derivative of the Gaussian function is the product of an odd symmetry that can generate the gradient and the second-order derivative of the Gaussian function is the product of an even symmetry.



(a) (b)

Figure (3): Matérn function

Figure (3): (a); shows log10 (λ_i) where λ_i are eigenvalues of integral operator of Matérn v=3/2 of Gaussian, and (b) log10 (λ_i) where λ_i are eigenvalues of integral operator of exponential. (Porcu, et al. 2022)

3.3 Finite difference approach in cokriging

The gradient is approximated using a central finite difference instead of the true derivative. Two points are placed on either side of the boundary, in the approximation of the boundary vectors. Instead of treating the gradient information as a secondary variable. (Farag,H. A. et. al, 2020).

3.4 procedures of cross validation

In order to determine the validity of the prediction and the accuracy of the values to be predicted, error measures and standards were used, including the first measure, which is a measure of the total square equation and is symbolized by (MSE) based on Equation (17), and using the root mean square error is referred to as (RMSE) according to Equation (18), which gives an indication of the dispersion or variance of the prediction accuracy, while the Kriging values for the reduced mean square error are referred to as (KRMSE) with reference to Equation (19), which shows the prediction accuracy at the point, and these measures were calculated as follows:

$$MSE = \frac{1}{N}\sum_{i=1}^{N}[\,\hat{z}(u_i) - z(u_i)]^2 \tag{17}$$

$$RMSE = \left[\frac{1}{N}\sum_{i=1}^{N}[\,\hat{z}(u_i) - z(u_i)]^2\right]^{0.5} \tag{18}$$

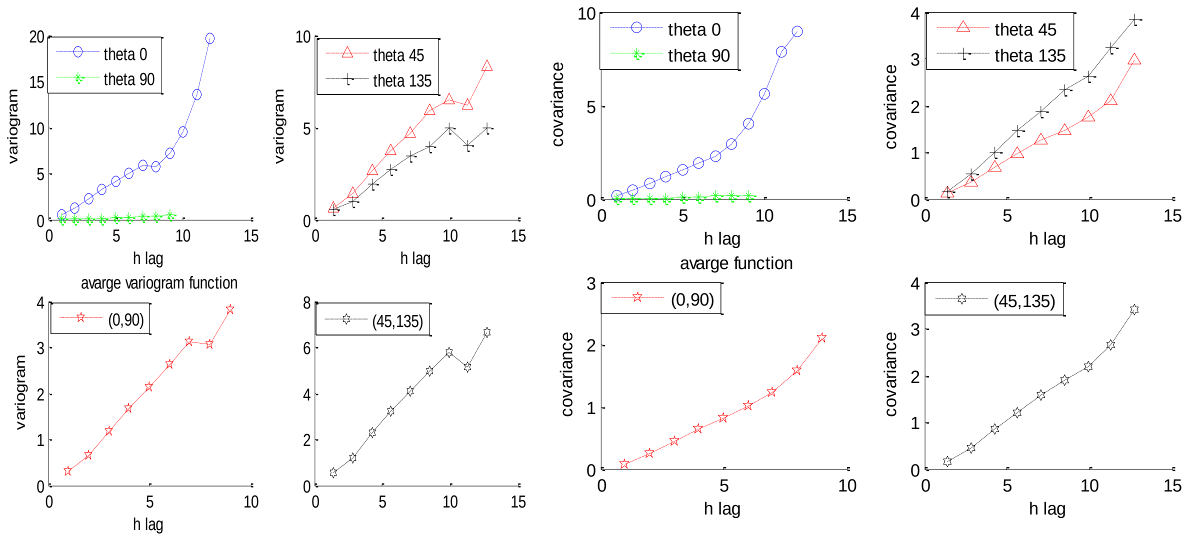
$$KRMSE = \frac{1}{N}\sum_{i=1}^{N}\left\{\frac{[\hat{z}(u_i) - z(u_i)]^2}{\sigma^2_{cokrige}}\right\} \tag{19}$$

where N is the number of data points, and (KRMSE) is chosen as the geostatistical interpolation criterion for the final model using cokriging.

4 Data analysis

4.1 variogram function

The experimental variogram function was applied to the study data to know the behavior of the variogram function curves, with their average which shows us the behavior of the mathematical model for the studied data and the head data or the boundary data by taking the main directions of the compass, as shown in the following figures:



(a) (b)

Figure (4): experimental variogram functions of spatial variables

Figure (4): show the behaver of variogram functions of spatial variables to determine the features of experimental variogram function using fundamental directions of all compass: (0°, 90°, 45°, and 135°) with their average.

Table (1): results of model of spatial variables

Spatial variable	Model	Nugget effect		Sill		Range	
		(0°, 90°)	(45°, 135°)	(0°, 90°)	(45°, 135°)	(0°, 90°)	(45°, 135°)
Covariance of transmissivity	Exponential	0.0836	0.0838	2.097	2.097	8	8
Covariance of head	Gaussian	0.3028	0.5788	3.815	6.621	8	11.31

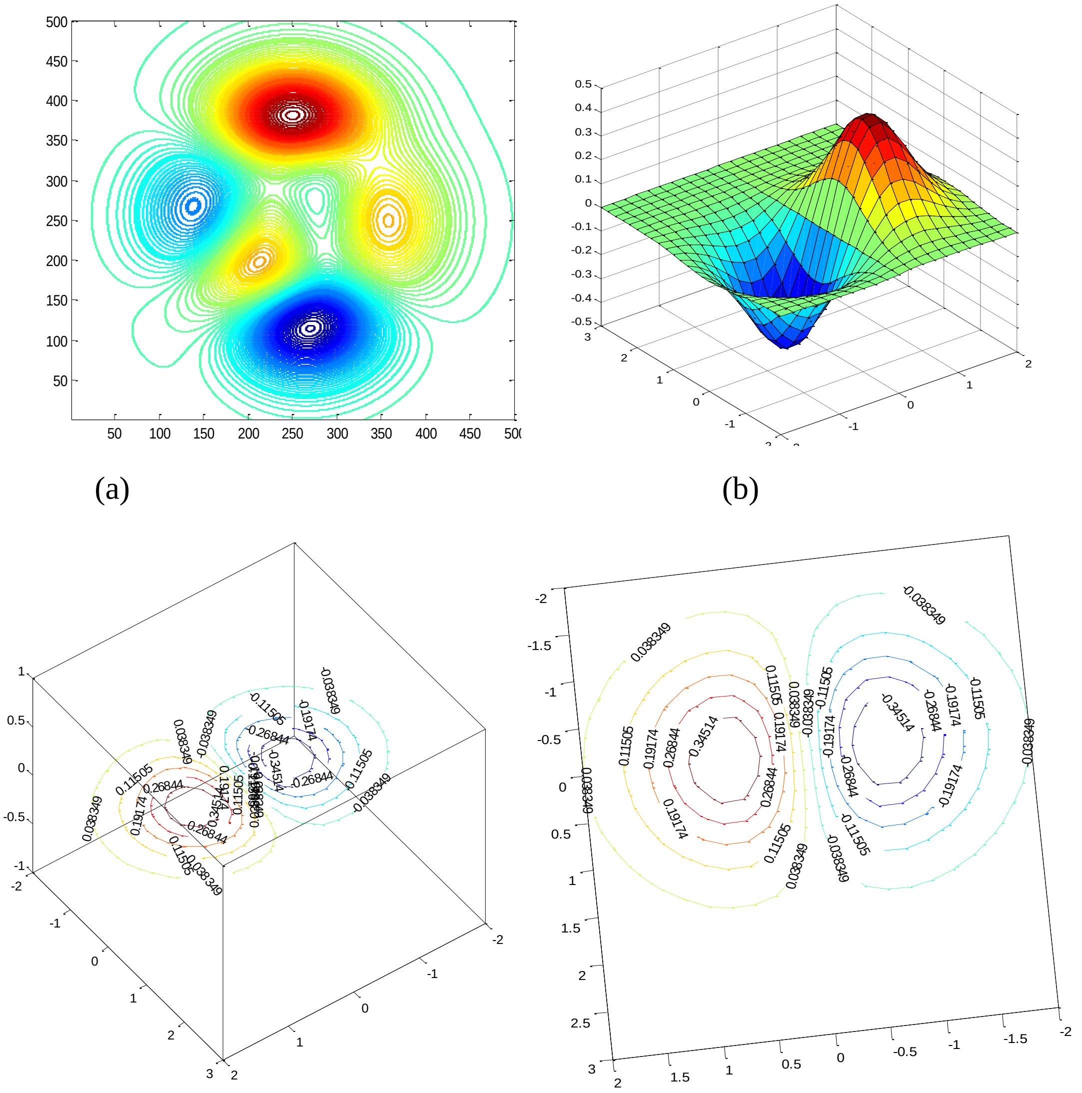
Table (1): illustrate the results of model of spatial variables with the properties of variogram function based on the figure (4 a,4 b), of all compass: (0°, 90° , 45° , 135°) with their average.

Table (2): results of measures of errors by the models

Model	MSE	RMSE	$KRMSE$
Matérn	0.212	0.215	0.324
Cokriging	0.367	0.222	0.312

Generalized Cauchy covariance			
Derivatives $\hat{v}$	0.378	0.212	0.256
Derivatives $\hat{l}$	0.345	0.312	0.244

Table (2): show the results of measures of errors by the models of Matérn, cokriging and Generalized Cauchy covariance. From these results we note the error measures are very small in comparison, indicating the correctness of the prediction.

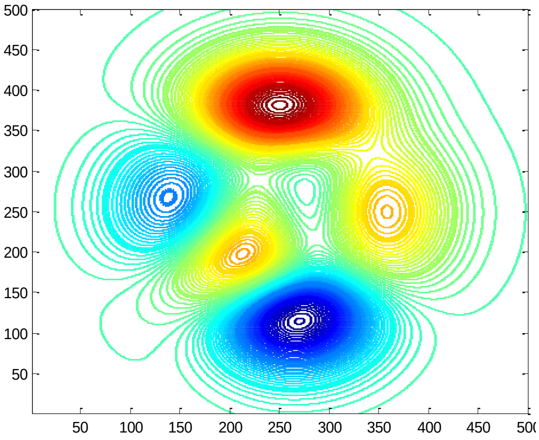


(a)

(b)

(c)

Figure (5): a) original data, b) head data in three dimensions, and c) contour of head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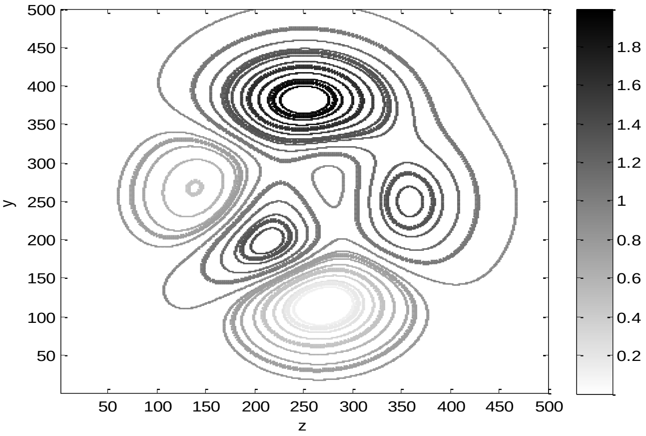
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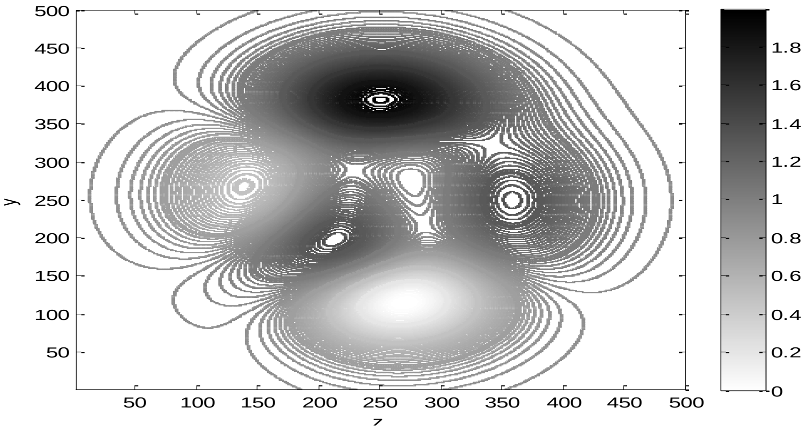
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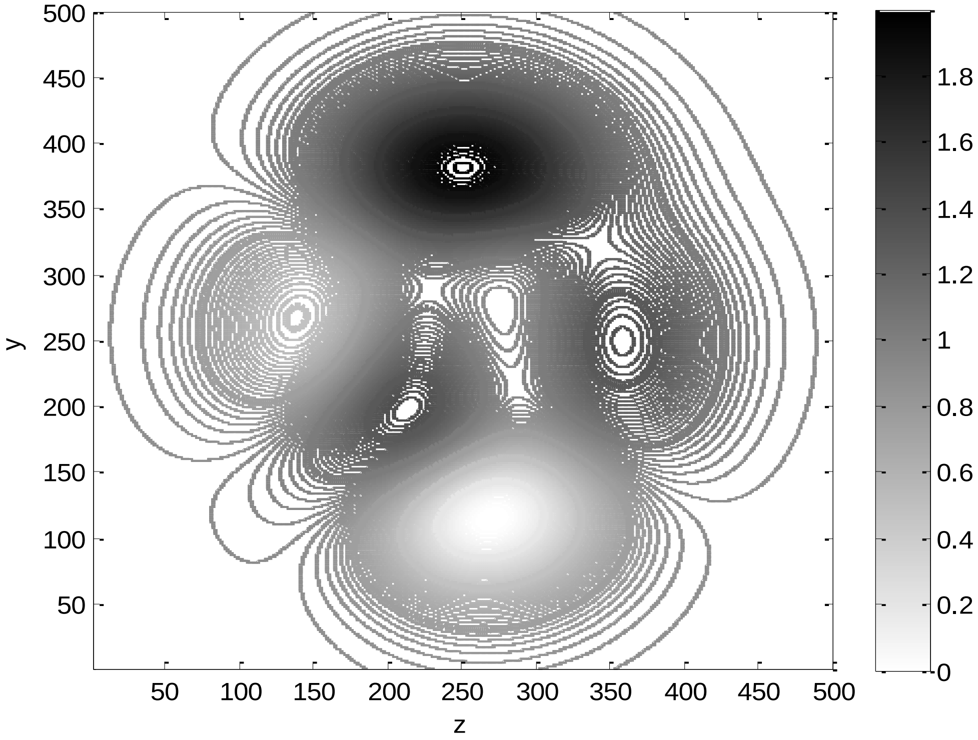
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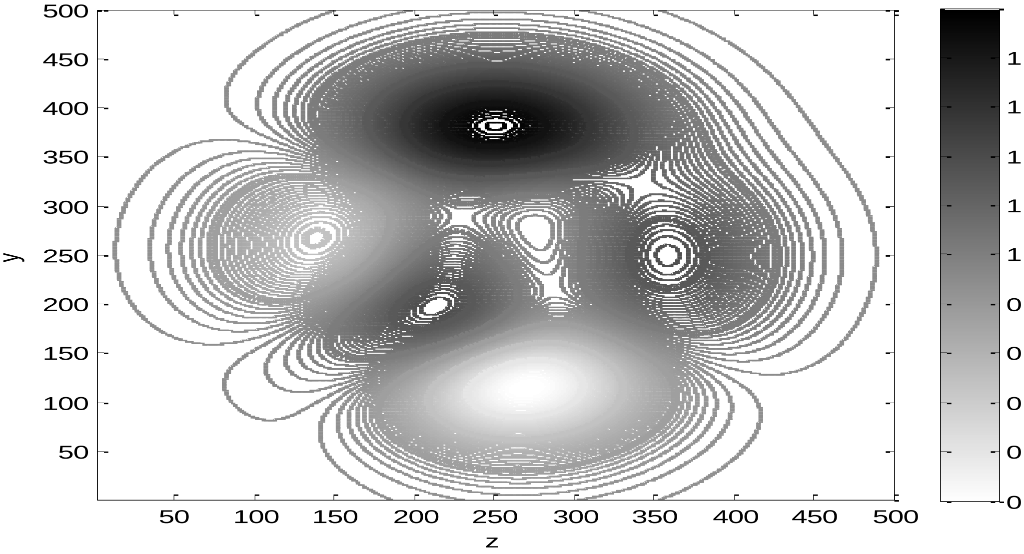

Figure (6): Stages of changing shapes according to the vertical indicators for each shape in terms of the development of colors and the extent of their lightness or depth of colors.

5. Discussion and Conclusions

This work focuses on describing the hydrogeological system using boundary data, typically linked to the acquisition of hydrogeological information. This study aims to ascertain the characteristics of groundwater presence in the aquifers of Mosul city, northern Iraq, primarily utilizing multivariate covariance models as the principal methodology. Variogram models were implemented and parameters were computed. Geostatistical approaches have demonstrated greater efficiency in both time and accuracy for determining aquifer property parameters. Regional parameters yielded more precise findings than geostatistics when applied to other constrained data. The model estimations facilitated the determination of flow parameters. Furthermore, the uncertainty evaluation within the model suggests the establishment of a groundwater monitoring system to address data deficiencies in certain promising regions. To validate the modeling outcomes in these areas, geophysical investigations are required to examine the tectonic and structural influences on groundwater flow. Establishing monitoring wells in distinct groundwater horizons is crucial for precise characterization. This work introduces a method for integrating no-flow and constant-head boundary conditions into potential field estimates. Our methodology produces results that closely resemble those obtained by the finite difference method in comparable studies. The approximate method is simpler to derive and execute, although the exact derivative method is marginally quicker. Our approach necessitates fewer evaluations of the covariance function. In analyzing the data, we demonstrate that joint kriging, a recognized and often utilized multivariate estimator in geostatistics, possesses numerous extensions that we have compiled and demonstrated to showcase the potential of this spatial variance. This work addresses scenarios in geographic stochastic processes, including enhancing the spatial resolution of the spatial variable (downscaling), resolving inverse difficulties, estimating directional derivatives, and spatial interpolation with boundary conditions. All of these spatial estimators are optimal linear estimators, meaning they are unbiased and minimize the variance of the estimate error. The findings in this thesis demonstrate that the kriging system with boundary conditions is an efficient approach for enhancing interpolated contour maps without requiring partitioned modeling. Cokriging between hydraulic head and structural transmission involved a study aimed at confirming that the two variables comply with the partial differential equation.

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