Estimation the Variogram Function Indicator which represent the Transmissivity Coefficient in the groundwater

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Introduction

Many statisticians prefer to name the estimation of the variogram function Indicator at certain locations by the prediction process to distinguish it from the word estimate for the parameters in a particular probability distribution, and that the word estimation has been widely used by geostatistics researchers in the study of the spatial random process [1]. In developed countries, estimation of the variogram function Indicator has become a priority in protecting and cleaning the environment.

Estimating and reconciling variogram are critical stages in estimating or spatial prediction, when a spatial prediction is performed to obtain a prediction in locations to be predicted in a spatial phenomenon that may be minerals, groundwater, plants, or contamination of the environment or a satisfactory environment, the estimation of the variogram function must be conducted in a careful manner from a lesser estimation error or the prediction results will be in accurate and unreliable.

The experimental (approximate) variogram function that measures spatial continuity with in this work is used to make spatial predictions. In order to calculate these spatial predictions, we have an effective theoretical model (variogram) to fit the experimental variogram function we obtain from the diagram. For this purpose, we should know model variogram theoretical indicator (real) as a synthesis written in small groups of approved (authorized functions) i.e, dependable meaning, for example (joke effect, Exponential model, spherical model, Gaussian model) see table (1) shown in the appendix (A) with positive equations and each basic structure of these functions depends on a limited number of parameters eg. jokes effect, Sill, Isotropic, non - uniform properties, and as soon as we know the basic formulations and all parameters will be possible to determine the appropriate theoretical model compared variogram Indicator by drawing and estimating model parameters theory by ordinary least squares (OLS) and generalized least squares (GLS) [2]. By moving spatial statistics as in time series [3], Shows that the composite model differs in different directions across the data perspective .The weighted least squares method would be best to obtain an optimal estimator for the Variogram function Indicator [4,5,6]. This research included two parts, where the part one contains the theoretical aspect of the research in terms of formulating the question of appreciation Formulation of estimation problem by weighted least squares .The second part contains the applied side of the research, the results were encouraging as the Gaussian and spherical models were used on these data The aim of this research is to estimate the variogram function Indicator by the least squares method estimated weighted Indicator variogram data on water tanker factories in groundwater in Bashiqa /Nineveh Governorate/

ABSTRACT

The problem tackled in this paper is the estimation of variogram function Indicator of spatial stochastic process for the Levels of groundwater, by the method of weighted Least squares. This methods is well known in regression analysis in estimating the coefficient of ression model. After defining the indicator variable the parameters of Indicator variogram estimated based on mean squares error. The final formula of weighted least squares estimator can be not be solved exactly, then through the use of iterative Newten - Raphson algorithm and for some iterations the convergence of solution is obtained with certain termination criterion or number of repeats (that used in this paper).
Northern Iraq. Finally, all the algorithms are programmed into the search using the Matlab system.

Section I

Estimation by Generalized least Squares (GLS)

1-1- Indicator Variable:
The pointer variable is often referred to only as the pointer in the spatial statistics literature and is essentially a binary variable and takes values 1 and 0. Just, these variables typically represent the presence or absence of a particular attribute (or feature) in the region consideration. For example, in the mining phenomenon we know the variable is equal 1 when there is a metal and 0 in the absence of the metal. And now we can know the indicator b(x). From the constant variable Z(x), Simply equal to 1, if : which means, Less from the b(x) indicator or equal to a specified threshold ZC and (0) otherwise.

b(x) = 1 if \( Z(x) \leq Z_C \), \( x \in D \in R^P \)

0 otherwise

x is location within the study area/R is Euclid’s space / P=2 tow dimensions or P=3 three dimensions / D a field or area under study.

By defining the indicator we have divided the measurement of the spatial variable Z(x) into two sections the first The Z(X) \( \leq Z_C \). And the other section \( Z(x) > Z_C \). Respectively. This division is known as Indicator variable. If the variable z(x) represents a watch for a random process Z(x), the indicator b(x) is considered as a view of the random indices function B[Z(x) \( \leq Z_C \)] this function is a new binary random stochastic process [7].

1-2- Variogram Function Indicator:
After the pointer variable is declared, a binary random process is obtained where this random (or accidental) process is spatial \( Z(x); x \in D \) Since \( D \subseteq R^P \) assuming that this process fulfills the basic stability Hypothesis of intrinsic stationary in which:

- Mathematical expectation exists and does not depend on the location x that is:

\[ E[Z(x)] = \mu \quad \forall x \in D \quad \ldots \ldots \quad (1) \]

- For all distances h, the increase \( Z(x+h) - Z(x) \) it has a specific variation and is not dependent on the location x that is:

\[ \text{Var}[Z(x+h)-Z(x)] = \sigma^2 \quad \forall x \in D, \quad (h \text{ is the distance between the sites}) \ldots \ldots \quad (2) \]

As that \( 2\gamma(h) \) is the variogram function Indicator of the distance h. Z(x) is the spatial variable of the site x with low dimensions \( x=(u,v) \). We assume that the binary random Stochastic process B[Z(x) \( \leq Z_C \)] is stable and isotropic, so that \( 2\gamma(h) \) depends on the distance h only.

Now, the classic estimator of variogram function indicator is defined as:

\[ 2\gamma(h) = \frac{1}{N(h)} \sum_{j=1}^{N(h)} [Z(x_j + h) - Z(x_j)]^2 \quad \ldots \ldots \quad (3) \]

[8,9,10] these sources adopted the primary source [11], and surely \( N(h) \) represents the number of pairs of views that are separated by distance h.

Now can define a function variogram pointer is a function representing the degree of heterogeneity of the continuity of the phenomenon (metal ore wells or groundwater or air gases) under study to analyze the spatial heterogeneity within the structure of the specific occurrence of the phenomenon of the region, the increasing dimension h between observations as the heterogeneity becomes large until the height of the function stabilizes \( \gamma(h) \) at a certain offset like \( h = a \) and this offset a it called long, and after a long note will fade covariance function in variogram as it stabilizes the value of fixed equal contrast views \( \sigma^2 \). This explains outside the study area, i.e., there is no effect of the phenomenon studied after the range, or there may be an impact in very small quantities.

Given the importance of the variogram function \( \gamma(h) \) scientists have been able to identified various models that can be expressed in Table(1) shown in the appendix (A).

Now you can give be the following formula of the Semi-Variogram function by shifting (h).

\[ \gamma(h) = \frac{1}{2 N(h)} \sum_{j=1}^{N(h)} [Z(x_j + h) - Z(x_j)]^2 \quad \ldots \ldots \quad (4) \]

It is the square of the differences between spatial observations that are shifted apart h as that \( N(h) \) represents the number of views pairs \( Z(x_j), Z(x_j + h) \). [12,13]. Called the equation (4) Semi-variogram function Indicator because there is a half at the right end of the equation.

1-3- Drafting issue Formulation of the Problem:
The appropriate methods of the experimental variogram function. I.e., containing the unknown parameters proposed so far ignore the visual diagram represented \( \gamma(h) \) Since \( h = h_1, h_2, \ldots, h_n \) and then find a theoretical variogram that is close to it fit the theoretical model with the experimental model and this method is a useful tool because the parameters of the experimental model is not estimated with the least possible error [14,15]. Which should be a measure of convergence between the experimental model and the theoretical model by the total difference between the boxes variogram demo and variogram indicator theory, which must be less than what can, and of course a function variogram demo containing unknown parameters represent a vector \( \theta \) as:

\[ \theta=(\theta_1, \theta_2, \ldots, \theta_n) \]

will therefore encode function variogram index theoretical form \( \gamma(h: \theta) \). That is:

\[ \gamma(h: \theta) = \sum_{j=1}^{n} [\gamma(h_j) - \gamma(h: \theta)]^2 \quad \ldots \ldots \quad (5) \]

The formula (5) represents the estimated least normal squares to \( \theta \) and of course we will get \( \hat{\theta} \) after taking the derivative of equation (5) for \( \theta \) and equal to zero to get \( \hat{\theta} \) (the least squares estimator), although equation (5) does not have a geometric appearance because it does not consider the distribution of the variability function of the estimator is important in
addition to the variability of the spatial variable $Z(x)$. Therefore, the appropriateness of the generalized least squares estimator assumed that the variogram estimator obtained at distances ($h_1, h_2, ..., h_n$) that $n$ are fixed and represent the number of views that are apart from each other $h$. The Ordinary Least Squares (OLS) is the estimation of the parameter $\theta$ and suppose that it is written $\hat{\theta}$ so that:

$$S(\theta) = \frac{2}{n(h)} \sum_{j=1}^{n} (\gamma(h(j)) - \gamma(h(j), \theta))^2$$

The smallest thing possible, as that $S(\hat{\theta})$ it represents the sum of the residual boxes or error between variogram indicator theoretical and variogram indicator, when:

$$2\gamma = (2\gamma(h_1), ..., 2\gamma(h_n))'.$$

It $2\gamma$ symbolizes the vector of random variables $2\gamma(h_j)$, $i = 1, 2, ..., n$, with a contrast matrix where:

$$Var(2\gamma) = \sigma^2$$

Then to get the estimator $\hat{\theta}$ we use the Generalized Least Squares method (GLS) of reducing the amount

$$Q(\theta) = g'(\theta) \sigma^{-1} g(\theta)$$

there is an intermediate stage between $\hat{\theta}$ and $\theta$ is the least-squares method which states that the estimated $\hat{\theta}':$ We get it by reducing the amount

$$W(\theta) = g'(\theta)V^{-1} g(\theta)$$

$V = \text{diag} \{ Var(2\gamma(h_1)), Var(2\gamma(h_2)), ..., Var(2\gamma(h_n)) \}$ is the weighted matrix.

Diagonal matrix with zeros in all inputs except contrast, $2\gamma(h_j), j = 1, 2, ..., n$ on the main diameter.

$Var(2\gamma(h_j))$

To obtain the final formula for the weighted least squares estimator, the proofs listed below must be proved:

1-3-1-Theorem(1) [16]:

$$\text{Cov}(Z(x+h_1)-Z(x), Z(y+h_2)-Z(y))$$

$$\frac{\text{Var}(Z(x+h_1)-Z(x))}{\text{Var}(Z(y+h_2)-Z(y))}$$

Applying the two versions of the theorem (2) and theorem (3)

$C(h) = C(0) - \gamma(h)$

$Var(Z(x+h)-Z(x)) = 2\gamma(h)$

1-3-2-Theorem (2) [17]:

For each pair of new spatial random variables $[Z(x+h), Z(x)]$, covariance exists and depends on the separation distance $h$. The stability of covariance leads to the stability of variance and the variogram indicator and a correlation can be obtained between covariance $C(h)$. The function of the indicator variogram $\gamma(h)$ and contrast. As in the following formula:

$$\gamma(h) = C(0) - C(h)$$

Since that $C(0) = \sigma^2$, $E[Z(x)] = \mu$, $\forall x \in E$

1-3-3-Theorem(3) [18]:

Let it be $\{Z(x)\}$ stable new random spatial process of second order through $i = 1, 2, ..., n Z(x_i)$ views at sites $x_1, x_2, ..., x_n$ then:

$$\text{cov}[(Z(x_i)-Z(x_j)) (Z(x_k)-Z(x_l))]=r(x_i-x_j)+r(x_k-x_l)-r(x_i-x_l), i 
eq j \neq k$$

Since $h = (x_i-x_j)$ represents distance between locations and $\gamma(.)$ Semi-Variogram function.

1-4-Generalized least squares (GLS):

Returning to the classical estimator defined by equation (3) and suppose that $\{Z(x)\}$ is Gaussian (normal) and as it is known that any conciliation of a linear variable Gaussian is also Gaussian if it is $N(0, 1), ..., (8)$.

According

$$(Z(x+h)-Z(x))$$

to the basic premise

$$\text{Var}[Z(x+h)-Z(x)] = E[(Z(x+h)-Z(x))^2] = 2\gamma(h)$$

of (8) results

$$\text{Sinc}(Z(x+h)-Z(x))^2 = 2\gamma(h) \sim X^2(3)$$

It $X^2(3)$ represents a variable where the Chi-square distribution is distributed with equal freedom 1 the correlation between the two variables can be written

$$(Z(y+h_2)-Z(y))^2, (Z(x+h_1)-Z(x))^2$$

and offset $h_1$ and $h_2$ in the following form:

$$\text{Corr}[Z(x)+Z(x+h_1), Z(x+h_2)-Z(x)] \sim X^2(3)$$

$$= [(\text{Corr}(Z(x+h_1), Z(x+h_2)-Z(x)) \sim X^2(3)$$

$C(h) = C(0) - \gamma(h)$

$$Var(Z(x+h)-Z(x)) = 2\gamma(h)$$

112
Calculating the quality of the Variogram Function using the Generalized least Squares (GLS) Introduction

The practical aspect includes the Newton Raphson algorithm to obtain the estimator and estimating the variogram function indicator for real data taken from the site (x, i) and values Z (x, i). Since i = 1, 2, ..., n and the total of data from inside Iraq water wells in the area Ba’ashiqah / province of Nineveh / Iraq [21]. They are the aquatic conductivity plants in 45 Exploration well in the area, has been taking a subset of these the data (30) wells to get a regular network Regular grid, and Table No(2) shown in the appendix (A) illustrates mijjah water conductivity coefficient data measured by unit (M²/day).

2-1-Semi-variogram function calculation:
If we take Z = {Z (x_1), Z (x_2), ..., Z (x_n)} It represents a sample of views at installed sites x_1, x_2, ..., x_n for the second-order, stable, binary spatial randomization. Assume that \( 2\gamma (h; \theta) \) variogram function indicator theory is valid and we want to reconcile the variogram classic of this process and rely on the parameter \( \theta \) which represents the vector of unknown parameters \( \theta = (\theta_1, \theta_2, \theta_3) \)
also that \( \theta \in \Theta \subseteq \mathbb{R}^k \) and represent \( \Theta \) Parameter space \( \theta \), represent \( \theta \) Jokes effect (Nugget) and \( \theta_2 \) Poor continuity of the spatial phenomenon or measurement error, which is part of the variation, ie: \( \theta_2=C(0)-\theta_1 \).

The remaining part of (TB) sill can be written in the format \( C(0)=\theta_1+\theta_2 \).
\( \theta_1 \) The extent of the spatial phenomenon under study and the extent represents the distance that determines the presence of spatial phenomenon and the distance in excess of the spatial phenomenon begins to fade and the fee variance of the variogram indicator to equal its height tuberculosis or contrast with no omission that \( \psi_0=\theta_1, \psi_1=\theta_2, \psi_2=a(\text{Range}) \) and \( \sigma \) The spatial phenomenon or measurement error, which is part of the variation, ie: \( \theta_2=C(0)-\theta_1 \).

It is well water data will calculate the results of sub-functions variogram function indicator using equation (3) offsets \( h = 1, 2, ..., 7 \) and for the four directions in terms of angle \( \theta \) Since that \( \theta = 0^\circ, \theta = 45^\circ, \theta = 90^\circ, \theta = 135^\circ \) as shown in Table 3 in the appendix (A).

Note from Table 3 that the sine -variogram function was calculated according to the equation (3) For the four important directions of the compass, these directions are North - South, North - East, Southwest, East-West, North, West-Southwest, which represent the above angles as shown in Figure (1).

Fig. 1: The four angles used to calculate the semi-variogram function represent the indicator
Note from Figure (2) that the semi-variogram drawing of the angles \( \theta = 0^\circ, \theta = 45^\circ, \theta = 90^\circ, \theta = 135^\circ \). Clustered together in an intertwined beam, which explains that the semi-variogram function of this data is isotropic. Isotropic, i.e., does not depend on direction. To obtain the model of the quasi-variogram indicator, we find the average of the semi-variogram function from these four functions, from which we obtain the quasi-variogram indicator, one representing the spatial reliability. Spatial dependence these data are as shown in Table (4) in the appendix (A).

The average variogram indicator in Table (4) was obtained by adding the values of \( \gamma(90^\circ) \) with \( \gamma(0^\circ) \) and dividing by 2 when \( h = 1,2, \ldots, 7 \). The same process with \( \gamma(135^\circ) \) and \( \gamma(45^\circ) \) when \( h = 0.5542, 1.8299, \ldots, 12.0118 \). We note that the values of the semi-variogram function increase with increasing values \( h \).

Table (4) shows the adjustment of the variogram Indicator rate that was extracted from the results of a program designed for this purpose by the Matlab.

2-2-(Newton -Raphson algorithm)

1- Beginning.

2- Data entry \( \hat{X} \).

3- Calculate the pointer’s variogram function at the angles \( \theta = 135^\circ, \theta = 90^\circ, \theta = 45^\circ, \theta = 0^\circ \).

4- Draw the indicator of the variogram function of the four angles.

5- Calculate the average of the variogram function of the indicator with the display of the results and plot the function.

6- Print estimates values for \( \theta_1, \theta_2, \theta_3 \) Calculated from semi-variogram indicator function.

7- End.

Developed algorithm

We follow the same steps as above and add the following steps:

1- Beginning.

2- Enter \( \theta_{01}, \theta_{02}, \theta_{03} \), calculated from algorithm (1).

3- Calculate the first derivative of equation (14).

4- Calculate the second derivative of equation (14).

5- Using Newton Ravson’s algorithm by taking the values \( \theta_{01}, \theta_{02}, \theta_{03} \) and stopping condition is 100 iterations.

6- Calculate the spherical model and the exponential model of the new values (obtained from the Newton-Ravson algorithm from step (5)).

7- Comparing old and new results (i.e., improved values) using the least squares method with the graph.

8- Calculate the lowest error ratio between the real and estimated values using equation (15) for the spherical and exponential models.

9- End.

2-3-estimate Generalized least Squares:

Now we will use Newton Ravson’s algorithm to get the estimator \( \hat{\theta} \) in the equation (14). In order to apply the Generalized Least Squares we must derive the equation (14) derived partial first and second, that is: 

\[ G^T G \hat{\beta} \] 

any for \( \theta_1, \theta_2, \theta_3 \). Since: 

\[ \theta = (\theta_1, \theta_2, \theta_3) \]

This was a special program that used a system Matlab. The growth exponential primary values obtained from the drawing variogram function, which were taken from the drawing function semi variogram indicator of Figure (2) in the total of the data for \( \theta_1, \theta_2, \theta_3 \).

\( \theta_{01} = 0.6 \), \( \theta_{02} = 1.2 \), \( \theta_{03} = 9.3 \)

The spherical model (Spherical Variogram) Can be written as follows:

\[ \gamma(h) = \gamma(0) + \frac{3}{2} \left( \frac{h}{\theta_3} \right) \left( 1 - \frac{h}{\theta_3} \right) \]

The exponential model (Exponential Variogram) It is as follows:

\[ \gamma(h) = \gamma(0) + \theta_3 \left( 1 - e^{-h/\theta_3} \right) \]

We have obtained the required results by repeating the above method \( \lambda \) in the algorithm is as follows:

\[ (\theta)_{k+1} = (\theta)_k - G_k^{-1} \delta_k \]

Since \( \theta = (\theta_1, \theta_2, \theta_3) \) appreciation \( \theta \) when repeating \( (\theta)_{k+1} \) appreciation \( \theta \) when repeating \( k \), \( \theta \), the first derivative vector relative to the parameter \( \theta \) for \( G \) in equation (14) when repeating \( k \) and \( G_k \). The second derivative matrix of the equation \( G \) for master \( \theta \) and \( G \) known as the Hessian matrix. If we assume that:

\[ \delta = \theta + \lambda \text{diag}(\theta) \]

So

\[ (\theta)_{k+1} = (\theta) - D^{-1}\delta_k \]

Called \( \lambda \) By Levenberg -Marquardt parameter [16.22].

We stopped the implementation of the program at 100 iterations to get the best approximation between the real and approximate values curve and the lowest mean error square between them and the exponential and spherical models. \( \theta_1, \theta_2, \theta_3 \). The values of \( \lambda \) are as follows:

at 100 iterations and a value \( \lambda = 300 \) best in exponential model:

\[ \theta_1 = 0.676 \quad \theta_2 = 1.092 \quad \theta_3 = 9.9972 \]
In the spherical model, the best was achieved when repeating 100 and value \( \lambda = 3000 \)

\[ \hat{\theta}_1 = 0.598; \quad \hat{\theta}_2 = 1.442; \quad \hat{\theta}_3 = 10.013 \]

But we did not just get the above results, we calculated the quality of the reconciliation of variogram by the estimator of least squares weighed by the mean error square (MSE) Mean Squares error which is calculated from the following law:

\[
\text{MSE} = \frac{1}{n} \sum_{i=1}^{n} (\hat{\gamma}(h_i) - \gamma(h_i; \hat{\theta}))^2 \quad (15)
\]

Of a special program specially prepared for this purpose by the system MATLAB was obtained less error ratio between the real values and the estimated values for the data in the study site using the value of the spherical model

\[
\text{MSE} = 7.9911 \quad \text{Figure (3) illustrates this.}
\]

Using the exponential model, the lowest error rate was

\[
\text{MSE} = 1.9551 \quad \text{Figure (4) illustrates this.}
\]

That is, the results given by the spherical model are better than exponential patterns.

![Plot of spherical model](image)

**Fig. 3:** is the best estimate of the spherical model

![Plot of exponential model](image)

**Fig. 4:** is the best estimate of the exponential model

Of the two forms (3), (4) note that the exponential model gave the best results of the spherical model of the data set in the area of study. After obtaining the final formula to estimate the function variogram cursor is possible to use this function to predict the spatial process and we believe that the prediction will be accurate because of the accuracy of a function variogram which is considered very important in the process of teacher Kriging and common Cokriging.

**2-4- Conclusions**

Because we did not get the complete solution for estimating the least squares, Newton Ravson’s algorithm was used to obtain the final solution for estimation. And we listed the four directions \( \theta = 0^\circ, \theta = 45^\circ, \theta = 90^\circ, \theta = 135^\circ \) This is in order to obtain the index variogram rate ,which is an accurate representative of the spatial data and is better than the calculation of variogram index one. It can anus of this research future work by applying it to other data, for example, climate data or infections environmental ...... etc .by introducing a certain threshold and the study of this phenomenon at that threshold, Also the Variogram Function Indicator estimated by this method can be used in all types of Kriging and prediction, for example, Ordinary Kriging, the Universal Kriging and Cokriging.

**Appendix (A)**

**Table 1: Models of Variogram functions**

<table>
<thead>
<tr>
<th>Formula Name</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spherical Model</td>
<td>( \psi_0 + \psi \cdot \frac{h}{2a} + \frac{1}{2a(\frac{h}{a})^3} ) for ( h/a \leq 2 )</td>
</tr>
<tr>
<td>( h &gt; 0 )</td>
<td>( \psi_0 + \psi \cdot \frac{h}{2} )</td>
</tr>
</tbody>
</table>
Both \( \psi_0 \), \( \psi \) unknown parameters called covariance components or semi indicator variogram functions

### Table 2: Data and their location in the study area

<table>
<thead>
<tr>
<th>T</th>
<th>juvenile u</th>
<th>juvenile v</th>
<th>Water conductivity plants (M (^2)/day)</th>
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<td>2925</td>
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### Table 3: Results of the Parameters of the Parameters of Data at the Study Location

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Table: 4 results of the average semi-variogram

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References


تقدير دالة الفاريوكرام المؤشر لمعامل الناقلية المائية في المياه الجوفية

سيروان سليمان نون كرجية
مديرية تربية محافظة نينوى، الموصل، العراق

الملخص

المسألة التي تتناولها هذه الدراسة هي تقدير دالة الفاريوكرام المؤشر لمعامل الناقلية المائية في المياه الجوفية. بواسطة المراعاة الصغرى الموزونة وهذه الطريقة معروفة في تحليل الانحدار للحصول على مترات معلمات نموذج الانحدار. بعد تعريف المتغير المؤشر يتم تقدير معلمات دالة الفاريوكرام المؤشر (MSE) المستخدم في التنبؤ من خلال تصغير متوسط مربعات خطأ (MSE) للفي تي من خلال معادلات خطية للمعادلات التالية: يتم تصغيرها والحصول على الحل النهائي لمعلمات الموارد من خلال استخدام الطريقة التكرارية المعروفة في حل المعادلات غير الخطية مثل خوارزمية نيوتن – رافن. يتم التكرار بعد عدد من المرات لحقن الوصول إلى التقارب والوصول إلى التقدير النهائي لمعلمات دالة الفاريوكرام المؤشر من خلال معيار توقف معين أو عدد من التكرارات (الذي تم استخدامه في هذه الدراسة).