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Effect of choosing a variogram model to predict salinity and its impact on the environment and geotechnical structures

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Abstract. Various disciplines, engineering, humanities, and other sciences require interpolating many parameters. Geostatistics, with its structural analysis step, is widely used for this purpose. Variography is the valuable step used to assess the correlation and dependence of the data. However, the wrong choice of the variogram model encounter all the predictive attended results. This article illustrates how the use of inappropriate variogram models can seriously conduct to a misleading of predicted results for such analysis.
The influence of the selection of the semi-variogram model is highlighted and illustrated by thematic maps developed using three different models (Gaussian, spherical and exponential).
To avoid such a drawback, a methodical approach to select the most suitable model, based on the calculation and analysis of the mean error (ME), the mean square error (MSE), the root of the square error mean (REQM), mean standard error (ESM) and root of mean standard error (REQSM), is proposed in the present research study. Such contribution could reduce the negative effects of the choice of variogram model on the interpolation operation using the kriging technique.

Keywords. Structural analysis, variogram model, Predictive analysis, Interpolation, Kriging

1. Introduction

Environmental research is always sample-based, but overall, the measurement results represent the continuity of the sampling space. Most analysts want to know what value can represent the place [1]. Even with the same input data, applying different interpolation methods may produce different results [2, 3, 4].

More and more interpolation applications are appearing in various fields. Depending on the mathematical model on which they are based, interpolation methods generally fall into two categories [5] :

- deterministic methods based on purely mathematical properties (generally geometrical), without taking into account the physical phenomenon which interests us. From the surrounding measured values, interpolation is used to determine the result values [6]. Interpolators such as Spline, TIN (Irregular Triangular Network), IDW (Inverse Distance Weighting), and LPI (Local Polynomial Interpolation) are classified as deterministic methods.

- stochastic methods which use probabilistic models and result from the statistical analysis of the data considered. We then speak of geostatistical techniques which consist of an autocorrelation (statistical relations between different measured points), which also makes it possible to estimate the uncertainty of each result. [6, 7].

South African mining engineer Danie Krige first proposed the concept of a moving average to overcome the problem of overestimating the mineral reserve system. To celebrate this pioneering miner, Professor Matheron coined the term “Kriging” for the method he developed [8].

By considering the spatial correlation and modeling it, geostatistics can quite correctly predict environmental variables with minimal and known variance, unlike other methods. The technique of prediction by Kriging, requires a mathematical model to describe the spatial covariance, generally expressed in the form of a variogram, and thanks to its parameterized form it has become the main tool of geostatistics [9].

Initially, professionals must write their own code for geostatistical analysis. They must include digital analysis to program the methods. This situation has changed a lot in recent years, and powerful programs are widely and economically available in the market. Unfortunately, it is possible to simply press a few keys on your keyboard to interpolate the scattered data and display the results as a map, without having to understand the situation between the data and the generated map. Software becomes a "black box" [10].

Kriging is different from all interpolation techniques, due to its fair characteristic of being the best linear unbiased estimator (BLU Best Linear Unbiased) [11]. It is by far the most widely used method for this purpose in all areas of environmental science around the world. [12, 13, 14, 15].

It is also advisable to examine the practical impact of the choice of a model on the Kriging estimate and the associated uncertainty to assess their sensitivity [16].

The variogram-based kriging technique is used today by scientists in many fields, such as civil defense [17]meteorology [18], geochemistry [19, 20, 21, 22].

If the authors do not consider the impact priority of the variogram model in this type of survey, the survey will be a summary and misleading result. This explains the importance of this document.

To this end, a study was carried out to show the main advantages residing in taking into account the modeling of the empirical spatial connection of the data and the possibility of providing an a priori error which allows qualifying the confidence in the results obtained. [23]; a geostatistical analysis, on the Tunisian territory, of the reference evapotranspiration, based on the modeling of the variogram and the determination of its parameters (nugget, slope or plateau and range) [24]; a suggestion to use cross-validation to check the validity of the semivariogram model [25].

In order to highlight the delicacy of modeling and evaluations, many other studies have been carried out. Giuseppe and Petrarca [26]evoke the influence of scale in the spatial interaction model. Patuelli and Giuseppe [27] published an editorial on the progress of statistical modeling of spatial interaction data.

This article discusses the question of selecting the appropriate semivariogram model. The objective is to briefly explain the impact of the choice of the variogram model on the kriging estimation and the associated uncertainty in order to assess its sensitivity, and how to choose the most appropriate model. The variogram model is tested by cross-validation, which makes it possible to reduce the influence of its bad choice on the interpolation by the kriging technique.

2. Materials and methods

2.1 Study site

In this experimental analysis, we used a set of spatial salinity data, on a cultivated plot, located at the level of the Mina plain in the Relizane state of Algeria [28].

Figure 1 shows the position of the 64 points identified on the site of the Mina plain in relation to the eastern municipality of El Matmar located in the west of Algeria

2.1.1 *Used Data.* The data acquisition was carried out in the field using a Garmin type GPS, for the geographical coordinates of the points, the field prospecting required the use of the electromagnetic conductivity meter (EM38) and the taking of samples of soils. The soil samples collected were coded and put in well-sealed plastic bags and sent for laboratory analysis to the National Institute of Soils, Irrigation and Drainage (INSID) in El Matmar (Relizane). The best method is to intervene after heavy rains which homogenize the water profiles of the soils [29].

2.1.2 *Digital database.* A data file in Excel format, including the UTM coordinates and the study parameter which is the electrical conductivity (EC) was introduced in point format within a geographic information system (GIS). In order to limit the study area, a shapefile is georeferenced in the same reference coordinate system, in order to be superimposed on the study area.

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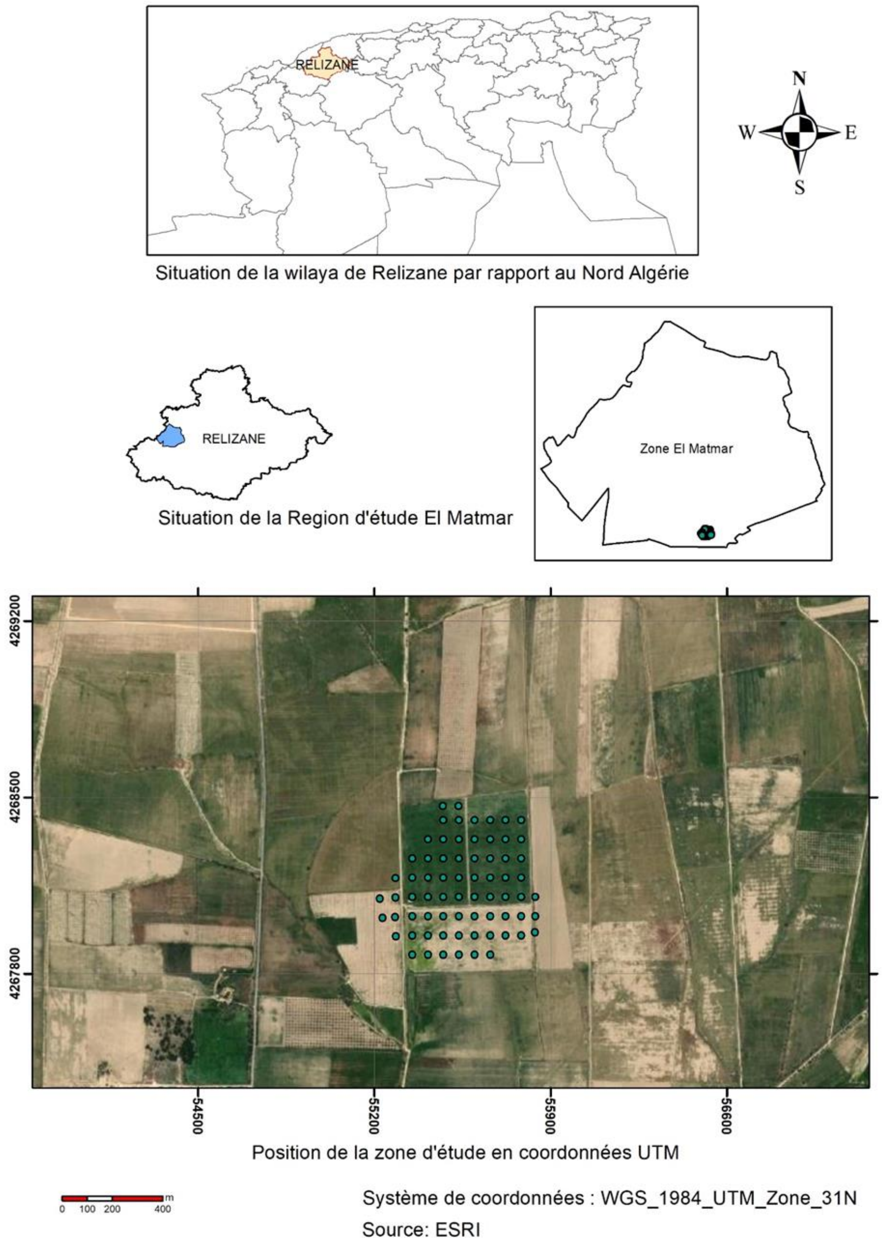

Figure 1. The geographical location of the study area

2.2 Geostatistics

Geostatistics is a tool for analyzing the spatial structure of geographic information [30]. It is based on the theory of the study of regionalized variables [31]. The variogram is one of the most important tools for quantifying the spatial correlation between data points.

2.2.1 *Variography.* According to Nolin [32], the closer the samples are in space, the more they resemble each other up to a certain distance beyond which they become independent of each other. A commonly used method to study the spatial dependence of observations is to analyze the semivariogram, a graph that shows the change in the half-variance γ(h) as a function of the distance (h) between samples [33]. It is the basis of the kriging interpolation technique.

2.2.2 *Experimental variogram.* The experimental or empirical variogram is an estimator of the theoretical variogram from the data. In a more general case, h could be a vector, and the sum will be done on all the points zi, zj such that zj=zi+h, which makes it possible to process the anisotropies. We can estimate the variogram by the formula:

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

- $\gamma_e(h)$ is the estimated value of the semi-variogram for the shift (h);
- N (h) number of pairs of measurement points distant from h;
- z (x_i) value measured at measuring point x_j.

2.2.3 *Typical theoretical variogram.* A model is admissible if any variance calculated from the model is positive [34]. The description of a semivariogram model is based on the quantification of several parameters identified in Figure 2 which represents a theoretical model where the semi-variance is a function of the sampling interval h and whose equation is given by:

$$\gamma(h) = \frac{1}{2} Var\big(z(x) - z(x + h)\big) \qquad (2)$$

The range (length) a is the distance at which the correlation between observations becomes zero. At this distance, the semivariogram reaches the threshold or Threshold σ^2 which is the sum of the variance of the nugget C_0 and the partial sill (variance) C_1 ($\sigma^2 = C_0 + C^1$).

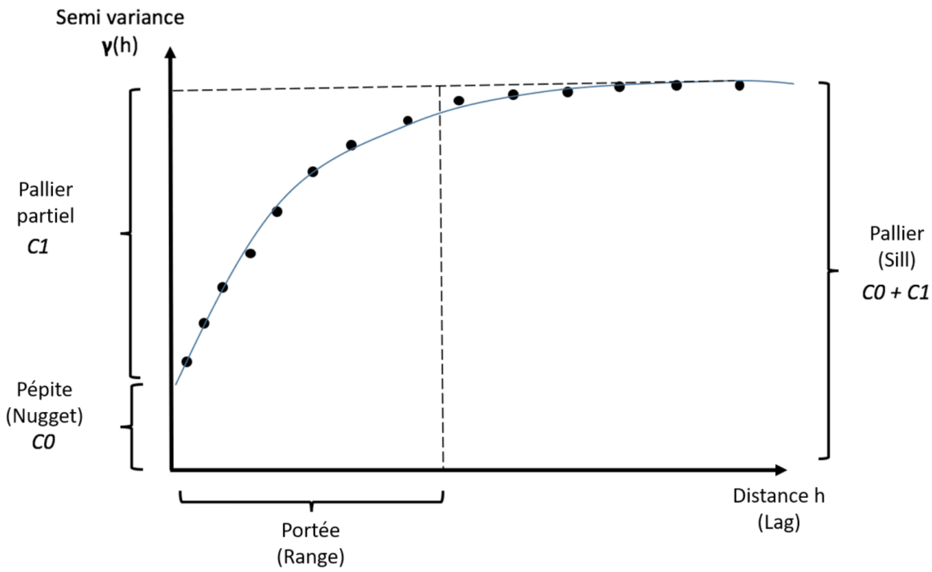

Figure 2. Typical variogram model

The nugget effect comes from various sources such as measurement errors, the existence of a microstructure smaller than the sample size and / or the presence of a microstructure with a range less than the distance between the two observations. the closest. It is impossible to quantify the contribution of each source.

2.2.4 *Theoretical variogram.* In order to interpolate with different methods, a theoretical model must be fitted to the experimental data. By fitting a theoretical model to the values of the empirical model and applying linear and non-linear models, unknown variables can be estimated [35]. The most common theoretical semivariogram models are spherical, exponential, linear, and Gaussian models [36].

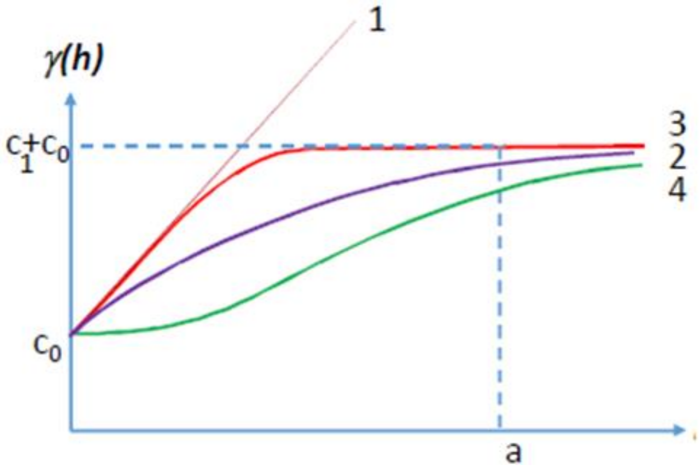

Figure 3. Most common theoretical adjustment models

2.2.5 *Fitting the variogram model.* The most common theoretical variogram models are expressed as follows [37]:

Model Spherical:

$$\gamma(h) = \begin{cases} c_0 + c\left(\frac{3h}{2a} - \frac{h^3}{2a^3}\right) & \text{si} \quad 0 < h < a \\ c = c_0 + c_1 & \text{si} \quad h \geq a \end{cases} \qquad (3)$$

Gaussian model:

$$\gamma(h) = c_0 + c\left[1 - e^{-3\left(\frac{h}{a}\right)^2}\right] \qquad (4)$$

Exponential model:

$$\gamma(h) = c_0 + c\left[1 - e^{-3\frac{|h|}{a}}\right] \qquad (5)$$

Linear model:

$$\gamma(h) = c_0 + bh \qquad (6)$$

The variogram model is chosen from a set of mathematical functions that describe spatial relationships. The appropriate model is chosen by matching the shape of the curve of the experimental variogram to the shape of the curve of the mathematical function.

For interpolation, a nugget or linear model is automatically offered to the user, who should rationally select the appropriate one from the box to the right (Figure 4).

In fact, the variogram is used in the interpolative kriging technique at its second stage. This step is preceded by an exploratory analysis of the data and a prediction of values [38].

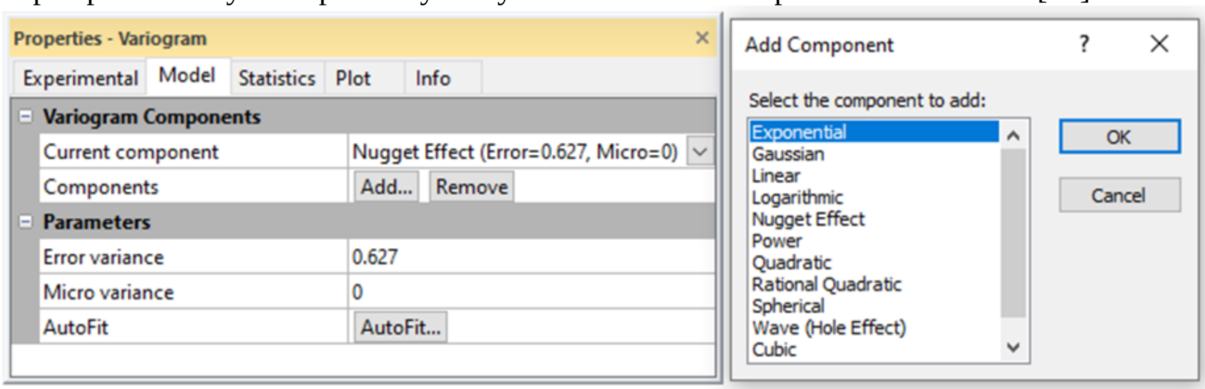

Figure 4. Selecting the appropriate variogram model

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2.2.6 *Geostatistical interpolation.* Kriging is a prediction-oriented interpolation method commonly used for spatial data. This is a straightforward approach with a single solution and can be used to estimate the unknown value z* of a variable at a point from the surrounding known values z_i. Ordinary kriging provides the weighted average of the sample values which leads to the error in the estimation of the minimum variance [39], using the following equation:

$$z^*(x_0) = \sum_{1}^{n} \lambda_i z_i \qquad (7)$$

- z_i = value measured at location i
- λ_i = unknown weight of the measured value at location i
- x_0 = forecast location
- n = number of readings

2.2.7 *Cross-validation.* During the exploratory analysis, the data should be checked for consistency, outliers removed and the statistical distribution identified. The normal distribution of data is decided when the mean and median are very similar. However, high skewness values indicate the existence of outliers, which are very high or low measured values relative to the dataset. Outliers are caused by wrong measurement or recording and should be transformed when they exist. In the prediction phase, semi-variogram models must be represented in order to select the best fit. The predictive performance of the models provided is verified on the basis of cross-validation tests. The values of the mean error (ME), mean square error (MSE), the root of mean square error (REQM), mean standard error (ESM), and root of mean standard error (REQSM) are estimated to verify the performance of developed models. If the predictions are unbiased, the mean error (ME) should be almost zero. But due to its weaknesses due to its dependence on the scale of the data and its indifference to semi-variogram error, the mean error (ME) is usually normalized by the MSE, being theoretically zero.

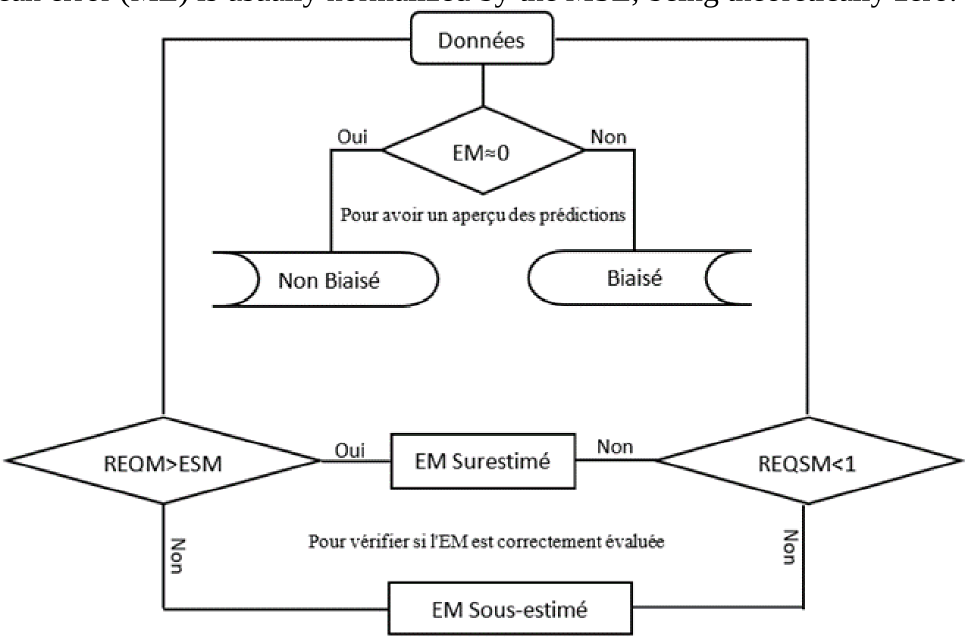

Figure 5. Diagram of the principle of selection of a semivariogram model

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The REQM and ESM values should be calculated to indicate whether the prediction errors are correctly evaluated if they are close. Otherwise, if the REQM is less than the ESM (or REQSM less than 1), then the variability of the predictions is overestimated; and if the REQM is greater than the ESM (or REQSM greater than 1), then the variability of the predictions is underestimated. Once the best model has been selected, it is used to draw the thematic map which provides the spatial distribution of the parameter to be estimated.

2.2.8 *Highlighting the best-fitting variogram model.* To highlight the influence of the semivariogram model on the kriging results, three semivariogram models (Gaussian, exponential and spherical) with the same nugget of effect (C0), same threshold (σ2), and same range (a) were used to interpolate the data by kriging. These semivariogram models are shown in Figure 6.

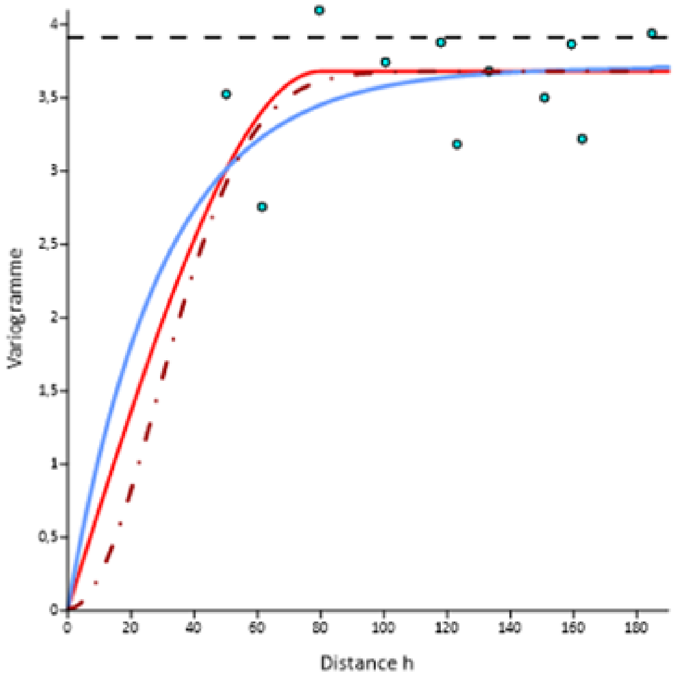

Figure 6. Analytical analysis differences between the three variogram models

3. Results

3.1 *Descriptive statistics.*

The database used consists of 64 values of electrical conductivity of the saturated paste CEps ranging from 3.69 to 14.43 (ds/m), with an average of 7.80 (ds/m) and a standard deviation (SD) of 1.98 (ds/m). No need to plot the histogram or the QQ plot to check the normality of the data. Indeed, Table 1 shows that the median is very close to the mean value. This indicates that the distribution of the data is egalitarian, that is to say, more or less normal.

Table 1 Descriptive statistics of the database

Setting	No.	Min	Max	Avg.	Median	Standard deviation	Coefficient asymmetry	Coefficient flattening
EC (ds/m)	64	3.69	14.43	7.80	7.56	1.98	0.63	0.96

3.2 Cross-validation.

Using the Gaussian model, the estimated electrical conductivity CEps oscillate between 6.86 and 9.42 (ds/m). The spherical model produces values between 7.01 and 9.21 (ds/m) while the exponential model provides a range of 6.95 to 8.97 (ds/m). In general, each model produced a

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different result from each other's. The difference can be at the ends of the range or its magnitude. These differences are summarized in Table 2.

Table 2. Analytical analysis differences between the three variogram models

	Gaussian	Exponential	Spherical
Minimum	6.86	6.95	7.01
Maximum	9.42	8.97	9.21
Extent	2.56	2.02	2.20

In addition, as to appreciate the operation of the cross-validation developed above, the well-known point value (7 (ds/m) value obtained at location P-30) was masked, then estimated using different semi-variogram models. The results summarized in Table 3 agree that the Gaussian model provides the most accurate estimate.

Table 3. Illustration of the cross-validation test

	Experimental (ds/m)	Estimated (ds/m)	Residual (ds/m)	Residual (%)	Remark
Gauss	7	7.48	0.48	+6.80	Very overrated
Spherical	7	7.58	0.58	+3.59	Slightly overestimated
Exponential	7	7.25	0.25	+8.29	Very overrated

4. Results discussions

In the particular case of this study, the values interpolated using the Gaussian, spherical and exponential models varied within the same range (6.9–9.5 (ds/m)). But in general, each semivariogram model provides a separate result. However, despite their observed differences, all thematic maps have the same variation trend. The minimum and maximum values are almost in the same regions respectively from one card to another. These observations are consistent with the results published by many other authors. It is therefore evident that the quality and reliability of a kriging interpolation strongly depend on the structure of the field data analysis, i.e., the semivariogram model. The predictive performance of the fitted models is verified on the basis of cross-validation tests.

Table 4 shows that the spherical model exhibits the best fit. This agrees well with Figure 7 which illustrates that the same (spherical) model fits the most with the experimental semi-variogram. Indeed, before being able to use this statistical method based on the theory of regionalized variables, one must create a semi-variogram model, which will determine the interpolation function.

Table 4. Analytical characteristics of variogram models

Residual value of Z	Characteristic	Gaussian	Exponential	Spherical
Average Error	EM	0.006	0.005	0.005
Root Mean Quadratic Error	REQM	1,942	1,949	1,932
Average Standard Error	ESM	1,957	1,964	1,947
Root Mean Standard Quadratic Error	REQSM	0.245	0.246	0.243
Mean Squared Error	EQM	3,770	3,798	3,731

However, kriging is optimal when the data are normally distributed and stationary, i.e., the mean and the variance do not vary significantly in space [40, 41, 42, 43, 44].

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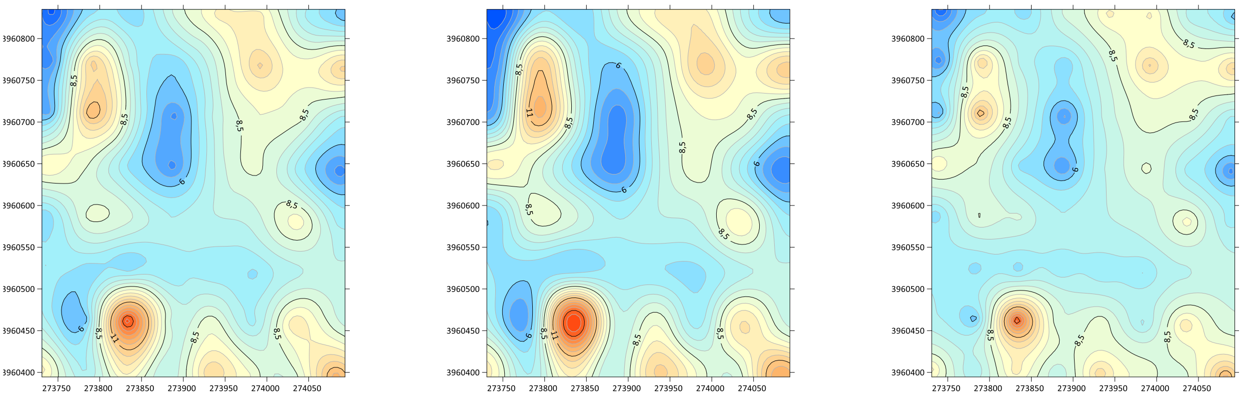

Figure 7. Thematic estimation maps produced using different variogram models (a / spherical model, b / Gaussian model, c / exponential model).

5. Conclusions

The most cited modeling, geo-spatialization, and interpolation software are ArcGIS from ESRI and Surfer from Gold Software. The operation of this software is based on deterministic and geostatistical interpolation techniques.

However, one cannot perform a continuous measurement, the parameters to be estimated are measured discretely, then in order to obtain continuous information, the kriging method is used.

This article discusses the question of selecting the appropriate semi-variogram model. It highlights the negative effects of the semi-variogram model on prediction or interpolation operations using the kriging technique.

A wrong choice of the semi-variogram model might distort the results of the evaluation, forecast, or prediction. In order to avoid this drawback, a method based on the calculation and analysis of EM, REQM, ESM, REQSM, and EQM is proposed and summarized in a recap graph (Figure 5). It is therefore necessary to apply it in a good manner for the cross-validation test in order to select the most appropriate semi-variogram model before the predictive analysis.

The present research contribution is expected to have various applications and impacts on the environment, soil shrinkage and swelling, soil stabilization parameters, influence on soil type, and therefore on seismic acceleration for the choice of appropriate binders used in the construction of reinforced concrete structures.

Nomenclature

EM	Average Error
ESM	Average Standard Error
EQM	Mean Quadratic Error
REQM	Root Mean Quadratic Error
N (h)	number of pairs of measurement points distant from h
z (x_i)	the value measured at measuring point x_j
C_0	nugget of effect
a	range

Greek symbols

γ	Semi variogram
σ^2	variance

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