GEOSTATISTICS KRIGING METHOD AS A SPECIAL CASE OF GEODETIC LEAST-SQUARES COLLOCATION

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***Abstract**: Modeling is a widespread method used for understanding the physical reality. Among the many applications of modeling are: determining the shape of the earth's surface, geological and geophysical studies, hydrology and hydrography. Modeling is realized through interpolation techniques such as kriging method and geodetic least-squares collocation. In this paper is presented a comparison between these two methods.*

***Keywords:** geostatistics, kriging, collocation*

1. Introduction

Kriging is a very popular method used in geostatistics to interpolate the value of a random field (or spatial stochastic process) from values at nearby locations.

Kriging estimator is a linear estimator because the predicted value is obtained as a linear combination of known values. This and the fact that kriging technique is based on the least-squares principle have made some authors [1] to call it optimal predictor or best linear predictor. Depending on the properties of the stochastic process or random field, different types of kriging apply.

Least-squares collocation is an interpolation method derived from geodetic sciences, first introduced by H. Moritz, for determining the earth's figure and gravitational field. Collocation method can be interpreted as a statistical estimation method combining least-squares adjustment and least-squares prediction

Another important component in estimation of a random field from discrete values measured or known in various spatial locations, is a parameter or function of the process which describes its spatial dependence. This parameter has a great influence over the interpolated values. This function is called *the variogram* of the spatial stochastic process.

2. Variogram

In geostatistics the variogram is a function describing the spatial correlation or dependence of a spatial stochastic process. Let

$$\operatorname{var}\left(Z(s_1)-Z(s_2)\right)=2\gamma(s_1-s_2) \tag{1}$$

for all spatial locations s_1, s_2 from the respective domain (field), where s_1-s_2 is the lag distance between any two spatial locations. The quantity 2γ has been called variogram, and respectively γ has been called semivariogram.

Experimental Variogram of a Stationary Process

Considering a spatial stationary process (process with unknown and constant mean) where we have observed values $Z(s_i)$ in spatial locations s_i, the experimental variogram is calculated from every pair of measured values with the formula below.

$$2\gamma_{ex} = \left(Z(s_i) - Z(s_j)\right)^2 \quad (2)$$

where $Z(s_i)$ and $Z(s_j)$ are two pairs of observed values.

The Variogram Estimator

Similar to the descriptive statistics we have to group the γ_{ex} values in classes according to lag distance s_i-s_j=D_{ij}. The variogram estimator is the averaged experimental variogram values from a certain class.

The lag distance *h*, of a class, is empirically determined [2] as the mean minimum distance between observed points:

$$h = \frac{1}{n}\sum_{i=1}^{n} \min(D_{ij}), \quad j=\overline{1,n}, \quad j \neq i \quad (3)$$

where *n* is the number of observed values.

Then the variogram estimator γ_E for a certain class *k* is:

$$\gamma_E^k = \frac{1}{n(k)}\sum_{i=1}^{n(k)} \gamma_{ex}^i(D_{ij}), \quad (h\text{-}1)k \leq D_{ij} \leq hk \quad (4)$$

where $n(k)$ is the number of γ_{ex} values in class *k* and $\gamma^i_{ex}(D_{ij})$, are the γ_{ex} values that fall in class *k*.

Now the lag distance D_E corresponding to the γ_E values is

$$D_E^k = \frac{1}{n(k)}\sum_{i=1}^{k} D_i, \quad (h\text{-}1)k \leq D_i \leq hk \quad (5)$$

where D_i are the distances that hold with the property on the right side of the Eq. (5).

If we plot the γ_E values with respect to the distances D_E, and also, on the same graph, the population variance *var(Z)*, the estimated (semi)variogram is obtained (see Fig. 1):

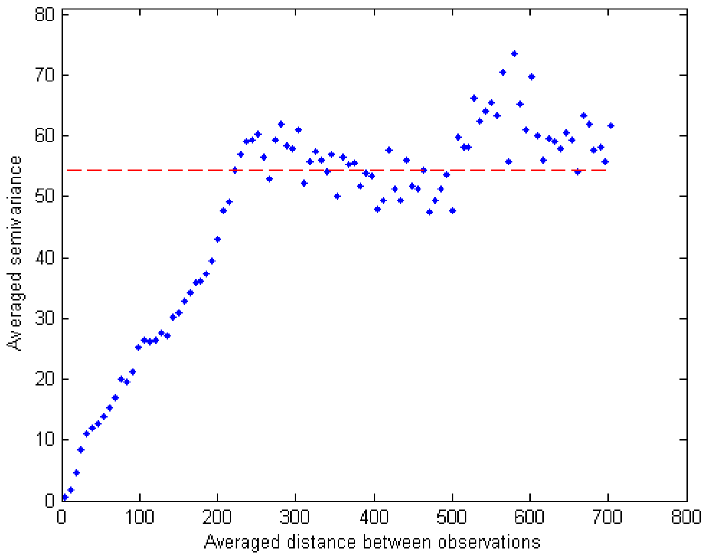

Fig. 1. The Estimated Semivariogram Plot and Population Variance

The figure indicates that the spatial process is correlated over short distances while there is no spatial dependency over long distances [3].

Variogram Model Fitting

Various variogram model fitting techniques had been proposed [1], [4]. Among them are distinguished methods based on least squares and maximum likelihood algorithm. Three models (linear, spherical and exponential) have been fitted over the semivariogram plot showed in Fig. 1. The models are shown in Fig. 2.

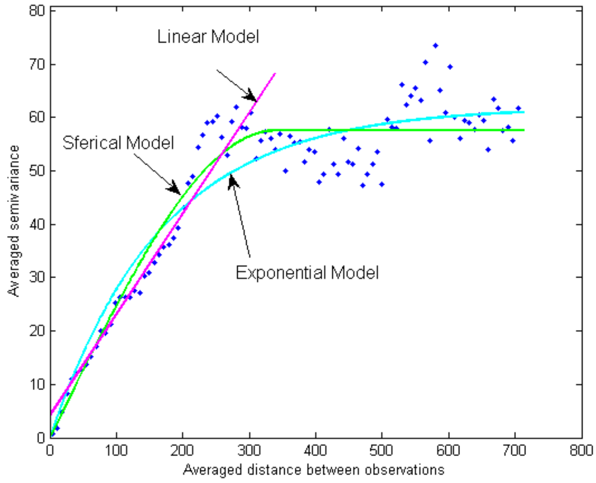

Fig. 2. Variogram Model Fitting

3. Ordinary Kriging

This section deals with the ordinary kriging estimation method.

Assumptions

Model assumption:

$$Z_i = \mu + \delta_i \tag{6}$$

Ordinary kriging assumes an unknown constant trend for the respective process. This is the case when the process is presumed to be stationary. In Eq. (6) this trend is represented by μ, which, as we said, is unknown but constant. δ from Eq (6) represent the signal of the process in the point *i*.

Predictor assumption:

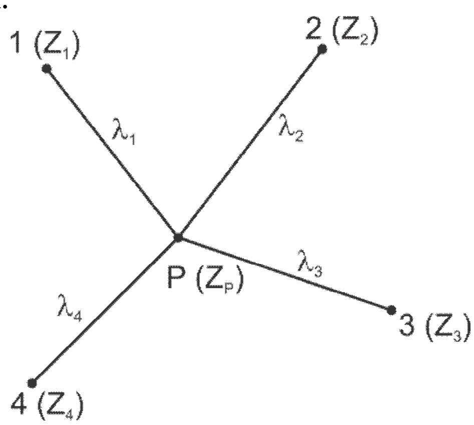

Fig. 3. Kriging Prediction

Kriging is a least squares estimation algorithm in which the predicted value of a process, in a location P, where no observations have been made (see Fig. 3), it is obtained with the Eq. below:

$$Z_P = \sum_{i=1}^{n} \lambda_i Z_i \tag{7}$$

where Z_P denotes the interpolated or predicted value of the stochastic process in the point P, Z_i are known values of the respective process in certain spatial locations and λ_i are the corresponding weights for Z_i values, satisfying the following condition:

$$\sum_{i=1}^{n} \lambda_i = 1 \tag{8}$$

the unknowns λ_i will satisfy the following system of linear equations:

$$\boldsymbol{\lambda} = \boldsymbol{\Gamma}^{-1}\left(\boldsymbol{\gamma} + \mathbf{1}\frac{1-\mathbf{1}'\boldsymbol{\Gamma}^{-1}\boldsymbol{\gamma}}{\mathbf{1}'\boldsymbol{\Gamma}^{-1}\mathbf{1}}\right) \tag{9}$$

where:

$$\boldsymbol{\Gamma} = \begin{pmatrix} \gamma(s_1-s_1) & \gamma(s_1-s_2) & \dots & \gamma(s_1-s_n) \\ \gamma(s_2-s_1) & \gamma(s_2-s_2) & \dots & \gamma(s_2-s_n) \\ \vdots & \vdots & \ddots & \vdots \\ \gamma(s_n-s_1) & \gamma(s_n-s_2) & \dots & \gamma(s_n-s_n) \end{pmatrix} \tag{10}$$

$$\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_n)' \tag{11}$$

$$\boldsymbol{\gamma} = (\gamma(s_0-s_1), \dots, \gamma(s_0-s_n))' \tag{12}$$

$$\mathbf{1} = (1, 1, \dots, 1)' \tag{13}$$

The matrix form of Eq. (7) is:

$$Z(s_0) = \boldsymbol{\lambda}'\mathbf{Z} \tag{14}$$

then, replacing (9) in (14) is obtained another Eq. for computing the predicted value:

$$Z(s_0) = \left(\boldsymbol{\gamma}' + \frac{1-\boldsymbol{\gamma}'\boldsymbol{\Gamma}^{-1}\mathbf{1}}{\mathbf{1}'\boldsymbol{\Gamma}^{-1}\mathbf{1}}\mathbf{1}'\right)\boldsymbol{\Gamma}^{-1}\mathbf{Z} \tag{15}$$

4. Least-Squares Collocation

Collocation is a data processing method which simultaneously performs regression (determining trend surface), filtering and spatial prediction [5].

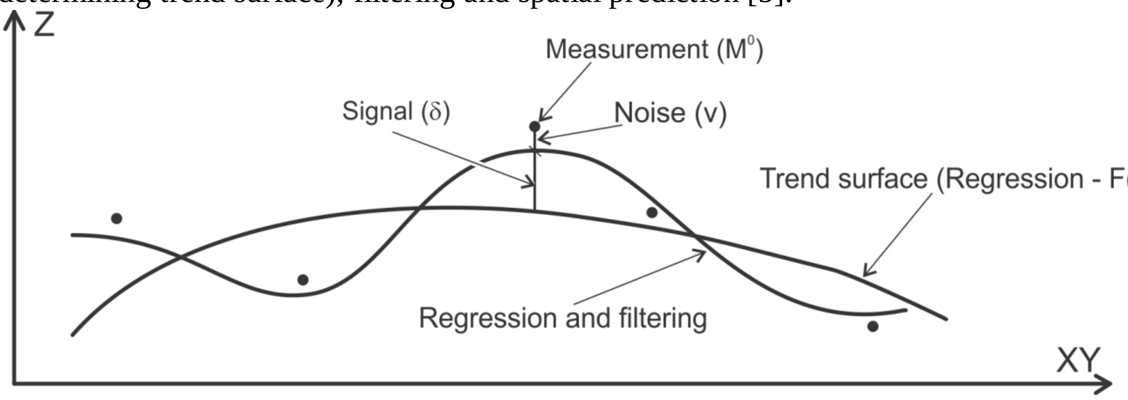

Fig. 4. Collocation

Collocation method assumes the fact that measurements consist of two components shown in Fig. 4:

- A systematic component (trend surface)
- A random component composed of *signal* (determined by local factors) and *noise* (caused by measurement errors).

Through collocation one can perform regression (determining the parameters of the trend surface), filtering (noise elimination), and prediction.

Functional model

$$M_i^0 + v_i = F_i(x_j) + \delta_i \tag{16}$$

$$\mathbf{Ax} - \mathbf{v} + \boldsymbol{\delta} + 0\boldsymbol{\delta}^0 = \mathbf{0} \tag{17}$$

where $\mathbf{v}$ is the noise, $\boldsymbol{\delta}$ is the signal in measured points and $\boldsymbol{\delta}^0$ is the signal in interpolation points. $\mathbf{x}$ contains trend surface parameters.

Notations:

$$\mathbf{B} = [\mathbf{-I}\ \mathbf{I}\ \mathbf{0}] \tag{18}$$

$$\mathbf{e} = \left(\mathbf{v}\ \boldsymbol{\delta}\ \boldsymbol{\delta}^0\right)' \tag{19}$$

With the notations (18) and (19), (17) becomes

$$\mathbf{Ax} + \mathbf{Be} + \mathbf{l} = \mathbf{0} \tag{20}$$

Stochastic model

Cofactor matrix form is:

$$\mathbf{Q} = \begin{pmatrix} \mathbf{Q_{ll}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_{\boldsymbol{\delta\delta}} & \mathbf{Q}_{\boldsymbol{\delta\delta}^0} \\ \mathbf{0} & \mathbf{Q}_{\boldsymbol{\delta}^0\boldsymbol{\delta}} & \mathbf{Q}_{\boldsymbol{\delta}^0\boldsymbol{\delta}^0} \end{pmatrix} \tag{21}$$

where $\mathbf{Q_{ll}}$ is the cofactor matrix for measured values:

$$\mathbf{Q}_{ll} = \begin{pmatrix} q_{l_1 l_1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & q_{l_n l_n} \end{pmatrix} \tag{22}$$

Cofactor matrix of the signal can be established on the basis of certain theoretical considerations. Such theoretical considerations may be the spatial dependence between certain locations, or, in other words, the semivariogram of the spatial process. Then

$$\mathbf{Q}_{\boldsymbol{\delta\delta}} = \begin{pmatrix} \gamma(s_1 - s_1) & \gamma(s_1 - s_2) & \dots & \gamma(s_1 - s_n) \\ \gamma(s_2 - s_1) & \gamma(s_2 - s_2) & \dots & \gamma(s_2 - s_n) \\ \vdots & \vdots & \ddots & \vdots \\ \gamma(s_n - s_1) & \gamma(s_n - s_2) & \dots & \gamma(s_n - s_n) \end{pmatrix} \tag{23}$$

where s_i denotes a spatial location where the value of the spatial stochastic process is known from measurements

$$\mathbf{Q}_{\boldsymbol{\delta\delta}^0} = \begin{pmatrix} \gamma(s_1 - s_1^0) & \gamma(s_1 - s_2^0) & \dots & \gamma(s_1 - s_m^0) \\ \gamma(s_2 - s_1^0) & \gamma(s_2 - s_2^0) & \dots & \gamma(s_2 - s_m^0) \\ \vdots & \vdots & \ddots & \vdots \\ \gamma(s_n - s_1^0) & \gamma(s_n - s_2^0) & \dots & \gamma(s_n - s_m^0) \end{pmatrix} \tag{24}$$

where s_i^0 refers to a spatial location where the value of the respective process is unknown but desired.

The parameter vector $\mathbf{x}$ and the vector that contains the signal in interpolation points $\boldsymbol{\delta}^0$ is obtained with the following Eq.:

$$\mathbf{x} = -\left(\mathbf{A}'\underline{\mathbf{Q}}^{-1}\mathbf{A}\right)^{-1}\mathbf{A}'\underline{\mathbf{Q}}^{-1}\mathbf{l} \tag{25}$$

$$\boldsymbol{\delta}^0 = -\mathbf{Q}_{\boldsymbol{\delta}^0\boldsymbol{\delta}}\underline{\mathbf{Q}}^{-1}(\mathbf{Ax} + \mathbf{l}),\ \text{where}\ \underline{\mathbf{Q}} = \mathbf{Q_{ll}} + \mathbf{Q}_{\boldsymbol{\delta\delta}} \tag{26}$$

The predicted values of the random field or process in spatial location s_0 where no measurements have been made will be:

$$Z(s_0) = A_0 x + \delta^0 \tag{27}$$

where A_o is vector which contains the coefficients for the trend surface parameters towards the spatial location s_0, so $A_o x$ is the value of the trend surface in considered spatial location.

5. Kriging as a particular case of collocation

In this section we will prove that ordinary kriging method is a particularization of the least-squares collocation under certain conditions.

If we neglect the measurements errors then:

$$\mathbf{Q_{ll}} = \mathbf{0} \tag{28}$$

Also we assume that the stochastic process or random field has an unknown constant trend. A process that holds this property, as we said in section 2, is called stationary process. The Eq. below is the mathematical expression of this property:

$$\mathbf{x} = \mu \tag{29}$$

In this case the design matrix has the following form

$$\mathbf{A} = (1,1,...,1)' \tag{30}$$

so,

$$\mathbf{Ax} = \mu \cdot \mathbf{1} \tag{31}$$

The measurements vector will be:

$$\mathbf{l} = (-Z_1, -Z_2, ..., -Z_n)' = -\mathbf{Z} \tag{32}$$

If we consider only one prediction point or one spatial location where we want to find the value of the process, then $\mathbf{Q_{\delta^0\delta}}$ matrix has the following form:

$$\mathbf{Q_{\delta^0\delta}} = (\gamma(s_0 - s_1) \quad \dots \quad \gamma(s_0 - s_n)) \tag{33}$$

so, from (33) and (12) we obtain:

$$\mathbf{Q_{\delta^0\delta}} = \boldsymbol{\gamma}' \tag{34}$$

From (23), (28) and (10) $\underline{\mathbf{Q}}$ matrix is given by:

$$\underline{\mathbf{Q}} = \mathbf{\Gamma} \tag{35}$$

Considering this particular case (31), (32), (34), (35), and the Eq. (26) and (27) the predicted value in spatial location s_0 is:

$$Z(s_0) = \mu - \boldsymbol{\gamma}'\mathbf{\Gamma}^{-1}(\mu \cdot \mathbf{1} - \mathbf{Z}) \tag{36}$$

or

$$Z(s_0) = \mu - \boldsymbol{\gamma}'\mathbf{\Gamma}^{-1}\mathbf{1} \cdot \mu + \boldsymbol{\gamma}'\mathbf{\Gamma}^{-1}\mathbf{Z} \tag{37}$$

The constant trend is given by (25):

$$\mu = \left(\mathbf{1}'\mathbf{\Gamma}^{-1}\mathbf{1}\right)^{-1} \mathbf{A}'\mathbf{\Gamma}^{-1}\mathbf{Z} \tag{38}$$

so, from (38) an (37), the predicted value in location s_0 is:

$$Z(s_0) = (1 - \boldsymbol{\gamma}'\mathbf{\Gamma}^{-1}\mathbf{1}) \cdot \left(\mathbf{1}'\mathbf{\Gamma}^{-1}\mathbf{1}\right)^{-1} \mathbf{1}'\mathbf{\Gamma}^{-1}\mathbf{Z} + \boldsymbol{\gamma}'\mathbf{\Gamma}^{-1}\mathbf{Z} \tag{39}$$

and, knowing that $\mathbf{1}'\mathbf{\Gamma}^{-1}\mathbf{1}$ is a scalar, we obtain the following Eq.

$$Z(s_0) = \left(\frac{(1 - \boldsymbol{\gamma}'\mathbf{\Gamma}^{-1}\mathbf{1})}{\mathbf{1}'\mathbf{\Gamma}^{-1}\mathbf{1}} \mathbf{1}' + \boldsymbol{\gamma}' \right) \mathbf{\Gamma}^{-1}\mathbf{Z} \tag{40}$$

Now, looking at (40) and (15) we realize that these are one and the same. So **kriging method is just a particular case of least-squares collocation**. This particular case is obtained considering the process stationary, and neglecting the measurement errors.

6. Case study

To verify the above results in practice, from a set of data, the surface model has been generated using both kriging and collocation method.

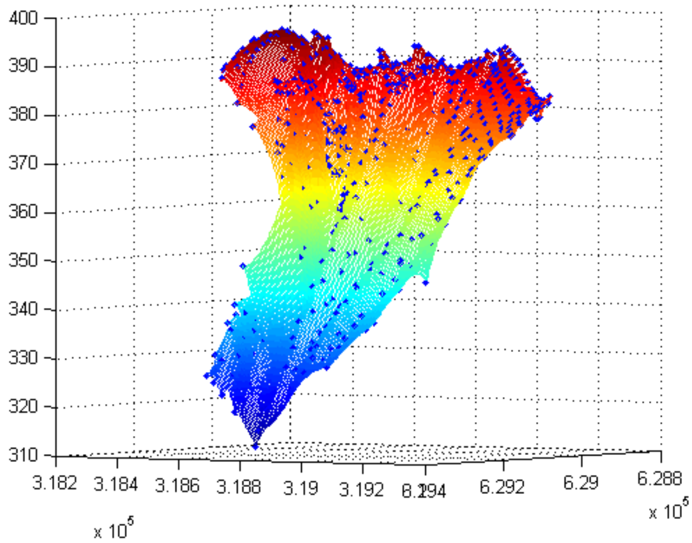

Fig. 5: Surface Model Generated using Kriging Method

In Fig. 5 is shown the surface model obtained by kriging method and in Fig. 6 is presented the surface generated using least-squares collocation. Note that the same linear variogram model had been used for the two methods. The variogram model was given by:

$$\gamma(h) = 1.3576 \cdot h \tag{41}$$

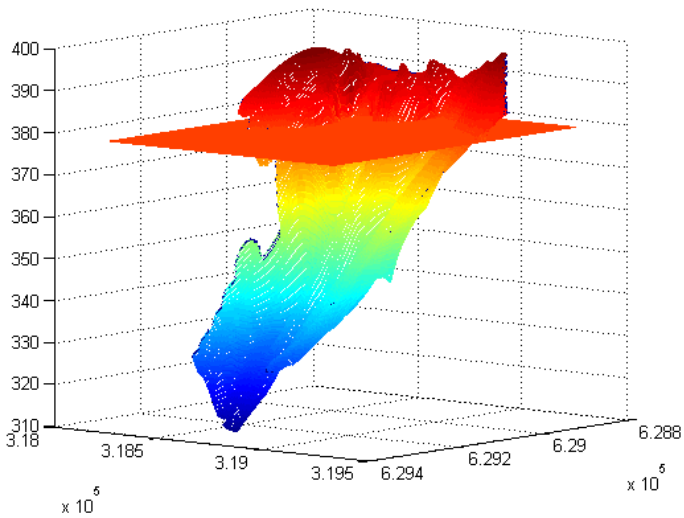

Fig. 6: Surface Model Generated using Least-Squares Collocation Method

In Fig. 6 is also represented a plane which is practically the trend surface determined by least-squares collocation. The trend surface is a constant one. This is a consequence of the stationarity condition which implies an unknown and constant mean μ for the respective process.

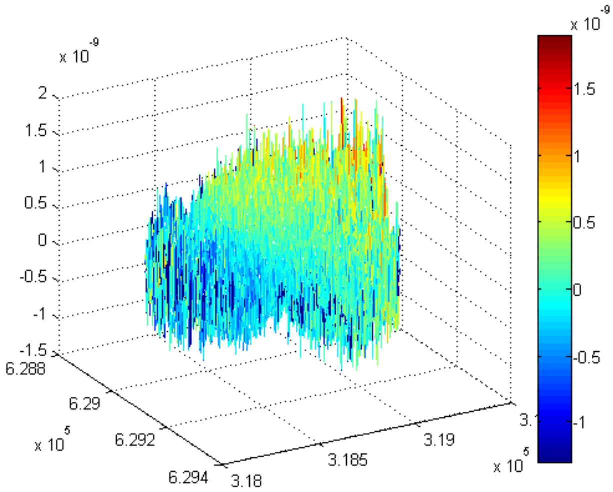

Fig. 7: The Differences in the Estimated Values

A plot of the differences in the values estimated using the two methods is represented in Fig. 7. As it can be seen the differences are of the order 10^{-9}. These values can be attributed to computational errors. So the theoretical considerations, that kriging is just a special case of least squares collocation, are confirmed in practice.

7. Conclusions

- Ordinary kriging is a very useful tool for surface modeling derived from geostatistics. The algorithm gives precise results and the input data is honored by the model. The algorithm requires a valid variogram model for the spatial process. Modeling the variogram is the most difficult stage in kriging estimation technique.
- Ordinary kriging method is a special case of the geodetic least-squares collocation. Several assumptions are made in order to derive kriging technique from least-squares collocation method. First is that *the process is considered stationary*, meaning that it has an unknown and constant mean. Second, and maybe most important, is that in kriging method *the measurement error is neglected*. Note that the same variogram model must be used for the two methods to coincide.

8. References

1. *N. A. Cressie, Statistics for Spatial Data, John Wiley & Sons, 1993.*
2. *R. Webster and M. A. Oliver, Geostatistics for Environmental Scientists (Statistics in Practice), New York: John Wiley & Sons, 2001.*
3. *M. H. Trauth, MATLAB® Recipes for Earth Sciences, Berlin: Spriger, 2006.*
4. *J.-P. Chiles and P. Delfiner, Geostatistics Modeling the Spatial Uncertanty, New York: John Wiley & Sons, 1999.*
5. *B. Hofmann-Wellenhof and H. Moritz, Physical Geodesy, Wien: Springer-Verlag, 2005.*