Direct Estimation of Trend Terms with Dual Kriging

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One of the most important problems in the geosciences is the problem of spatial prediction or spatial interpolation. Spatial predictions are often required for planning, risk assessment, and decision-making. Typical applications include determining the profitability of mining an orebody, producing a reservoir, management of soil resources, soil properties mapping, pest management, designing a network of environmental monitoring stations, etc. (Weisz et al, 1995; Gotway et al., 1996; Moyeed and Papritz, 2002).

The standard approach to the problem of spatial interpolation is kriging. Kriging is a well-proven methodology that provides the best linear unbiased estimate and its variance at the unsampled location. Kriging uses the spatial correlations provided by the variogram to calculate the weights of the sample values surrounding an unsampled location. The weights obtained from the kriging equations minimize the estimation variance and account for the spatial correlation between the surrounding samples and the estimation location (that is, closeness to the estimation location) and between sample themselves (that is, data redundancy).

Despite kriging estimates are usually calculated using weighted linear combination of the data in the local neighborhood of the estimation location (primal version of kriging), they can also be calculated based on covariance between data and an estimation location and a mean, that is, trend (dual version). In this paper we investigate the later approach to calculating kriging estimates, and dual kriging, in general. A FORTRAN code is prepared to calculate kriging with a trend estimate and variance in a dual form. Software implementation is illustrated with example.

Kriging in Primal Version

The simple kriging estimator predicts the value of the variable of interest $Z(\mathbf{u})$ at the estimation location $\mathbf{u}$ as a linear combination of neighboring observations $Z(\mathbf{u}_i),\ i=1,\ldots,n(\mathbf{u})$, (Journel and Huijbregts, 1978):

$$Z^*_{SK}(\mathbf{u}) = \sum_{i=1}^{n(\mathbf{u})} \lambda_i^{SK}(\mathbf{u}) Z(\mathbf{u}_i) + \left[1 - \sum_{i=1}^{n(\mathbf{u})} \lambda_i^{SK}(\mathbf{u})\right] m, \tag{1}$$

where m denotes the stationary mean, $\lambda = (\lambda_1(\mathrm{u}),\ldots,\lambda_n(\mathrm{u}))^T$ denotes the vector of the simple kriging weights calculated from the normal system of equations

$$\sum_{j=1}^{n(\mathrm{u})} \lambda_i^{SK}(\mathrm{u}) C_{i,j} = C_{i,0}, \quad i = 1,\cdots,n(\mathrm{u}), \tag{2}$$

where $C_{i,j},\quad i,j=1,\cdots,n(\mathrm{u}),$ denotes the data-to-data covariance values and $C_{i,0},\quad i=1,\cdots,n(\mathrm{u}),$ is the data-to-estimation point covariance values. The covariance function is calculated under stationarity through the semivariogram model $\gamma(\mathbf{h})$.

Simple kriging is the best linear unbiased estimator, that is, it provides estimates with minimum error variance $\sigma^2_{SK}(\mathbf{u})$ in the least square sense given by

$$\sigma^2_{SK}(\mathbf{u}) = C(0) - \sum_{i=1}^{n(\mathbf{u})} \lambda_i^{SK}(\mathbf{u}) C_{i,0} \tag{3}$$

Where $C(0)$ is the stationary variance.

Ordinary kriging is a common variant of kriging. It is believed to be a robust and reliable method of data interpolation (Yamamoto, 2005). The ordinary kriging estimator differs from simple kriging in that it constraints the sum of all weights to be 1. Specifically, it provides a model for the value of the variable of interest at the estimation location **u** as the following linear combination of the neighboring observations $Z(\mathbf{u}_i), i = 1, \dots, n(\mathbf{u}),$ (Journel and Huijbregts, 1978)

$$Z^*_{OK}(\mathrm{u}) = \sum_{i=1}^{n(\mathrm{u})} \lambda_i^{OK}(\mathrm{u}) Z(\mathrm{u}_i), \tag{4}$$

where $\lambda = (\lambda_1(\mathrm{u}), \dots, \lambda_n(\mathrm{u}))^T$ denote the vector of the ordinary kriging weights calculated from the following system of equations for the estimation location $\mathbf{u}$,

$$\begin{aligned} &\sum_{j=1}^{n(\mathbf{u})} \lambda_i^{OK}(\mathrm{u}) C_{i,j} + \mu^{OK}(\mathbf{u}) = C_{i,0}, \quad i = 1, \cdots, n(\mathbf{u}), \\ &\sum_{i=1}^{n(\mathbf{u})} \lambda_i^{OK}(\mathrm{u}) = 1, \end{aligned} \tag{5}$$

where $\mu_{OK}(\mathbf{u})$ is the Lagrange parameter and, as before, $C_{i,j}$, $i, j = 1, \cdots, n(\mathbf{u})$, denotes the data-to-data covariance values and $C_{i,0}$, $i = 1, \cdots, n(\mathrm{u})$, is the data-to-estimation point covariance values. The ordinary kriging estimator is also an exact interpolator. However, ordinary kriging provides estimates with larger error variance $\sigma^2_{OK}(\mathbf{u})$ than simple kriging,

$$\sigma^2_{OK}(\mathbf{u}) = C(0) - \sum_{i=1}^{n(\mathbf{u})} \lambda_i^{OK}(\mathbf{u}) C_{i,0} - \mu_{OK}(\mathbf{u}) \geq \sigma^2_{SK}(\mathbf{u}), \tag{6}$$

where $C(0)$ is the stationary variance.

Note that ordinary kriging is usually preferred to simple kriging in practical applications. This is because ordinary kriging does not require knowledge or assume stationarity of the mean over the entire region of interest. Ordinary kriging accounts for unknown or locally varying mean by limiting the region of stationarity to within the neighborhood centered at the location of interest. In general, it can be shown that OK estimates are larger than SK estimates in high-valued areas where the local mean is larger than the global mean; and OK estimates are smaller than SK estimates in lower-valued areas where the local mean is smaller than the global mean (Goovaerts, 1997).

Kriging with a Trend

The local estimation of the mean in ordinary kriging allows only accounting for global trend in the data over the study area. In some situation, however, it may be inappropriate to consider the local mean as a constant even within small local neighborhoods. Kriging with a trend models considers that the unknown local mean is a smoothly varying function of coordinates (Goovaerts, 1997):

$$m(\mathbf{u}) = \sum_{l=0}^{L} a_l f_l(\mathbf{u}), \tag{7}$$

where functions $f_l(\mathbf{u})$ are known functions of coordinates, but coefficients a_l are unknown and deemed constant within each local neighborhood, $l = 0, \dots, L.$ A kriging with a trend model for the value of the variable of interest at the estimation location **u** is the following linear combination of the neighboring observations $Z(\mathbf{u}_i), i = 1, \dots, n(\mathbf{u}),$ (Deutsch, lecture notes):

$$Z^*_{KT}(\mathbf{u}) = \sum_{i=1}^{n(\mathbf{u})} \lambda_i^{KT}(\mathbf{u}) Z(\mathbf{u}_i), \tag{8}$$

where $\lambda_i^{KT} = (\lambda_1(\mathrm{u}_1), \dots, \lambda_n(\mathrm{u}_n))^T$ denote the vector of the kriging with a trend weights calculated from the following system of equations for the estimation location $\mathbf{u}$,

$$
\begin{aligned}
&\sum_{i=1}^{n(\mathbf{u})} \lambda_i^{KT}(\mathbf{u}) C_{i,j} + \sum_{l=0}^{L} \mu_l f_l(\mathbf{u}_i) = C_{i,0}, \quad i = 1,\cdots,n(\mathbf{u}), \\
&\sum_{i=1}^{n(\mathbf{u})} \lambda_i^{KT}(\mathbf{u}) f_l(\mathbf{u}_i) = f_l(\mathbf{u}), \quad l = 0,\cdots,L,
\end{aligned}
\tag{9}
$$

where $R(\mathbf{u}) = Z(\mathbf{u}) - m(\mathbf{u})$ (for any location $\mathbf{u}$ in the study domain) is a residual data at location $\mathbf{u}$; $\mu_l,\ l = 0,\ldots,L,$ are the Lagrange parameters and, as before, $C_{i,j} \quad i, j = 1,\cdots,n(\mathbf{u}),$ denotes the residual-to-residual covariance values and $C_{i,0}, \quad i = 1,\cdots,n(\mathbf{u}),$ is the residual data-to-estimation point covariance values. Note that System (9) has a unique solution if and only if the L+1 trend functions are linearly independent (covariance function is assumed to be positive definite). Kriging with a trend estimator is an exact interpolator; the estimation (error) variance in kriging with a trend is

$$
\sigma_{KT}^2(\mathbf{u}) = C(0) - \sum_{i=1}^{n(\mathbf{u})} \lambda_i^{KT}(\mathbf{u}) C_{i,j} - \sum_{l=0}^{L} \mu_l f_l(\mathbf{u}), \tag{10}
$$

where $C_R(0)$ is the variance of residual data.

It is worth noting also that when L = 0, then kriging with a trend reduces to ordinary kriging (residual covariance is equal to data covariance when mean is constant); and it is assumed that beyond the data range the surface $Z(\mathbf{u})$ remains constant at level a_0 that needs to be estimated. Moreover, simple kriging can be also viewed as a special case of a kriging with a trend; here, it is assumed that beyond the data range the surface $Z(\mathbf{u})$ remains constant at level a_0 that is imposed prior to estimation.

Let us now rewrite kriging with a trend system (8)-(10) in the matrix form. First, however, let us introduce the following notation

- $\tilde{Z}(\mathbf{u})^T = [Z(\mathbf{u}_1),\ldots,Z(\mathbf{u}_n),0,0,\ldots,0]^T$ is an n+L+1 vector filled with data and zeros;
- $\lambda(\mathbf{u})^T = [\lambda_1(\mathbf{u}_1),\ldots,\lambda_n(\mathbf{u}_n),\mu_0,\mu_1,\ldots,\mu_L]^T$ is an n+L+1 vector of weights and Lagrange parameters;
- $c(\mathbf{u})^T = [C_{0,1},\ldots,C_{0,n},1, f_1(\mathbf{u}),\ldots, f_L(\mathbf{u})]^T$ is the right-hand side vector in system (9);
- $\mathbf{C}(\mathbf{u})$ is the left hand side matrix in system (9) give by

$$
\begin{aligned}
&\mathbf{C}_{ij} = C_{i,j}, \quad i, j = 1,\ldots,n; \\
&\mathbf{C}_{i,j+n} = f_j(\mathbf{u}_i), \quad i = 1,\ldots,n; \quad j = 0,\ldots,L; \\
&\mathbf{C}_{i+n,j} = f_i(\mathbf{u}_j), \quad i = 0,\ldots,L; \quad j = 1,\ldots,n; \\
&\mathbf{C}_{i+n,j+n} = 0, \quad i = 0,\ldots,L; \quad j = 0,\ldots,L.
\end{aligned}
$$

Then, kriging with a trend system (8)-(10) in the matrix form is as follows:

$$
Z_{KT}^*(\mathbf{u}) = \lambda(\mathbf{u})^T \tilde{Z}(\mathbf{u}); \tag{11}
$$

$$
\mathbf{C}(\mathbf{u}) \cdot \lambda(\mathbf{u}) = c(\mathbf{u}); \text{ or } \lambda(\mathbf{u}) = [\mathbf{C}(\mathbf{u})]^{-1} c(\mathbf{u}); \tag{12}
$$

$$
\sigma_{KT}^2(\mathbf{u}) = C_R(0) - \lambda(\mathbf{u})^T c(\mathbf{u}). \tag{13}
$$

Kriging in Dual Form

The matrix expression of kriging allows an interesting dual interpretation of kriging (Deutsch, lecture notes). First, let us note that it follows from (11)-(12):

$$
Z_{KT}^*(\mathbf{u}) = \lambda(\mathbf{u})^T \tilde{Z}(\mathbf{u}) = \left[[\mathbf{C}(\mathbf{u})]^{-1} c(\mathbf{u}) \right]^T \tilde{Z}(\mathbf{u}) = \tilde{Z}(\mathbf{u})^T [\mathbf{C}(\mathbf{u})]^{-1} c(\mathbf{u}). \tag{14}
$$

If we denote

$$
\varsigma(\mathbf{u})^T = \tilde{Z}(\mathbf{u})^T [\mathbf{C}(\mathbf{u})]^{-1}, \tag{15}
$$

where $\varsigma(\mathbf{u})^T = [d(\mathbf{u}_1),\ldots,d(\mathbf{u}_n),b_0,b_1,\ldots,b_L]^T$ is an n+L+1 vector of weights; then from (14):

$$Z_{KT}^{*}(\mathbf{u}) = \varsigma(\mathbf{u})^{T} c(\mathbf{u}) = \sum_{i=1}^{n(\mathbf{u})} d_i(\mathbf{u}) C_{i,0} + \sum_{l=0}^{L} b_l(\mathbf{u}) f_l(\mathbf{u}). \tag{16}$$

Equation (16) for calculating kriging with a trend estimate represents a dual version of kriging. In dual version, the kriging estimate $Z^{*}_{KT}(\mathbf{u})$ is a linear combination of the *n* covariances between residual data and the unsample location and the (*L*+1) trend functions $f_l(\mathbf{u})$. The weights $\varsigma^{T}(\mathbf{u})$ for the kriging with a trend estimate in a dual form are calculated from system (15), which can be rewritten in system format as:

$$\begin{aligned} &\sum_{i=1}^{n(\mathbf{u})} d_i(\mathbf{u}) C_{i,j} + \sum_{l=0}^{L} b_l f_l(\mathbf{u}_i) = Z(\mathbf{u}_i), \quad i = 1, \cdots, n(\mathbf{u}), \\ &\sum_{i=1}^{n(\mathbf{u})} d_i(\mathbf{u}) f_l(\mathbf{u}_i) = 0, \quad l = 0, \cdots, L. \end{aligned} \tag{17}$$

The estimation variance in dual form can be rewritten as:

$$\begin{aligned} \sigma_{KT}^{2}(\mathbf{u}) &= C_R(0) - \lambda(\mathbf{u})^{T} c(\mathbf{u}) = C_R(0) - \left[[\mathbf{C}(\mathbf{u})]^{-1} c(\mathbf{u})\right]^{T} c(\mathbf{u}) \\ &= C_R(0) - c(\mathbf{u})^{T} [\mathbf{C}(\mathbf{u})]^{-T} c(\mathbf{u}) = C_R(0) - c(\mathbf{u})^{T} [\mathbf{C}(\mathbf{u})]^{-1} c(\mathbf{u}). \end{aligned} \tag{18}$$

Moreover, the following can be noted from kriging equations in dual form:

- The dual expression for the kriging with a trend estimate can be read as

$$Z_{KT}^{*}(\mathbf{u}) = m^{*}(\mathbf{u}) + R^{*}(\mathbf{u}), \tag{19}$$

  where

$$m^{*}(\mathbf{u}) = \sum_{l=0}^{L} b_l(\mathbf{u}) f_l(\mathbf{u}); \tag{20}$$

$$R^{*}(\mathbf{u}) = \sum_{i=1}^{n(\mathbf{u})} d_i(\mathbf{u}) C_{i,0} \tag{21}$$

  It follows from (20) that the Lagrange parameters $b_l(\mathbf{u})$ of the dual system are the estimates of the unknown coefficients a_l of the trend $m(\mathbf{u}) = \sum_{l=0}^{L} a_l f_l(\mathbf{u}),$ that is, $b_l(\mathbf{u}) = [a_l(\mathbf{u})]^{*}.$. Moreover, because $b_l(\mathbf{u})$'s are kriging estimates, the estimate of the mean, $m^{*}(\mathbf{u}),$ is also a kriged estimate of the unknown value $m(\mathbf{u})$.

- The first *n* equations of the dual system can be seen as conditions for the interpolation function $Z^{*}_{KT}(\mathbf{u})$ to reproduce the data values at data locations:

$$Z_{KT}^{*}(\mathbf{u}_i) = \sum_{i=1}^{n(\mathbf{u})} d_i(\mathbf{u}_i) C_{i,0} + \sum_{l=0}^{L} b_i(\mathbf{u}_i) f_l(\mathbf{u}_i) = Z(\mathbf{u}_i). \tag{22}$$

  The last *L*+1 equations of the dual kriging are not yet clearly interpreted.

- If the estimation location is located far from any residual data, that is beyond the range of correlation($C(Z(\mathbf{u}_i), Z(\mathbf{u}\ )) = 0$, $i = 1, \ldots, n$), then the dual kriging estimate given in (16) becomes

$$Z_{KT}^{*}(\mathbf{u}) = \sum_{l=0}^{L} b_l(\mathbf{u}) f_l(\mathbf{u}) = m^{*}(\mathbf{u}); \tag{23}$$

  and the choice of the functions $f_l(\mathbf{u})$, $l = 0, \ldots, L,$ defines the functional form of the interpolated surface $Z^{*}_{KT}(\mathbf{u})$ in areas beyond the range of correlation. Since there is no data beyond the range of correlation, there is no validation of the trend extrapolation.

- In its primal version the kriging estimator is obtained by minimizing estimation variance. In its dual version the kriging interpolator is obtained as a weighted linear combination of the covariance interpolation functions and the trend functions.

Note also that for simple kriging the estimate in dual form is given by

$$Z^*_{SK}(\mathbf{u}) = \sum_{i=1}^{n(\mathbf{u})} d_i(\mathbf{u}) C_{i,0} + m_{SK}, \tag{24}$$

where m_{SK} is a known mean. For ordinary kriging the estimate in dual form is given by

$$Z^*_{OK}(\mathbf{u}) = \sum_{i=1}^{n(\mathbf{u})} d_i(\mathbf{u}) C_{i,0} + m_{OK} \tag{25}$$

where m_{OK} is ordinary kriging mean equal to coefficient $b_i(\mathbf{u})$ in (16).

Small Example

Let us consider the following small 1-D example. We have five data available for analysis, see Figure 1 below. The mean and variance of data is 5.2 and 1, respectively; the residual variogram model is assumed to be single structure spherical with a nugget effect of zero and range of correlation equal to 20. Consider now the problem of estimation the value at the unsampled location (12,2) using simple and ordinary kriging and kriging with a trend using both primal and dual formalisms.

Recall, that in the case of Simple Kriging, we assume the mean to be constant everywhere and equal to 5.2 (that is, mean of the data at hand). In the case of Ordinary Kriging, the mean is assumed to be constant, but unknown; in Kriging with a Trend, the mean is assumed to be a function of coordinates.

Figure 2 shows the ordinary kriging mean and kriging with a trend mean as a function of *X* coordinate. Note that both means were obtained using estimated weights assigned to the functions of coordinates in the dual form of kriging, see Section 3. Please not that the ordinary mean is a little higher is because of the string effect. The outlying samples can receive a significantly greater weight than central samples. (Deutsch, 1994)

Software Implementation

Program `kt3d` of GSLIB group (Deutsch and Journel, 1998) was modified in order to implement the dual formalism presented in section 3. The new parameter file for program `kt3d_dual` is presented below:

```
START OF PARAMETERS:
100data.dat                           ├file with data
0  1  2  0  3  0                      -   columns for DH,X,Y,Z,var,sec var
-1.0e21   1.0e21                      -   trimming limits
0                                     -option: 0=grid, 1=cross, 2=jackknife
xvk.dat                               -file with jackknife data
1   2   0    3    0                   -   columns for X,Y,Z,vr and sec var
0                                     -debugging level: 0,1,2,3
kt3d.dbg                              -file for debugging output
kt3d_newest.out                              -file for kriged output
50   0.5    1.0                       -nx,xmn,xsiz
50   0.5    1.0                       -ny,ymn,ysiz
1    0.5    1.0                       -nz,zmn,zsiz
1    1      1                         -x,y and z block discretization
10    10                                -min, max data for kriging
0                                     -max per octant (0-> not used)
20.0  20.0  10.0                      -maximum search radii
 0.0   0.0   0.0                      -angles for search ellipsoid
4     2.302                           -0=SK,1=OK,2=non-st SK,3=exdrift, 4=dual KT
1 1 0 1 1 0 1 0 0                     -drift: x,y,z,xx,yy,zz,xy,xz,zy
0                                     -0, variable; 1, estimate trend
none                                  -gridded file with drift/mean
1                                     -  column number in gridded file
1    0                                -nst, nugget effect
1    2.5  0.0   0.0   0.0             -it,cc,ang1,ang2,ang3
          12.0  12.0  10.0            -a_hmax, a_hmin, a_vert
```

Note that the only change in parameter file of the updated `kt3d` program is that option 4 was added to available kriging options. This option corresponds to kriging with a trend in dual form. When one are going to use the modified software, it should be use NOT standardized variance because the estimate are using the original variance. Also note that the output file obtained by executing dual kriging option contains 12 columns: first two columns inform on the kriging estimate and estimation variance; next 10 column give the estimates of the unknown coefficients $a_l, l = 0,\ldots,L$ for constant and drifts in x, y, z, xx, yy, zz, xy, xz, and yz, where x,y and z are coordinates of locations. Moreover, it is worth mentioning that this newest version of the kt3d (kt3d_dual) does not consider secondary drift file in estimation; the mean in kriging with a trend (dual and primal version) is estimated solely as a function of coordinates.

Case Study

In total, there are 310 samples within a 2D rectangular project area extending 3km in the Easting *X* direction (longitude) and 5km in the Northing *Y* direction (latitude) available for analysis. These samples are in normal score units. The location map of the Gaussian values together with their histogram is given in Figure 3. The experimental omnidirectional variogram of the data together with its fit (isotropic spherical with nugget effect of zero and range of correlation 1450 meters) is shown in Figure 4. This variogram will be used as an approximation to a residual variogram in kriging with a trend approach.

A new program kt3d_dual was applied to calculate the estimates at the unsampled locations in the study domain, estimates of the coefficients in a trend and a trend itself in the dual kriging framework. In our analysis, we consider the mean to be function of x, y and xy coordinates; 10 to 20 data are used in estimation of each location in the study domain; search radii are defined based on the variogram range.

Figure 5 shows the dual kriging with a trend estimate and primary estimation for the study domain. From the figure one can see that the results of the dual and primal kriging versions are the same. Figure 6-8 shows the estimated coefficients for a constant and drift terms with different search strategy. Please note from these figures the coefficients for a constant over a study domain are relatively large compared to other coefficients, Finally, figure 7 shows the estimated trend.

Conclusions

In this paper a dual formalism for kriging with a trend was derived and investigated. A methodology for calculating the dual kriging estimates, coefficients for the trend represented as a smoothly varying function of coordinates and a trend itself was presented and illustrated with a small example. A FORTRAN program called kt3d_dual was prepared for performing kriging in a dual form. Software implementation was illustrated using a case study.

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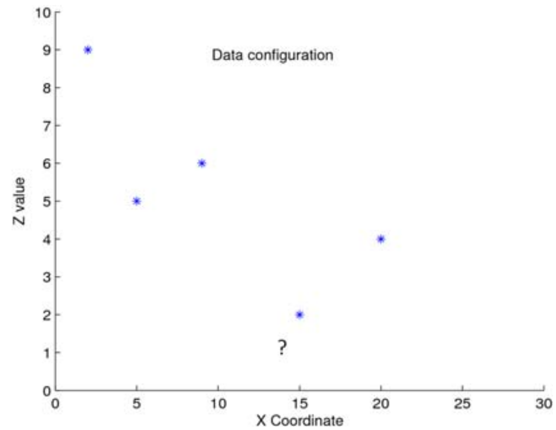

Figure 1: Data configuration for a 1-D example.

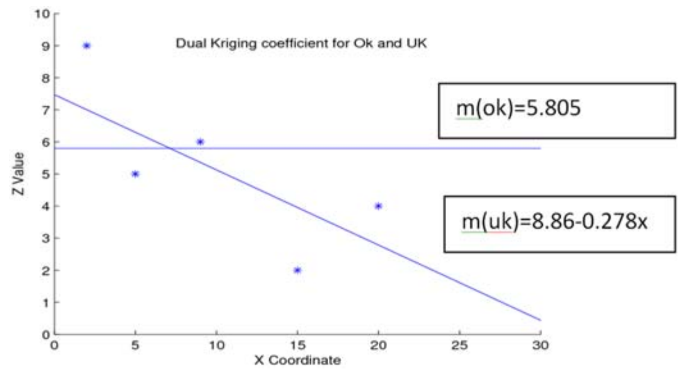

Figure 2: Mean as a function of the X coordinate for the ordinary kriging and kriging with a trend from dual formalism.

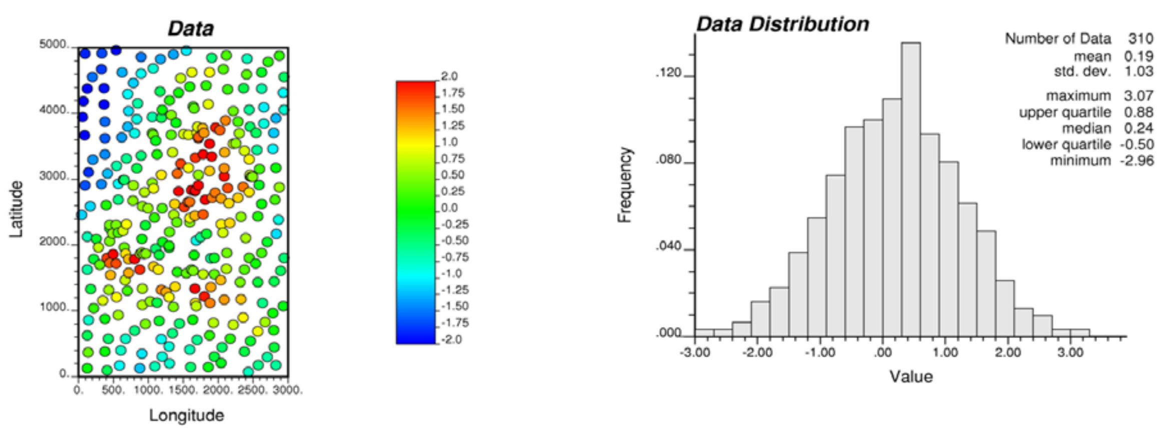

Figure 3: Location map of 310 samples together with their distribution.

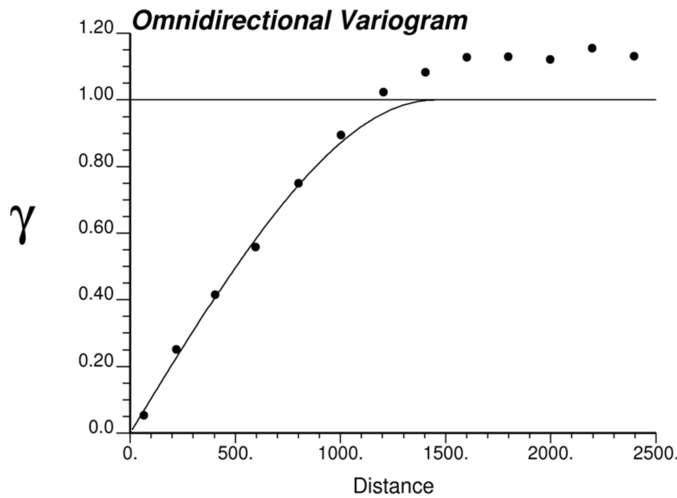

Figure 4: Experimental omnidirectional variogram (points) together with its variogram fit for 310 samples in the study domain.

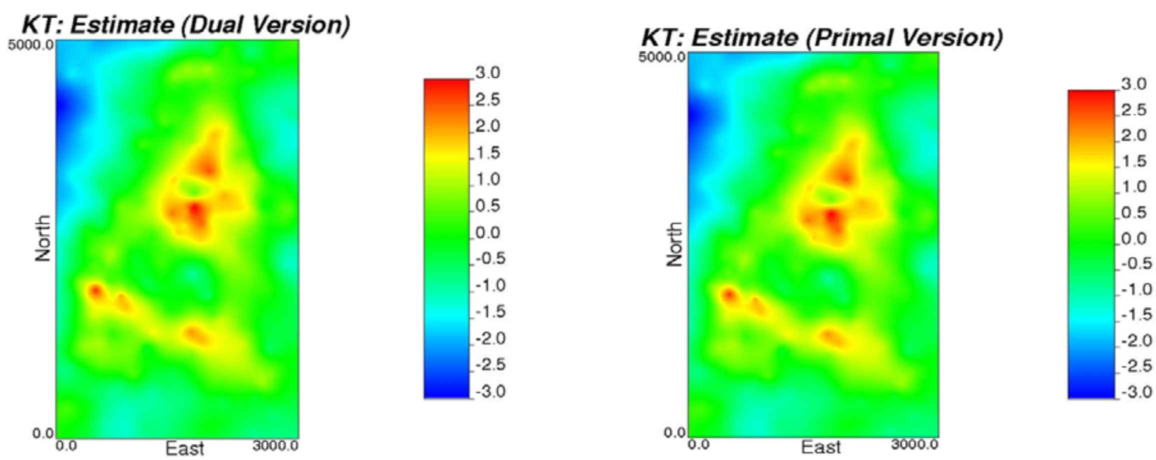

Figure 5: The dual kriging with a trend estimate compared with the primary form

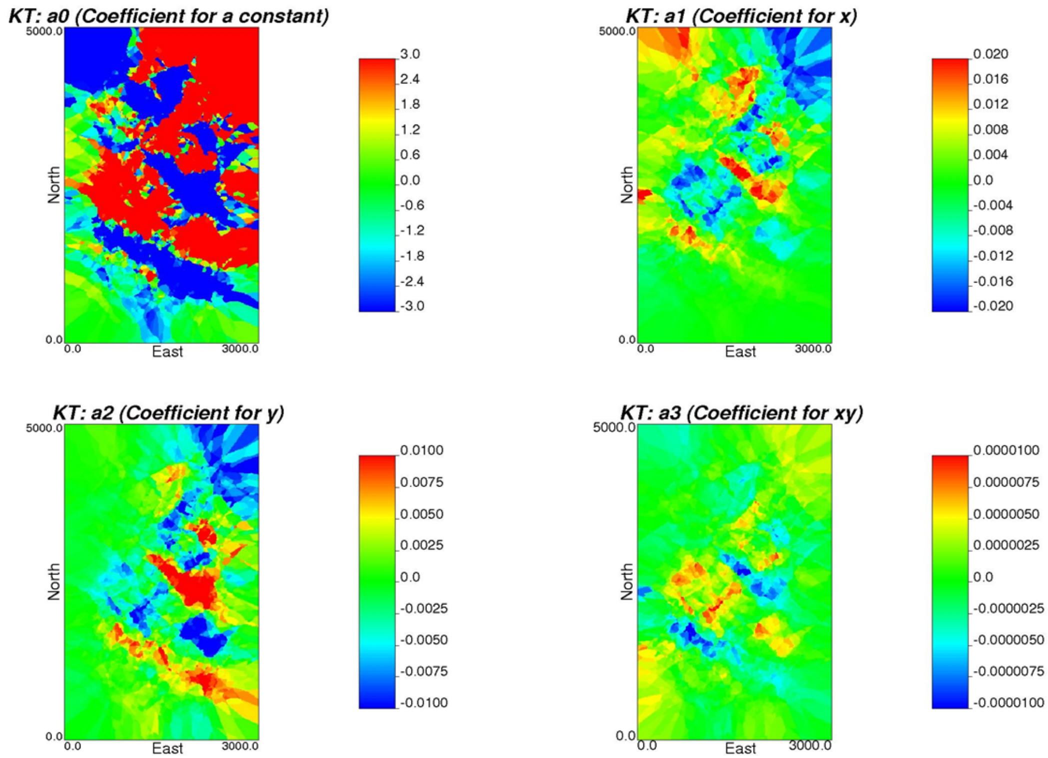

Figure 6: Estimated coefficients for a constant and drift terms in x, y and xy with 20 as its max kriging data.

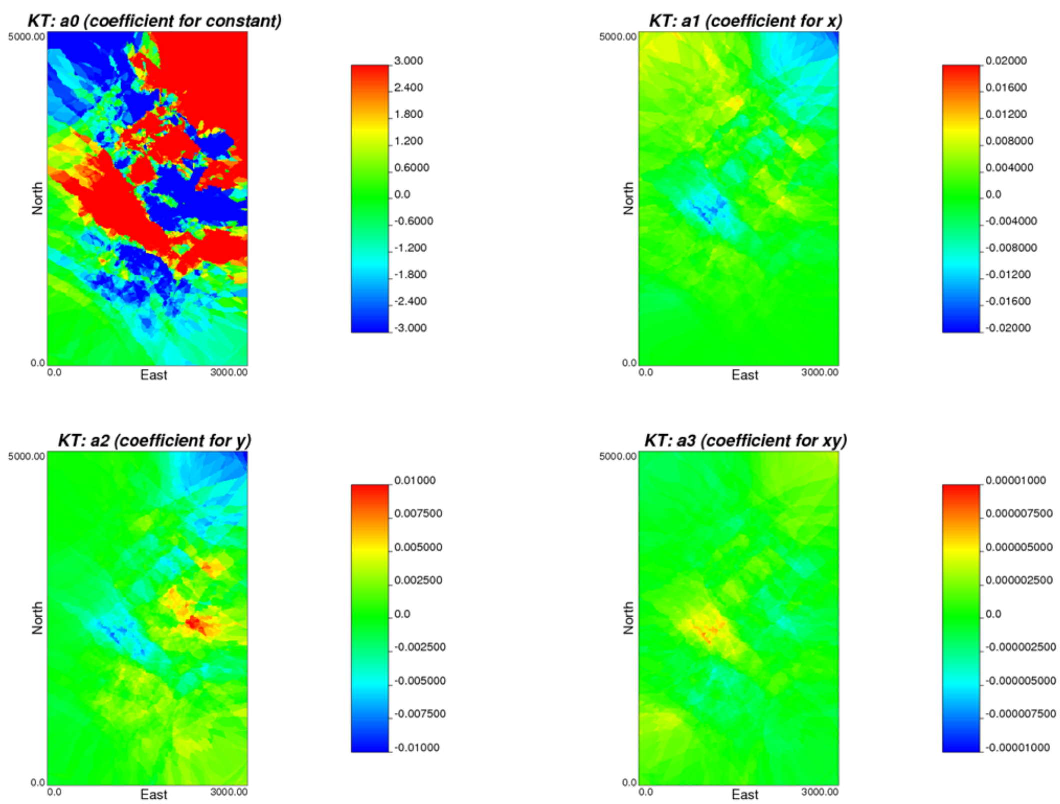

Figure 7: Estimated coefficients for a constant and drift terms in x, y and xy with 40 as its max kriging data.

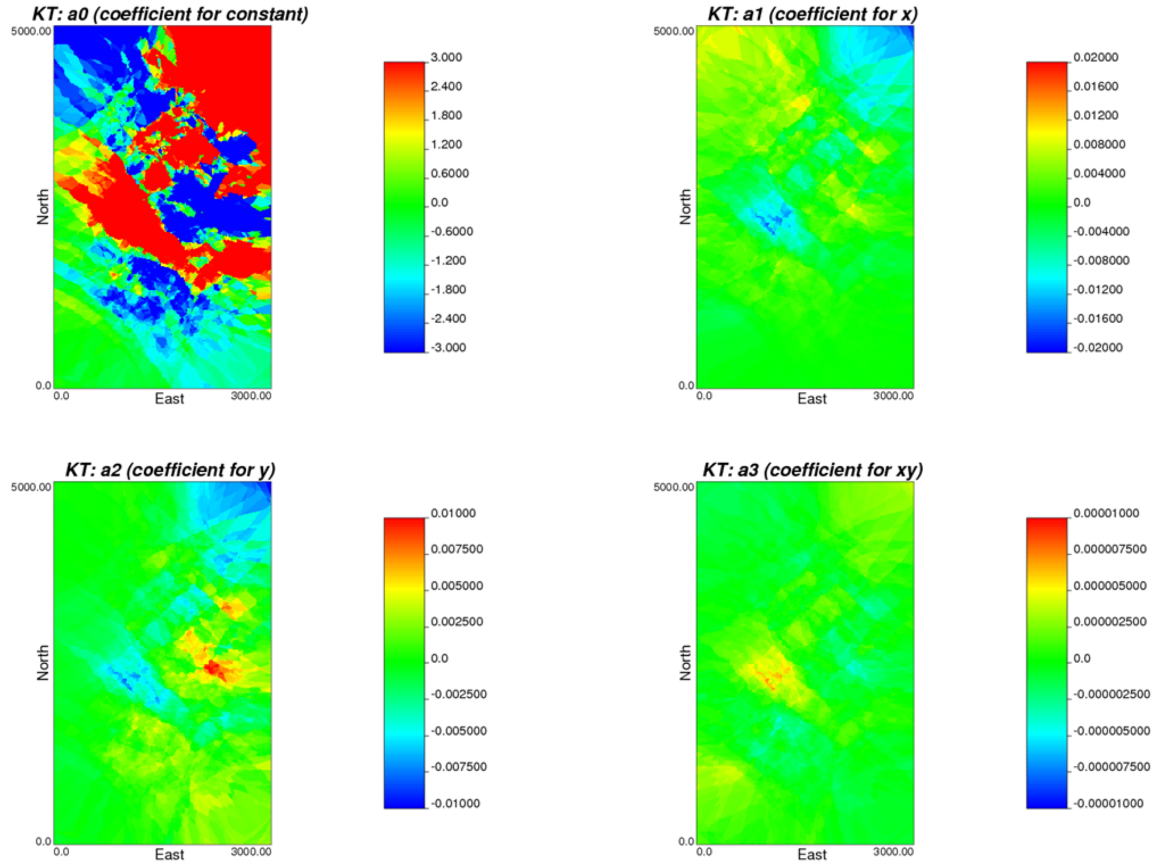

Figure 8: Estimated coefficients for a constant and drift terms in x, y and xy with 80 as its max kriging data.

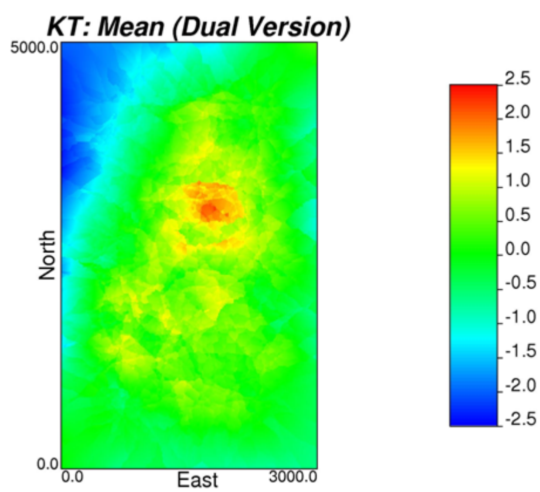

Figure 9: Estimated trend.