Successive Kriging for Estimation and Simulation in a Finite Domain

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*A longstanding problem in geostatistics is that kriging assigns end samples in strings of data unreasonably large weights. These weights are theoretically valid, but suboptimal estimates may result when there are geological trends in the variable near contacts. A number of ad-hoc corrections exist each with pros and cons; none are fully automatic with a well defined measure of optimality. A new method for estimation in a finite domain is proposed. This method is referred to as Finite Domain Kriging. The method is based on kriging with a successively larger number of data. The total number of relevant data (*n*) are established, then* n *kriging matrices are solved. The first matrix has the closest single data value (*n-*1 weights are set to zero), the second has the two closest data (*n-*2 weights are set to zero), and so on. The final matrix has all* n *data. The kriging weights used for estimation are the average of the weights from the* n *successive kriging runs. Each kriging run is optimal, yet with different smoothing and a different treatment of data at the end of strings. The result is a set of weights that does not give undue influence to data values at the end of strings. The methodology is developed for one string and for multiple strings with examples. Cross validation shows that Finite Domain Kriging out performs kriging with all data used in one step.*

Introduction

Stochastic simulation has become a powerful tool in many areas of natural resources characterization. It is widely used to quantify uncertainty in energy and mineral resources such as natural gas, oil and coal. Other applications consist of generating input for flow simulation and calculating the likelihood of exceeding critical threshold in contamination studies. Geostatistical simulation relies on kriging to model local conditional distributions. Simulation is performed by drawing from such conditional distributions.

An implicit assumption of kriging is that the study area is embedded within an infinite domain. This causes kriging to give much higher weights to end samples in strings of data. Despite the overweighting of the boundary samples is theoretically valid, this 'string effect' of kriging can cause serious problems when estimating variables of interest. Strings of data are often observed in mining and petroleum applications where the data are collected along wells or drillholes. The artifact weighting of boundary samples can result in biased estimation, especially when the data exhibits strange trends with boundary/border effects.

A number of ad-hoc solutions have been proposed for the 'string effect' of kriging. The most common are to extend the string or wrap the string (Deutsch, 1992, 1993). These approaches attempt to fix the string effect either by changing the data configuration or the covariance function. They do not yield significant improvement in the results. Recently a new *Distance Constrained* approach was also proposed by Babak and Deutsch (2006). Despite the fact that this approached removes large weights for end samples, it introduces many constraints that may lead to suboptimal estimation.

A new approach is introduced to correct the string effect. The method is referred to as Finite Domain Kriging. The problem of kriging with strings of data is explained. The new methodology is developed. Case studies are then shown to illustrate the method.

Finite Domain Kriging: Single String Case

Let us consider n adjacent data $i=1,\dots,n,$ at locations $u_i,\ i=1,\dots,n,$ aligned in a string. Consider now the problem of estimating the value of a variable of interest X at an unsampled location u^* using the proposed Finite Domain Kriging approach. The Finite Domain Kriging modifies the 'traditional' Kriging techniques in that it performs particular type of Kriging (Ordinary Kriging or Simple Kriging) as many times as there are conditioning data, that is, *n*. Each time *k*, $k=1,\ldots,n,$ kriging is performed based on the k closest data from the string. After assembling all *n* estimates by kriging, a Finite Domain Kriging estimator is taken as an average of them. Due to the fact that each of the *n* Kriging estimators is optimal, resulting Finite Domain Kriging estimator is also an optimal estimator. Let us now formulate Finite Domain Kriging approach mathematically.

Finite Domain Simple Kriging (FDSK)

The Finite Domain Simple Kriging (FDSK) provides a model of the unsampled value $X(\mathbf{u})$ as the following linear combination of the data in a string $X_i = X(\mathbf{u}_i),\ i=1,\ldots,n,$ and the population mean *m*

$$X_{FDSK}{}^{*} = \frac{1}{n}\sum_{k=1}^{n}\left[\sum\nolimits_{i=1}^{k}\lambda_i^k X_i^k + \left(1-\sum\nolimits_{i=1}^{n}\lambda_i^k\right)m\right] \tag{1}$$

where $X^k = (X_1^k,\ldots,X_k^k)$, $k=1,\ldots,n,$ denotes the vector of *k* closest data in a string to the estimation location $\mathbf{u}$; $\lambda^k = (\lambda_1^k(\mathbf{u}),\ldots,\lambda_k^k(\mathbf{u}))^T$, $k=1,\ldots,n,$ denotes the vector of the Simple Kriging weights calculated from the normal system of equations for the estimation location $\mathbf{u}$ based on the *k* closest data in the sting

$$\sum_{i=1}^{k}\lambda_i^k(\mathbf{u})Cov(X_i^k(\mathbf{u}_i), X_i^k(\mathbf{u}_j)) = Cov(X(\mathbf{u}), X_i^k(\mathbf{u}_j)), \quad j=1,\cdots,k, \tag{2}$$

where $Cov(X(\mathbf{u}_i), X(\mathbf{u}_j)),\quad i,j=1,\cdots,k,\quad k=1,\ldots,n,$ denotes data-to-data covariance function and $Cov(X(\mathbf{u}), X_i^k(\mathbf{u}_j))$ is data-to-estimation point covariance function.

Because the Finite Domain Simple Kriging estimator is the linear combination of the Simple Kriging estimators each of which is linear unbiased estimator and exact interpolator; Finite Domain Simple Kriging estimator is also a linear unbiased estimator and it is an exact interpolator. The variance of the Finite Domain Simple Kriging estimate at the estimation location **u** can be calculated as

$$\begin{aligned}
\sigma_{FDSK}^2(\mathbf{u}) &= Var(X_{FDSK}{}^{*}) = Var\left\{\frac{1}{n}\sum_{k=1}^{n}\left[\sum\nolimits_{i=1}^{k}\lambda_i^k X_i^k + \left(1-\sum\nolimits_{i=1}^{n}\lambda_i^k\right)m\right]\right\} \\
&= Var\left\{\frac{1}{n}\sum_{k=1}^{n}\sum_{i=1}^{k}\lambda_i^k X_i^k\right\} + Var\left\{\frac{1}{n}\sum_{k=1}^{n}\left(1-\sum\nolimits_{i=1}^{n}\lambda_i^k\right)m\right\} \\
&= Var\left\{\frac{1}{n}\sum_{k=1}^{n}\sum_{i=1}^{k}\lambda_i^k X_i^k\right\} = \frac{1}{n^2}\sum_{k=1}^{n}\sum_{i=1}^{k}\sum_{l=1}^{n}\sum_{j=1}^{k}Cov(\lambda_i^k X_i^k, \lambda_j^l X_j^l) \\
&= \frac{1}{n^2}\sum_{k=1}^{n}\sum_{i=1}^{k}\sum_{l=1}^{n}\sum_{j=1}^{l}\lambda_i^k\lambda_j^l Cov(X_i^k(\mathbf{u}), X_j^l(\mathbf{u})).
\end{aligned} \tag{3}$$

This could easily be solved by considering the standard estimation variance equation and average weights.

Finite Domain Ordinary Kriging (FDOK)

The Finite Domain Ordinary Kriging (FDOK) provides a model of the unsampled value $X(\mathbf{u})$ as the following linear combination of the data in a string $X_i = X(\mathbf{u}_i),\ i=1,\ldots,n,$

$$X_{FDOK}* = \frac{1}{n}\sum_{k=1}^{n}\sum_{i=1}^{k}\lambda_i^k X_i^k, \tag{4}$$

where $X^k = (X_1^k,\ldots,X_k^k)$, $k = 1,\ldots,n,$ denotes the vector of k closest data in a string to the estimation location $\mathbf{u}$; $\lambda^k = (\lambda_1^k(\mathbf{u}),\ldots,\lambda_k^k(\mathbf{u}))^T$, $k = 1,\ldots,n,$ denotes the vector of the Ordinary Kriging weights calculated from the normal system of equations for the estimation location $\mathbf{u}$ based on the k closest data in the sting

$$\sum_{i=1}^{k}\lambda_i^k(\mathbf{u})Cov(X_i^k(\mathbf{u}_i), X_i^k(\mathbf{u}_j)) + \mu = Cov(X(\mathbf{u}), X_i^k(\mathbf{u}_j)), \quad j = 1,\cdots,k, \tag{5}$$

$$\sum_{i=1}^{k}\lambda_i^k(\mathbf{u}) = 1, \tag{6}$$

where μ is a Lagrange multiplier, $Cov(X(\mathbf{u}_i), X(\mathbf{u}_j)), \quad i, j = 1,\cdots,k, \quad k = 1,\ldots,n,$ denotes data-to-data covariance function and $Cov(X(\mathbf{u}), X_i^k(\mathbf{u}_j))$ is data-to-estimation point covariance function. The covariance function is calculated under assumption of stationarity though the semivariogram model.

Because the Finite Domain Ordinary Kriging estimator is the linear combination of the Ordinary Kriging estimators, each of which is a linear unbiased estimator and exact interpolator; Finite Domain Simple Kriging estimator is also a linear unbiased estimator and it is an exact interpolator. The variance of the Finite Domain Simple Kriging estimate at the estimation location **u** can be calculated in the same way as was calculated for the Finite Domain Simple Kriging estimator and is given by

$$\begin{aligned}
\sigma_{FDOK}^2(\mathbf{u}) &= Var(X_{FDOK}*) = Var\left\{\frac{1}{n}\sum_{k=1}^{n}\left[\sum_{i=1}^{k}\lambda_i^k X_i^k + \left(1-\sum_{i=1}^{n}\lambda_i^k\right)m\right]\right\} \\
&= Var\left\{\frac{1}{n}\sum_{k=1}^{n}\sum_{i=1}^{k}\lambda_i^k X_i^k\right\} + Var\left\{\frac{1}{n}\sum_{k=1}^{n}\left(1-\sum_{i=1}^{n}\lambda_i^k\right)m\right\} \\
&= Var\left\{\frac{1}{n}\sum_{k=1}^{n}\sum_{i=1}^{k}\lambda_i^k X_i^k\right\} = \frac{1}{n^2}\sum_{k=1}^{n}\sum_{i=1}^{k}\sum_{l=1}^{n}\sum_{j=1}^{k}Cov(\lambda_i^k X_i^k, \lambda_j^l X_j^l) \\
&= \frac{1}{n^2}\sum_{k=1}^{n}\sum_{i=1}^{k}\sum_{l=1}^{n}\sum_{j=1}^{l}\lambda_i^k\lambda_j^l Cov(X_i^k(\mathbf{u}), X_j^l(\mathbf{u})).
\end{aligned} \tag{7}$$

Once again, this could more easily be solved by considering the average weights.

Small Examples: Structure of the Finite Domain Kriging Weights

To compare the kriging weights obtained using the 'traditional' Kriging with the Finite Domain Kriging approaches several small studies were performed. The weights were calculated for four estimation locations, (1, 7), (1.8, 7), (2.8, 7) and (3.8,7), based on the string of 7 data located at (1,0), (2,0), (3,0), (4,0), (5,0), (6,0) and (7,0), respectively. Isotropic spherical variograms with a contribution of one and ranges of correlation 2 and 20 are considered for analysis. Results for the weights are shown in Figure 1 for comparison of the Ordinary Kriging and the Finite Domain Ordinary Kriging data weights and in Figure 2 for comparison of the Simple Kriging and the Finite Domain Simple Kriging weights.

Figures 1 and 2 show that both Finite Domain Kriging approaches significantly reduce the artificially higher weights given to the end samples of the sting. Furthermore, also note that when the estimation location is located far from the data in the string (outside of the range of correlation), the Finite Domain Simple Kriging results in the same weights and estimate as Simple Kriging. Moreover, note the smoothness of the Finite Domain Kriging weights. The ad hoc distance constrained correction proposed for string affect removal by Babak and Deutsch (2006) resulted in very non-smooth weights, see Figures 3 and 4. The smoothness in the structure of the Finite Domain Kriging weights is connected to the theoretical basis of the approach.

Structure of the Finite Domain Kriging Weights for the Infinite String

Finite Domain Kriging has a very interesting property. If we consider estimation at a particular location based on a very long string of data ('infinite'), we can observe that at some point it becomes irrelevant weather you use the whole string of data or just portion of it. That is, Finite Domain Kriging weights assigned to the 'infinite' string of data will be the virtually the same as assigned to its substring and zeros for the rest of the data in a string of data. Mathematically we can write that there exists number *l* of closest data in the 'infinite' string to the estimation such that the following inequality holds

$$\left[\sum_{i=k}^{k+l}(\lambda_i - \tilde{\lambda}_i)^2 + \sum_{i<k \text{ or } i>k+1}\lambda_i^{\,2}\right] < \varepsilon, \qquad (8)$$

where $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_n)^T$ is the *n* by 1 vector of weights assigned to the 'infinite' string, $\tilde{\lambda} = (\tilde{\lambda}_k, \tilde{\lambda}_{k+1}, \ldots, \tilde{\lambda}_{k+l})^T$ is the *l* by 1 vector of weights assigned to the *l* closest data in the string to the estimation location; and ε is a very small value, say $\varepsilon = 0.0001$. Further we will refer to property (8) of the Finite Domain Kriging as convergence property.

To illustrate this convergence property, the following small case study was conducted. A string of 3000 data located at (1,0), (2,0), …, (3000,0), respectively, was considered for estimation of location (100,7) using Finite Domain Kriging techniques based on a Spherical variogram model with the range of correlation 500. Finite Domain Kriging was performed using 25, 100, 250, 500, 1000, 1500 and 3000 closest samples (the whole string) in the string. Figure 5 shows the resulting change in the structure of the Finite Domain Simple Kriging weights with respect to the number of closest data. Note that there is virtually no difference in Finite Domain Simple Kriging weights when performing estimation based on 1500 (half string) or more data or full 'infinite' string. Specifically, the difference in the left hand side of inequality (8) for Finite Domain Simple Kriging weights calculated based on the full string of 3000 data and 1500 data is less than 5.1169e-006. The difference in the left hand side of inequality (8) for all considered number of data in the Finite Domain Simple kriging estimation are given in the table below

25 data	100 data	250 data	500 data	1000 data	1500 data
0.0061	0.0025	0.0023	0.0008	0.0007	0.0000

Figure 5 also shows the change in the structure of the Finite Domain Ordinary Kriging weights with respect to the number of closest data. Looking at Figure 5 we can see that there is virtually no difference in Finite Domain Ordinary Kriging weights when performing estimation based on 1500 (half string) or more data or full 'infinite' string. Specifically, the difference in the left hand side of inequality (8) for Finite Domain Ordinary Kriging weights calculated based on the full string of 3000 data and 1500 data is less than 5.2874e-006. The difference in the left hand side of inequality (8) for all considered number of data in the Finite Domain Simple kriging estimation are given in the table below

25 data	100 data	250 data	500 data	1000 data	1500 data
0.0062	0.0025	0.0023	0.0008	0.0007	0.0000

Note that results of the Finite Domain Simple Kriging estimation and Finite Domain Ordinary Kriging estimation are very similar, this is because Simple Kriging and Ordinary Kriging results in very similar weights due to the closeness of the estimation location to the string in terms of range of continuity of the considered variable variogram.

Finite Domain Kriging: Generalization to the Case of Multiple Singles

Let us consider the situation of multiple strings containing possibly different number of data. Recall that the Finite Domain Kriging in the single string case is basically an average of several 'traditional' Kriging results obtained using different neighborhood search strategies. When we deal with the situation of multiple strings the following question arises: *Should we consider each string separately for the Finite Domain Kriging or all strings at the same time?* Two options will be considered.

Finite Domain Kriging I performs the 'traditional' Kriging as many times as there are conditioning data, that is, n. Each time k, $k = 1,\ldots,n,$ kriging is performed based on the k closest data without considering if they are from different strings or the same string. Thus, basically, the procedure of the Finite Domain Kriging I is the same as was described for the single string case.

The second option, Finite Domain Kriging II, is slightly more complicated. We will first assume that each string l, $l = 1,\ldots,L,$ contains at least n data. Then, in order to obtain Finite Domain Kriging II estimate, the 'traditional' Kriging is performed n times. Each time k, $k = 1,\ldots,n,$ kriging is performed based on a set of k closest data from each string. If the strings contain a different number of data, say string j contains only m ($m < n$) data, then procedure is almost the same. Except that in order to obtain final Finite Domain Kriging II, each time k, $k = 1,\ldots,m,$ kriging is performed based on a set of k closest data from each string; while each time k, $k = m+1,\ldots,n,$ kriging is performed based on a set of k closest data from all strings expect for string j (from string j only m data are selected). This could be extended to the case when we have different amount of data in each string.

Practical Applications

Data

To assess the difference between the Finite Domain Kriging approaches and the 'traditional' Simple and Ordinary Kriging, a case study of the real data from a petroleum reservoir (data set 1). Locations of the available vertical wells in the *XY* plane are shown in Figure 6. Figure 6 also shows the histograms of the data. Figure 7 shows the experimental variograms and their theoretical fits for the variable under study.

Estimation

Simple Kriging, Ordinary Kriging, Finite Domain Simple Kriging I, Finite Domain Ordinary Kriging I, Finite Domain Simple Kriging II and Finite Domain Ordinary Kriging II were applied for estimation of the study domain.

Figure 8 shows the middle slice in the XY plane of the 3D model for the data using Ordinary Kriging and Finite Domain Ordinary Kriging I. Figure 8 also shows location of the wells used in estimation and maps of the differences and smoothed differences between Finite Domain Ordinary Kriging I and Ordinary Kriging estimates. Figure 9 shows the middle slice in the XY plane of the 3D model for the data using Simple Kriging and Finite Domain Simple Kriging I. Figure 9 also shows location of the wells used in estimation and maps of the differences and smoothed differences between Finite Domain Simple Kriging I and Simple Kriging estimates. Note that when estimating using any of the considered approaches the following parameters were used: min and max number of data for estimation were set to 10 and 20, respectively; maximum search radii were set to maximum variogram ranges.

There are significant differences in the results of the Finite Domian Kriging approaches and 'traditional' Kriging mostly far from the well locations (at the boundaries of the study domain). This is reasonable and expected. The maximum influence of the data in the string X_i, $i = 1,\ldots,Ls,$ on the estimation location **u*** is defined as maximum relative weight given by an estimation location to the data in the string, that is,

$$i(u^*) = \max_{j=1,\cdots,Ls} \frac{\left|\lambda_j(u^*)\right|}{\sum_{k=1}^{Ls}\left|\lambda_k(u^*)\right|} \cdot 100\%,$$

where $\lambda(u^*) = (\lambda_1(u^*),\ldots,\lambda_{Ls}(u^*))^T$ denote the traditional (Simple, Ordinary) Kriging weights.

Example maps of the maximum influence obtained using Simple and Ordinary Kriging based on isotropic spherical variograms with nugget of zero and range of correlation 20 for estimation of finite domain based on string of 11 data are shown in Figure 10. It can seen from Figure 10 that when the location of interest is situated close to the string of data, then the data in the string which is positioned on the shortest distance to the location of interest receives the largest weight in Kriging, and, thus, have the largest influence on the result of estimation. However, if the location of interest is situated far (not necessarily a distance larger than the range of correlation) from the string of data, then one of the boundary data in the string receives the largest weight in Kriging, and, thus, have the largest influence on the result of estimation.

Considering Figure 10, we can easily explain the maps in Figures 8-9. Specifically, due to long range of continuity of the variable under study, we observe only slight difference in the estimates produced by Finite Domain Kriging approaches and traditional kriging (this is because there is no string effect in the estimates). However, when the estimation location is far from the well, the string effect becomes important and the difference in the estimates becomes more and more pronounced. To illustrate this point via example a subset of 100 well was removed from the database for the estimation of the domain of interest. Figure 11 shows the middle slice in the XY plane of the 3D model for the data using Ordinary Kriging and Finite Domain Ordinary Kriging I. Figure 11 also shows location of the 100 wells not used in estimation and the map of the wells used in estimation; as well as the maps of the differences and smoothed differences between Finite Domain Ordinary Kriging I and Ordinary Kriging estimates. Figure 12 shows the middle slice in the XY plane of the 3D model for the data using Simple Kriging and Finite Domain Simple Kriging I; locations of the 100 wells used in estimation and maps of the differences and smoothed differences between Finite Domain Simple Kriging I and Simple Kriging estimates.

Conclusions

A new approach to kriging in a finite domain using strings of data is proposed. This approach, referred to as Finite Domain Kriging, provides a linear unbiased estimate. Finite Domain kriging estimates are obtained as an average (or expected) value of the optimal kriging estimators for different search neighborhoods. Simple and Ordinary Finite Domain Kriging are possible.

The proposed approaches for estimation of a finite domain using strings of data were applied to real data set from petroleum reservoir. All Finite Domain Kriging approaches were shown to reveal and reduce the edge effect in the considered case study. The most significant reduction in the string effect was observed in Finite Domain Kriging I approach.

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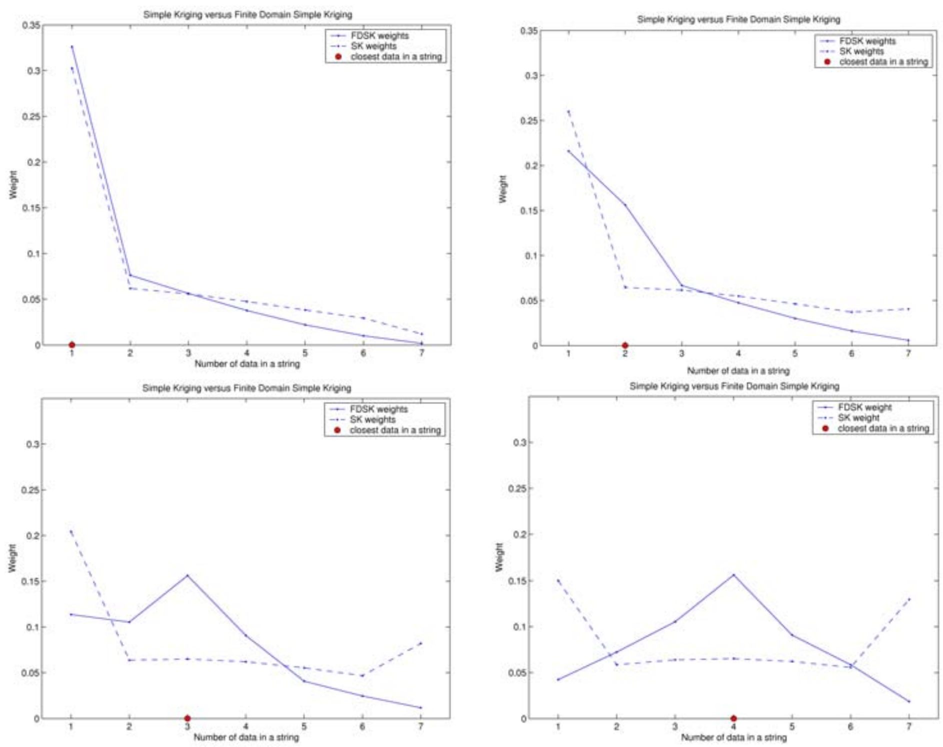

Figure 1: Structure of the Finite Domain Simple Kriging (solid line) and Simple Kriging (dashed line) weights when estimating locations: a) (1,7); b) (1.8, 7); c) (2.8, 7) and d) (3.8,7) using Spherical variogram model with the range of correlation 20

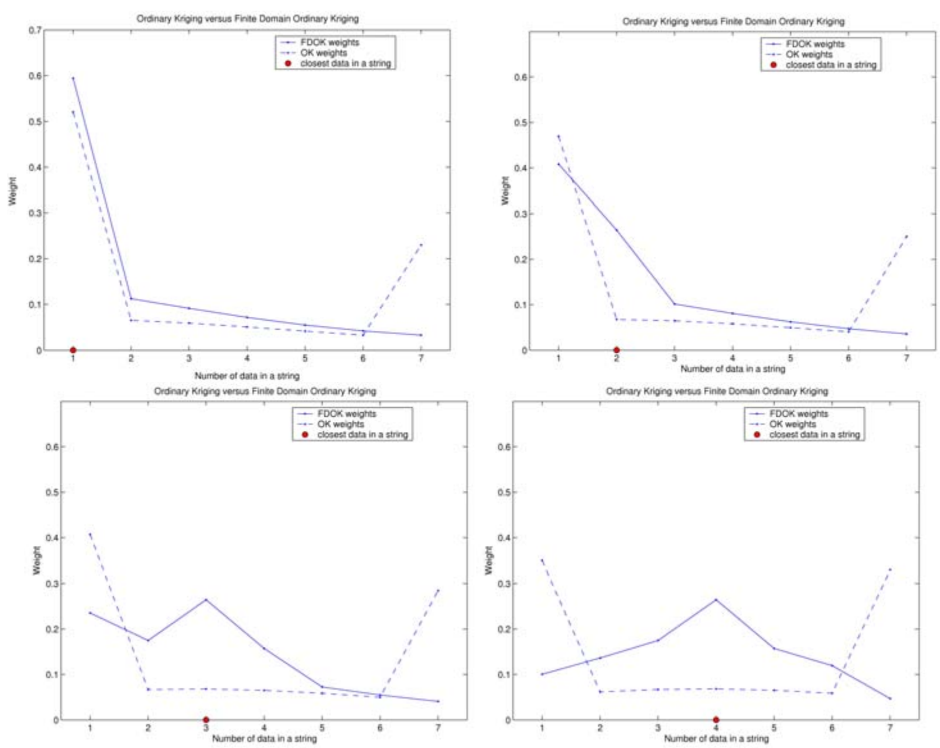

Figure 2: Structure of the Finite Domain Ordinary Kriging (solid line) and Ordinary Kriging (dashed line) weights when estimating locations: a) (1,7); b) (1.8, 7); c) (2.8, 7) and d) (3.8,7) using Spherical variogram model with the range of correlation 20.

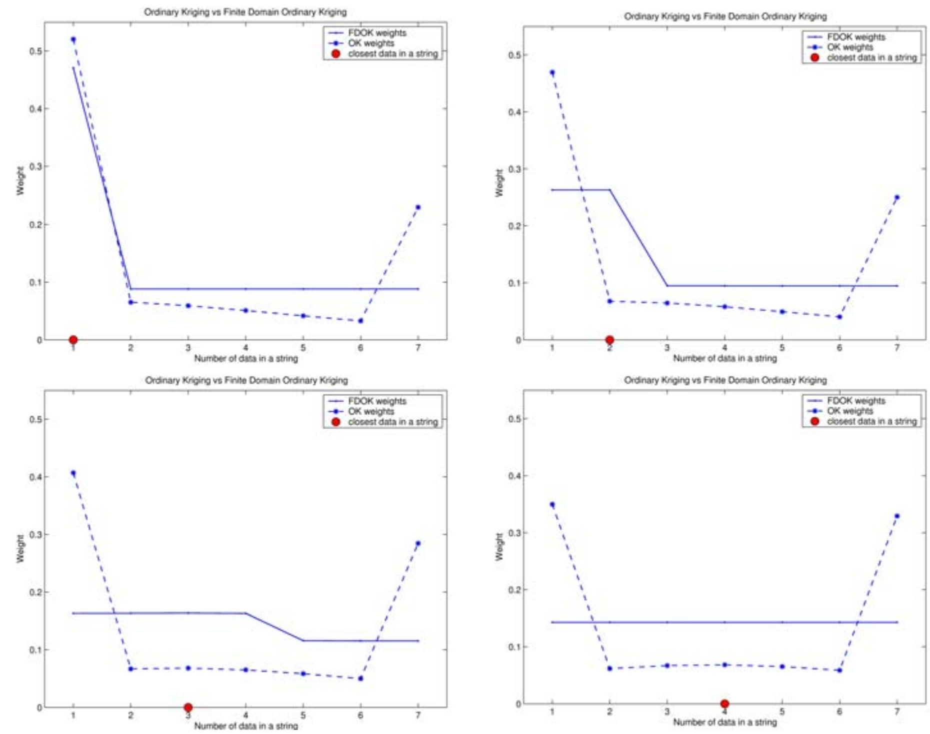

Figure 3: Structure of the Finite Domain Ordinary Kriging (solid line) and Ordinary Kriging (dashed line) weights when estimation location: a) (1,7); b) (1.8, 7); c) (2.8, 7) and d) (3.8,7) using Spherical variogram model with the range of correlation 20.

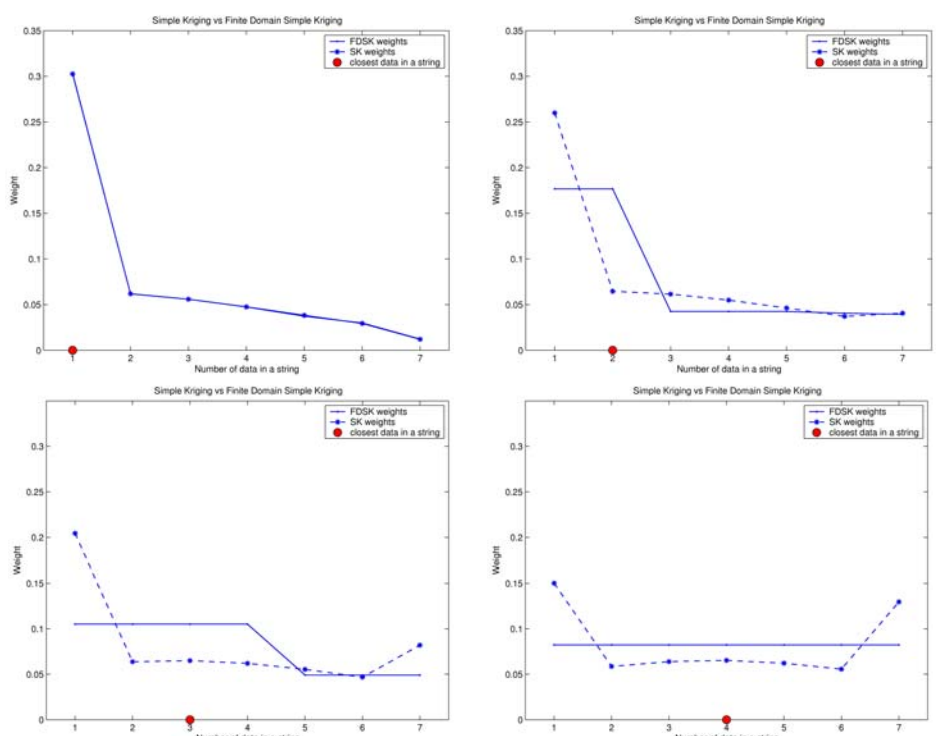

Figure 4: Structure of the Finite Domain Simple Kriging (solid line) and Simple Kriging (dashed line) weights when estimation location: a) (1,7); b) (1.8, 7); c) (2.8, 7) and d) (3.8,7) using Spherical variogram model with the range of correlation 20.

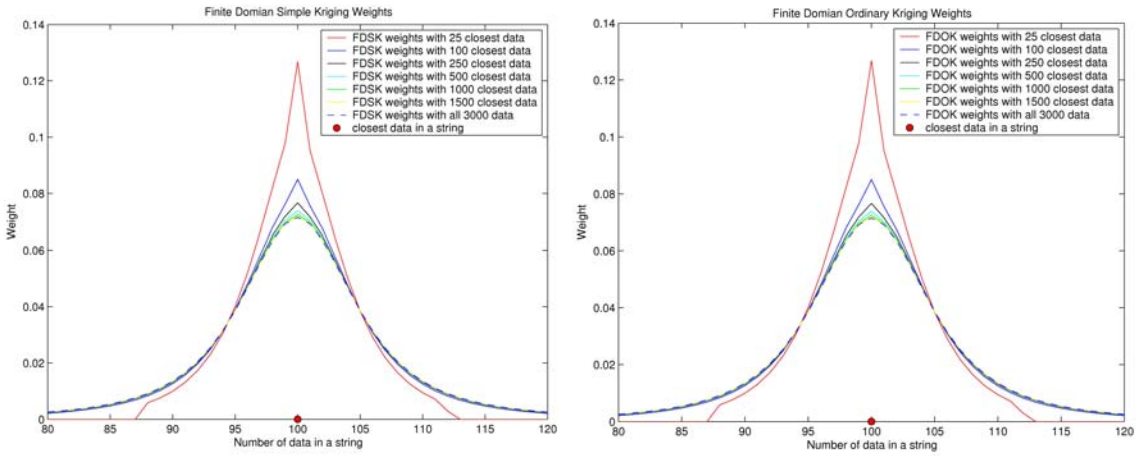

Figure 5: Change in the structure of the Finite Domain Simple and Ordinary Kriging weights with respect to the number of closest data in a string used for location (100,7) using Spherical variogram model with the range of correlation 500. String of 3000 data is located at (1,0), (2,0), …, (3000,0), respectively.

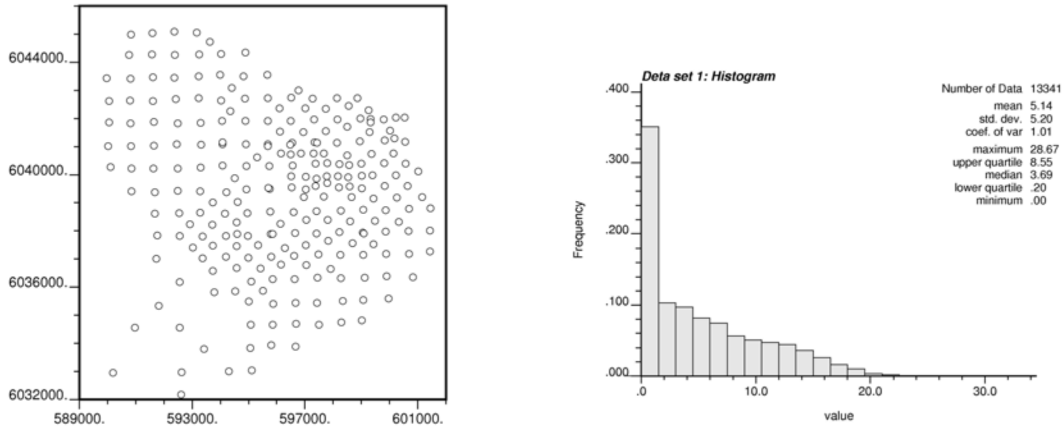

Figure 6 Locations of the wells and histogram of the data.

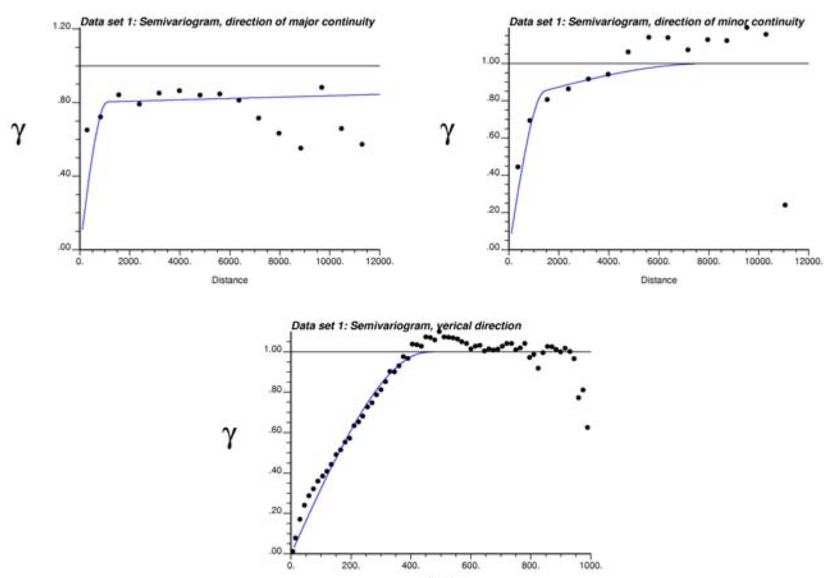

Figure 7: Variograms in the three directions of major continuity for the variable of interest.

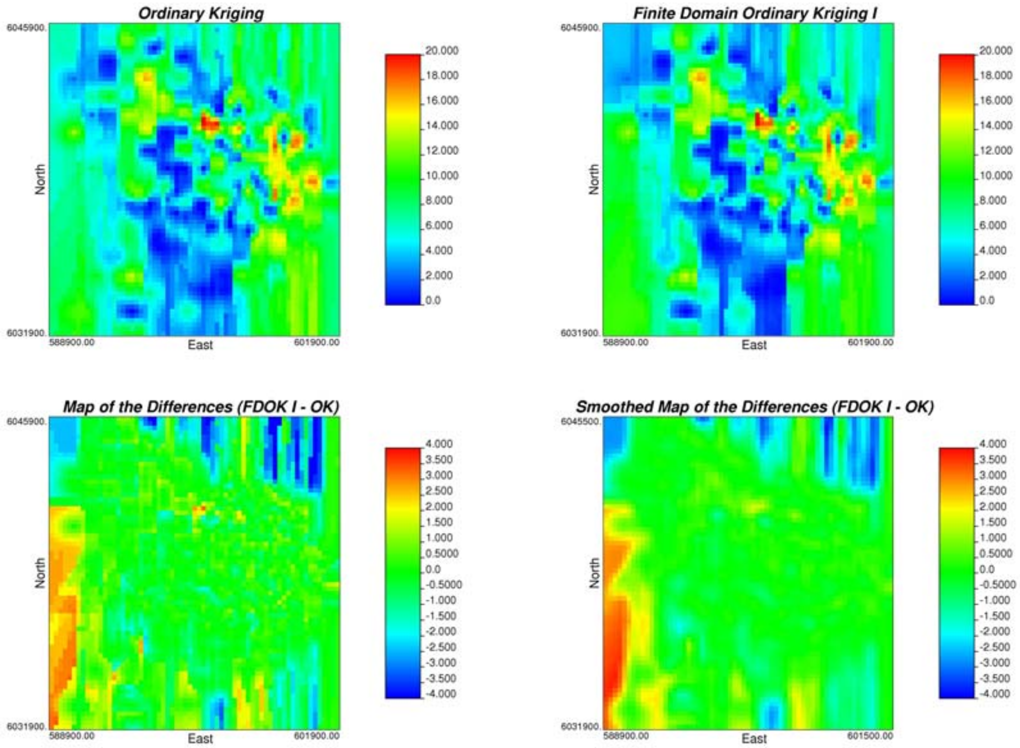

Figure 8: The middle slice in the XY plane of the 3D model obtained using Ordinary Kriging and Finite Domain Ordinary Kriging; maps of the differences (bottom left) and smoothed differences (bottom right).

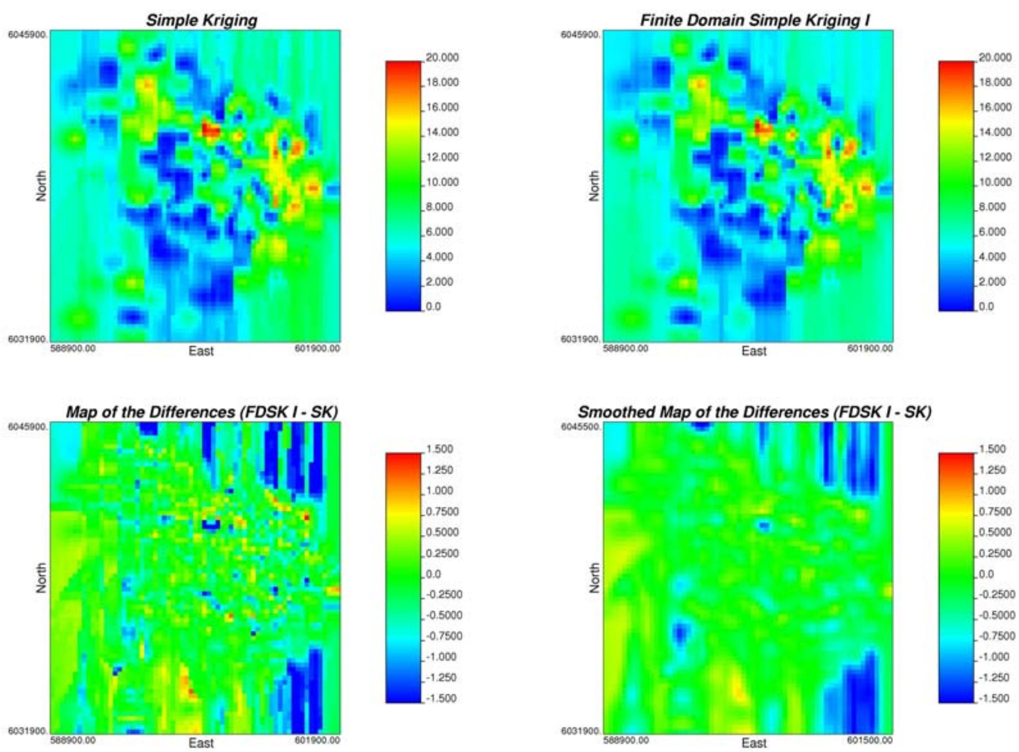

Figure 9: The middle slice in the XY plane of the 3D model using Simple Kriging (middle left) and Finite Domain Simple Kriging I; maps of the differences (bottom left) and smoothed differences (bottom right).

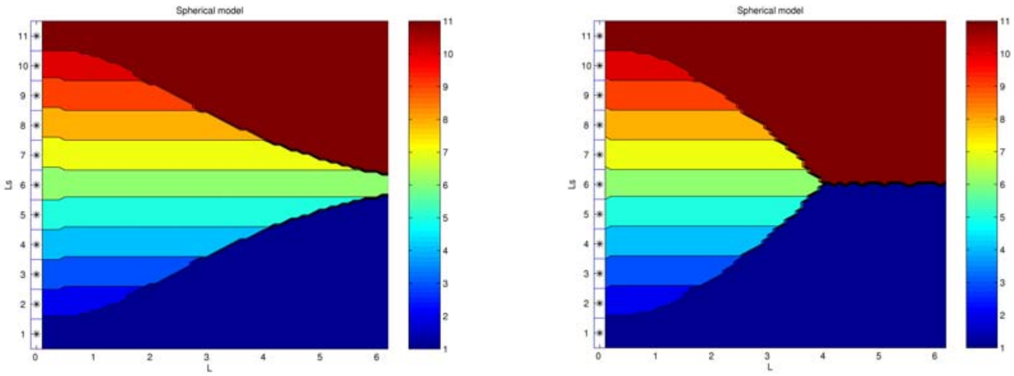

Figure 10: Map of the maximal influence of the data in the string obtained by Simple Kriging (left) and Ordinary Kriging (right) based on Spherical variogram model with range of correlation 20.

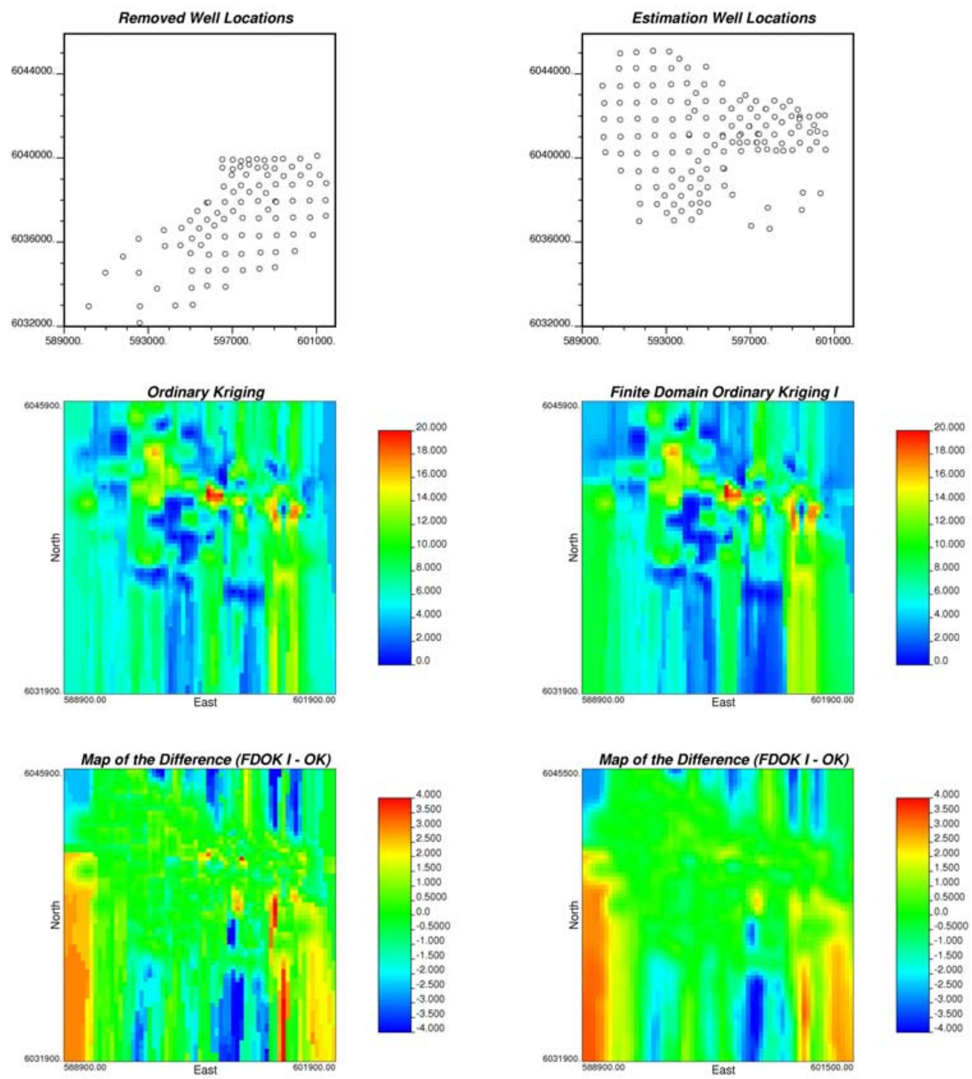

Figure 11: Locations of the 100 wells in the XY plane not used in finite domain estimation (top left) and locations of the wells in the XY plane used in finite domain estimation (top right); the middle slice in the XY plane of the 3D model for the variable of interest obtained using Ordinary Kriging (middle left) and Finite Domain Ordinary Kriging I (middle right); maps of the differences (bottom left) and smoothed differences (bottom right) between Finite Domain Ordinary Kriging I and Ordinary Kriging estimates.

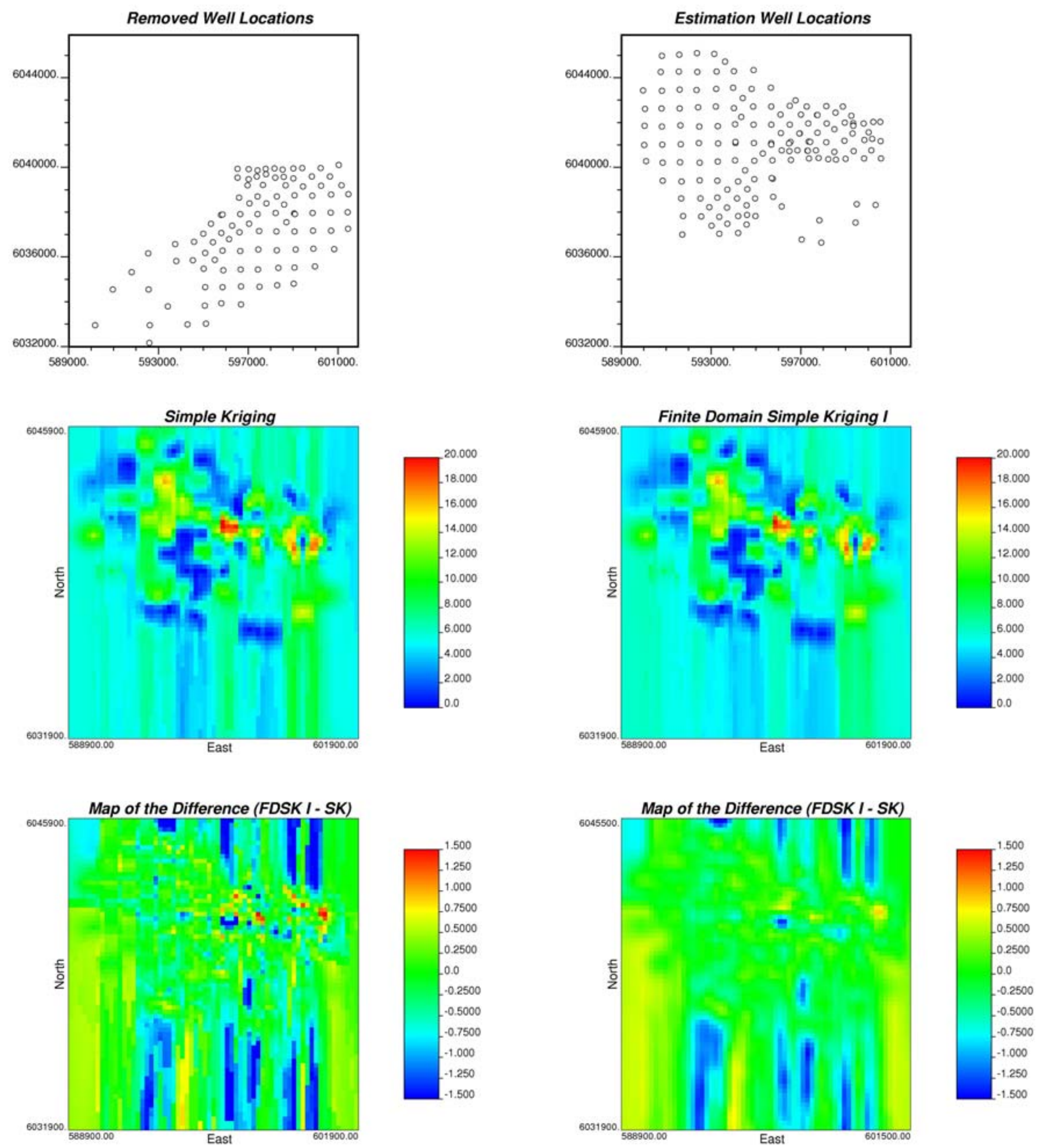

Figure 12: Locations of the 100 wells in the XY plane not used in finite domain estimation (top left) and locations of the wells in the XY plane used in finite domain estimation (top right); the middle slice in the XY plane of the 3D model for the variable of interest obtained using Simple Kriging (middle left) and Finite Domain Simple Kriging I (middle right); maps of the differences (bottom left) and smoothed differences (bottom right) between Finite Domain Simple Kriging I and Simple Kriging estimates.