Optimal Placement of Samples in Presence of Locally Varying Anisotropy

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Optimal placement of samples has been considered by many researchers in the presence of constant or no anisotropy (see references in Wilde, 2009). None have considered this problem in the presence of locally varying anisotropy (LVA). The Hooke-Jeeves optimization algorithm is used to determine the optimum locations for samples within an LVA field. A number of different initial configurations were investigated and it was found that even when starting with a near optimal solution, the CPU time and final objective function improvements were small. Initial configurations implemented include randomly generated, regular spacing in a high dimensional transformed space, and Delaunay triangulation within the high dimensional transformed space. The objective function implemented is the minimization of the distance between an estimation location and its nearest sampling point for all estimation locations. The optimal configuration is characterized by close spacing perpendicular to the local direction of continuity and sparse spacing parallel to this direction.

Introduction

Paper 406 (Wilde, 2009) in this report compares a number of optimization techniques as applied to the problem of field measurement design (FMD). The objective was to minimize the sum of the estimation variance within a geostatistical model by determining the optimum locations for a given number of samples. As explained in that paper, the optimum sample locations for this objective function are known. McBratney et.al (1981) showed that for an isotropic field the estimation variance is minimized if sampling is performed on an equilateral triangular grid. This known result was used as a benchmark to compare optimization algorithms in Wilde (2009). The comparison revealed that the Hooke-Jeeves Pattern Search optimization technique was the most efficient algorithm for this problem.

Wilde (2009) also explained that the motivation for this comparison was to choose an algorithm to apply to the problem of FMD in the presence of locally varying anisotropy (LVA). All previous work in the area of optimal FMD has been restricted to domains with constant anisotropy. This paper demonstrates optimal FMD in the presence of locally varying anisotropy using the Hooke-Jeeves method.

The objective function has been improved upon from that used in Wilde (2009) which was to minimize the sum of the estimation variances. This is computationally expensive as the kriging equations must be solved for every location for every new configuration of data. Using another result from McBratney et.al (1981), the objective function has been modified to be less expensive. McBratney et.al (1981) showed that when geologic semi-variograms are monotonic increasing functions, the kriging variance tends to increase as the distance between the interpolated point and the observation points increases. The distance between an interpolated point and its *nearest* sampling point is minimized by sampling on an equilateral triangular grid. The maximum estimation variance is also minimized if sampling occurs on an equilateral triangular grid. As such, the objective function implemented in this paper is taken to be the minimization of the distance to the nearest sample location because it is much less computationally expensive.

In order to optimize the placement of samples in the presence of locally varying anisotropy, the locally varying anisotropy must be defined. This paper presents two examples of FMD, the first uses a synthetic LVA field developed to mimic a channel deposit. A second example is provided for the Jura data set (Goovaerts, 1997) to demonstrate the methodology on a more realistic scale. Boisvert et.al (2007) discusses the methodology used to generate the LVA fields for both examples.

Boisvert & Deutsch (2009) provide an in-depth discussion of geostatistical modeling with LVA. For the purposes of this paper it is sufficient to understand that to consider geomodeling with LVA the entire geostatistical grid is embedded in a high dimensional Euclidean space where the data are isotropic. The *K* coordinates of each grid cell block are determined by ISOMAP-L (Silva & Tenenbaum, 2003), details of which can be found in Boisvert & Deutsch (2008).

Hooke-Jeeves Pattern Search

The Hooke-Jeeves optimization technique is a derivative free method based solely on evaluations of the objective function. It has been compared to geographical exploration in that it visits an initial base point, explores around that base point, moves to a new base point, and explores around the new base point. This process repeats until the optimal solution is found or until the step size is sufficiently reduced. The algorithm begins with a base point, x, and step size, h. The exploratory move is performed first during which the objective function is sampled at successive perturbations of the base point in search directions, d. The current best value $f_{cb} = f(x_{cb})$ and best point x_{cb} are recorded. x_{cb} is initialized to x. The sampling is managed by first evaluating $f(x_{cb} + v_j)$ and only testing $x_{cb} - v_j$ if $f(x_{cb} + v_j) \geq f(x_{cb})$. The exploratory phase will either produce a new base point or fail (meaning that $x_{cb} = x$). Note that this phase depends on the ordering of the coordinates of x. Applying a permutation to x could change the output of the exploration.

If the exploratory phase has succeeded, the search direction is $d = x_{cb} - x$ and the new base point is x_{cb}. The subtle part of the algorithm begins here. Rather than center the next exploration at x_{cb}, which would use some of the same points that were examined in the previous exploration, the Hooke-Jeeves algorithm is aggressive and attempts to move further. The algorithm locates the center of the next exploratory move at

$$x_b = x + 2d = x_{cb} + d \tag{1}$$

If this second exploratory move fails to improve upon $f(x_{cb})$, then an exploratory move with x_{cb} as the center is evaluated. If that also fails, h is reduced, x is set to x_{cb}, and the process is repeated (Kelley, 1999). A flow chart of this algorithm is shown in Figure 1.

In this implementation the "base point" is an initial configuration of n sample locations, where n is defined by the user. An exploratory move is considered as a shifting of the location of a single sample location by the step size in the x and y directions.

Application of Hooke-Jeeves Method

The aim of the optimization is to locate n data such that the distance between an estimation location, $\mathbf{u}$, and its nearest sampling point is minimized for all $\mathbf{u} \in A$. An initial configuration of samples is generated by randomly drawing x,y coordinates for n data locations. An initial step size is specified and the exploratory move is performed. Consider that the coordinates for the first point are (13,17) and the initial step size is 10. The exploratory move proceeds by first increasing (or decreasing) the x coordinate of the first point by the step size to a new location at (23,17). The objective function is evaluated for this new configuration. If the objective function is improved, the y coordinate of the first point is perturbed. If the objective function is not improved, the x coordinate is decreased by twice the step size to (3,17) and the objective function evaluated. If there is improvement, this coordinate is retained; if not the coordinate is returned to its initial value. The y coordinate of the first point is then perturbed as with x and the procedure is repeated retaining the coordinates that gives the best value of the objective function. This process of perturbing individual coordinates is repeated for all $2n$ coordinates. Finally, the pattern move is performed. Say a move from (13,17) to (23,27) resulted in the minimization of the objective function. The new data location (Equation 1) becomes:

$$[x_{new}, y_{new}] = [23,27] + \left([23,27] - [13,17]\right) = [33,37]$$

This first iteration of an exploratory and pattern move is illustrated in Figure 2. The same perturbation is applied to all n data. The exploratory move is then repeated. This cycle of exploratory and pattern moves is repeated until no improvement is made. The step size is then reduced and the cycle repeats until the step size is deemed sufficiently small. The final data configuration is considered optimal.

Application to LVA Fields

The goal is to locate n data within an LVA field such that the anisotropic distance between an estimation location $\mathbf{u}$ and its nearest sampling point is minimized for all $\mathbf{u} \in A$. Consider a geostatistical modeling grid with L cells. The first step is to embed the cells into a k-dimensional space using MDS, as discussed in Boisvert & Deutsch (2009). Next, n cells are chosen as initial data locations. The initial locations can be chosen randomly or in a more intelligent manner, which is discussed below. One limitation of using MDS is that there are a discrete number of potential data locations as data can only be located at grid cell centers. This can be mitigated by considering a smaller cell size but this increases CPU requirements. The objective function for optimization is as follows:

$$f(x)=\sum_{j=1}^{n}\left\{\sum_{i=j}^{L}\left[\min\left(\sum_{m=1}^{k}\left(x_{i,m}-x_{j,m}\right)^2\right)\right]\right\} \quad (2)$$

where L is the number of cells in the grid, n is the number of data locations, k is the number of dimensions, $d_{i,m}$ is the m^{th} coordinate of the i^{th} grid cell, and $d_{j,m}$ is the m^{th} coordinate of the j^{th} data location. The Hooke-Jeeves algorithm is then employed to find the optimal data configuration. The step size is the number of cells to shift each coordinate by. The algorithm proceeds until the step size is 1 and no further improvements can be made.

This method is applied to two LVA fields: the first is an artificial channel field with high anisotropy in the channel and no anisotropy outside the channel; the second example is a more realistic smoothly varying field with constant anisotropy based on the Jura data set (Goovaerts, 1997). These fields are shown in Figure 3. For the first case, consider a randomly generated initial configuration. This is the starting point for the Hooke-Jeeves algorithm. The objective function is evaluated for this configuration after which the cycle of exploratory move, pattern move and step reductions is performed. Once the step size is sufficiently small, the final data locations are returned.

The initial and final configurations for the channel and smooth LVA fields are shown in Figure 4 and Figure 5 respectively. Note that for the final configuration in the channel field, the data are regularly spaced where the field is isotropic while the data within the channel are closely spaced perpendicular to the channel and sparsely spaced parallel to the channel. This is an intuitive result as it is reasonable to expect the optimal configuration to contain more densely sampled data within the highly anisotropic zone. For the final configuration in the smooth field, the data are closely spaced perpendicular to the direction of continuity and are remotely spaced parallel to the direction of continuity.

Generating Intelligent Initial Configurations

It is desirable to have initial configurations that begin at a lower objective function evaluation as this reduces the CPU time of the algorithm and results in a lower final objective function value. Two methods for generating the initial configuration have been considered. Both involve choosing evenly spaced points in the transformed k-dimensional Euclidian space (Boisvert & Deutsch, 2008). The first method places the samples at locations which fall on a regular grid in the first two k-dimensions while the second uses conforming constrained Delaunay triangulation to evenly space the sample points.

Regular Spacing in the Transformed Space

It has been shown that after applying the transform to *k*-dimensions the data are isotropic (Sampson and Guttorp, 1994). Ideally, all *k* dimensions in the transformed space would be considered when placing samples on a regular grid. However, this is difficult to implement as *k* can be large (Boisvert & Deutsch, 2008). Instead, only the first two dimensions in the transformed space are considered. For example, after embedding the channel LVA field, the first two dimensions appear as shown in Figure 6 (left). The channel is clearly visible through the middle of the field. The cells in this field are discretized into 100 smaller cells. The coordinates of the cells for the first two dimensions are shown in Figure 6 (right).

Samples are placed on a regular grid using the first two dimensions of the coordinates in transformed space as shown in Figure 7 (left). The corresponding real space sample locations are shown in Figure 7 (right). Note the similarity between this configuration and the optimal configuration in Figure 4. The evaluation of data locations shown in Figure 7 is computationally fast and provides an initial data configuration for optimization that is closer to the optimal configuration. The final configuration generated using this initial configuration is shown in Figure 8. A number of samples have migrated from the channel leaving only four data in the channel. These points are sparsely spaced due to the high continuity present within the channel. Many more points are required outside of the channel due to reduced continuity.

The same method for generating an initial configuration was used for the smooth LVA field. The coordinates of the 90,000 (300x300) grid cells are shown in Figure 9 (left) along with an overlay of a regular grid used to locate the samples. The locations of these samples are shown in real space in Figure 9 (right). The similarity between this configuration and the optimal configuration in Figure 5 is not as striking as for the channel field, but this configuration does have a lower starting objective function value than the random initial configuration. The final configuration (Figure 10) generated using this initial configuration has moved some points closer to the edge to reduce the distance to a sample along the boundaries of the domain. It has also moved the points such that they are closely spaced perpendicular to the direction of continuity and sparsely spaced parallel to the direction of continuity.

Conforming Constrained Delaunay Triangulation

Another method for obtaining an improved initial configuration is to use conforming constrained Delaunay triangulation (Shewchuk, 2005). This method creates a two-dimensional finite element mesh within the transformed space. The center-point of each mesh is used as an initial data location. This method was used for the smooth LVA field (Figure 11 left). The corresponding locations in real space are shown in Figure 11 (right). The objective function value using this configuration is higher than the value obtained using the regular grid method and requires trial and error to determine the input parameters which yield the desired number of meshes. For these reasons, this method is not pursued further.

Conclusion

Determining the optimal data locations within an LVA field is an interesting problem. If the LVA field is known for a deposit of interest, future sampling campaigns can be designed to incorporate these locally varying directions of continuity. This paper implemented an objective function that is the minimization of the distance from an unsampled location to its nearest sampled location. The optimal data configurations has shown that the minimum objective function is found for close spacing perpendicular to the direction of continuity and sparse spacing parallel to this direction. This result is intuitive as more data are required to minimize uncertainty when continuity is low and fewer data can be used in areas that are very continuous. This agrees with McBratney et. al's (1981) statement that an optimal sampling scheme in presence of anisotropy will have greater spacing in the direction of continuity than perpendicular to this direction but has been extended to incorporate LVA.

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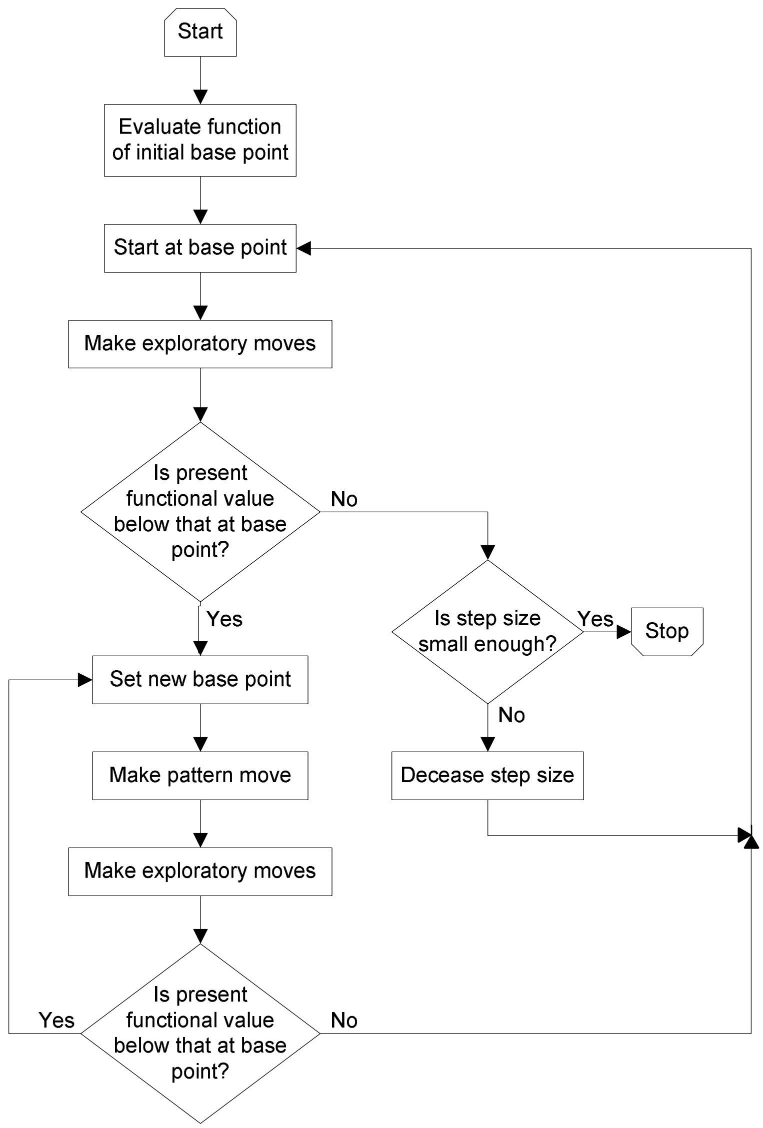

Figure 1: Flow chart of the Hooke-Jeeves algorithm.

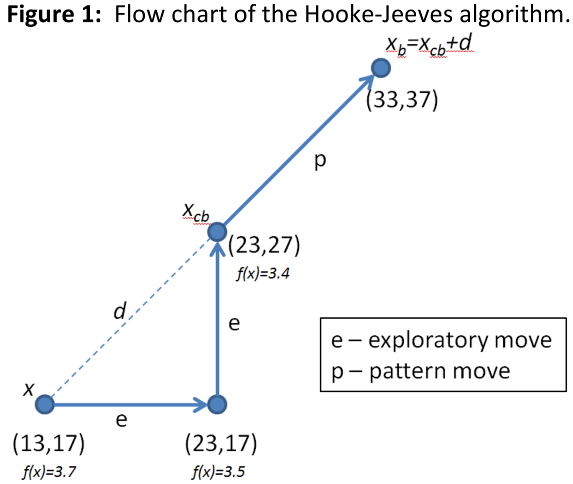

Figure 2: Illustration of exploratory and pattern moves.

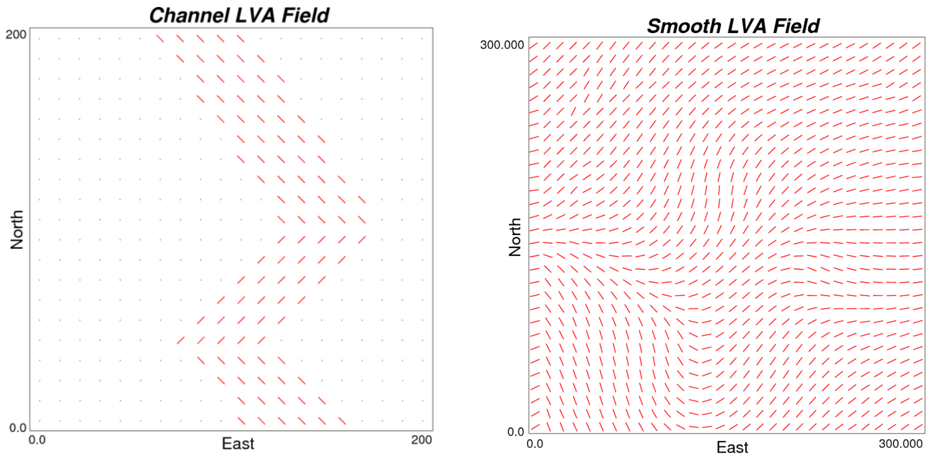

Figure 3: Locally varying anisotropy fields for the case studies. Left: the channel example with 10:1 anisotropy inside the cannel and 1:1 outside. Right: The smooth LVA field with constant 3:1 anisotorpy.

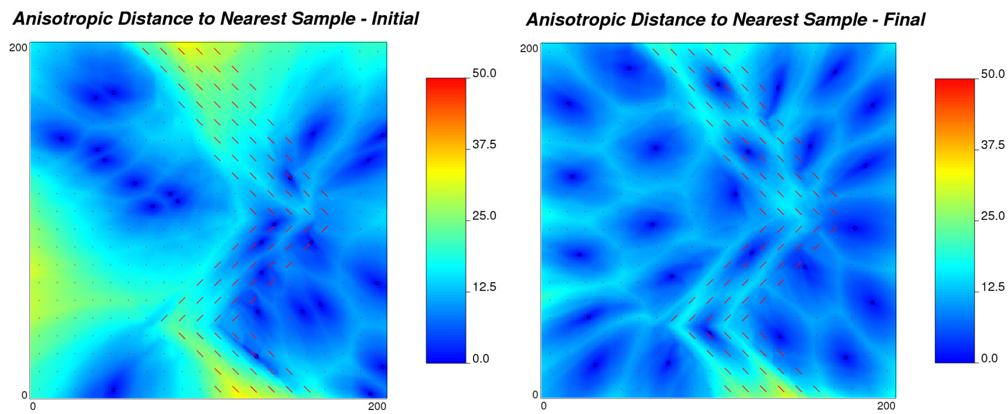

Figure 4: Initial and optimal data locations for the channel LVA field with objective function values of 562947 and 381627 respectively.

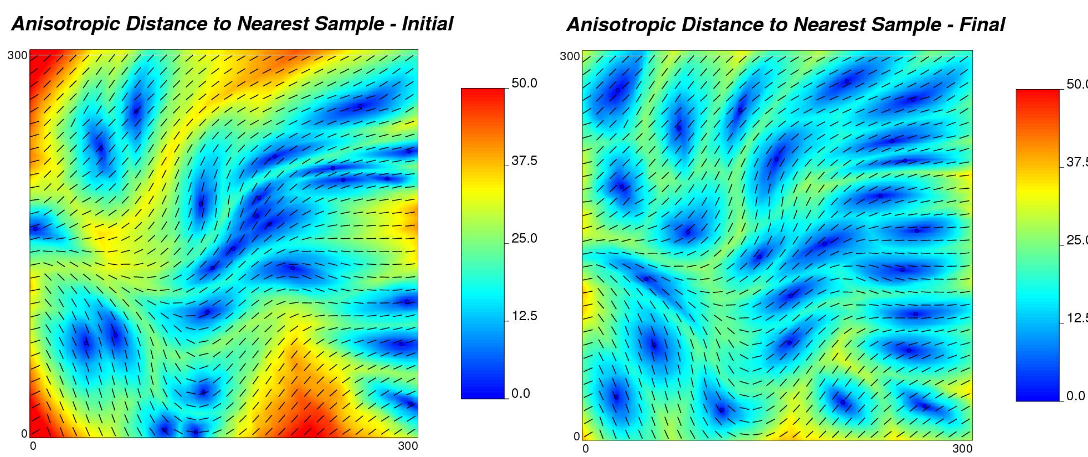

Figure 5: Initial and optimal data locations for the smooth LVA field with objective function values of 2029585 and 1543080 respectively.

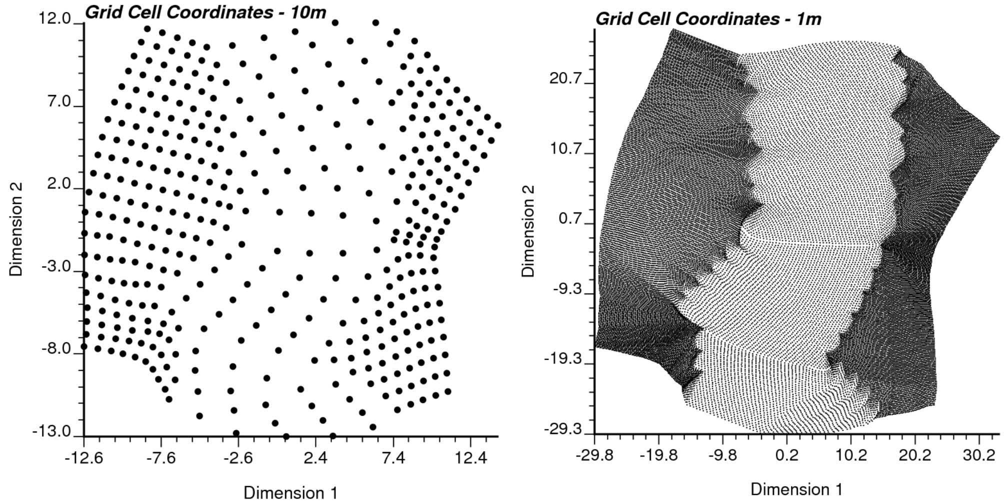

Figure 6: Transformed grid cell coordinates for the channel LVA field: left) 10m cells; right) 1m cells.

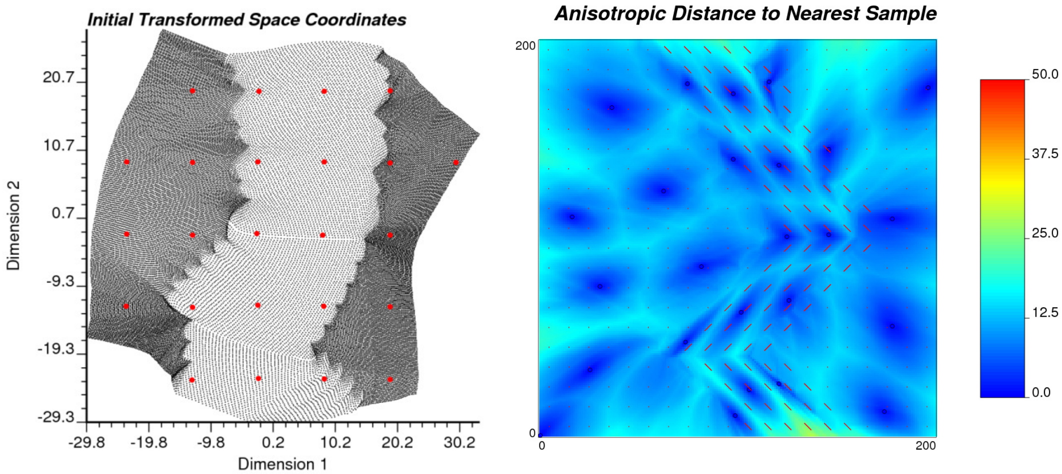

Figure 7: Initial data location coordinates for the channel LVA field shown in: left) transformed space; right) real space with objective function value of 431260.

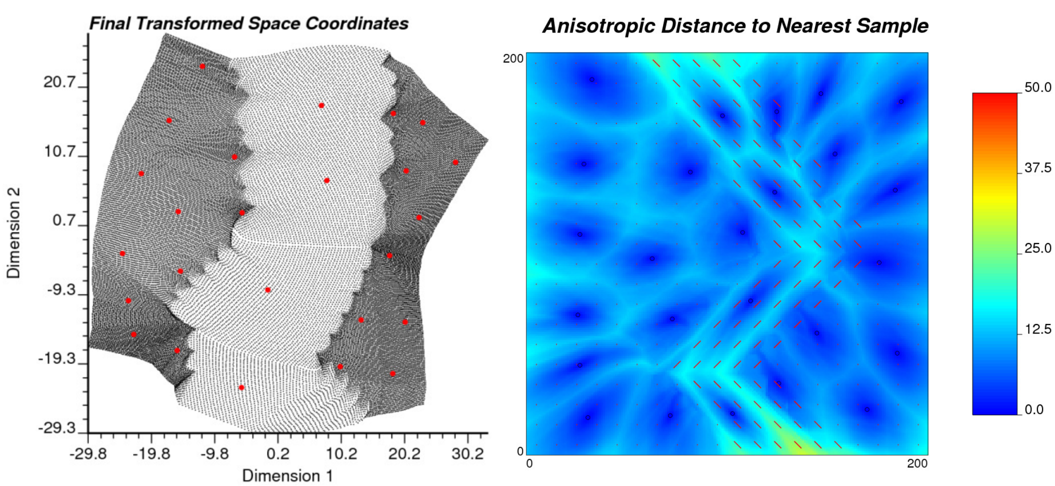

Figure 8: Final data location coordinates for the channel LVA field shown in: left) transformed space; right) real space with objective function value of 380285.

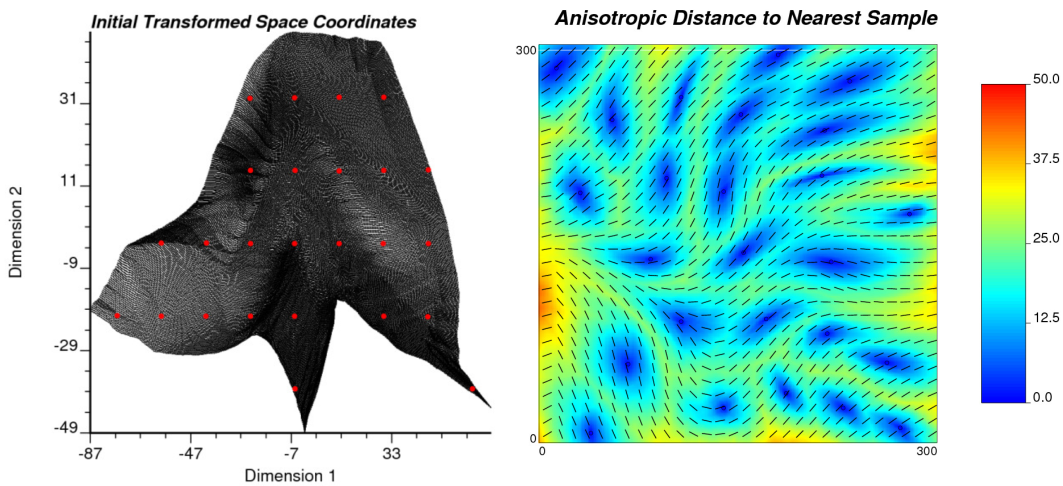

Figure 9: Initial data location coordinates for the smooth LVA field with a regular grid used to locate data shown in: left) transformed space; right) real space with objective function value of 1685035.

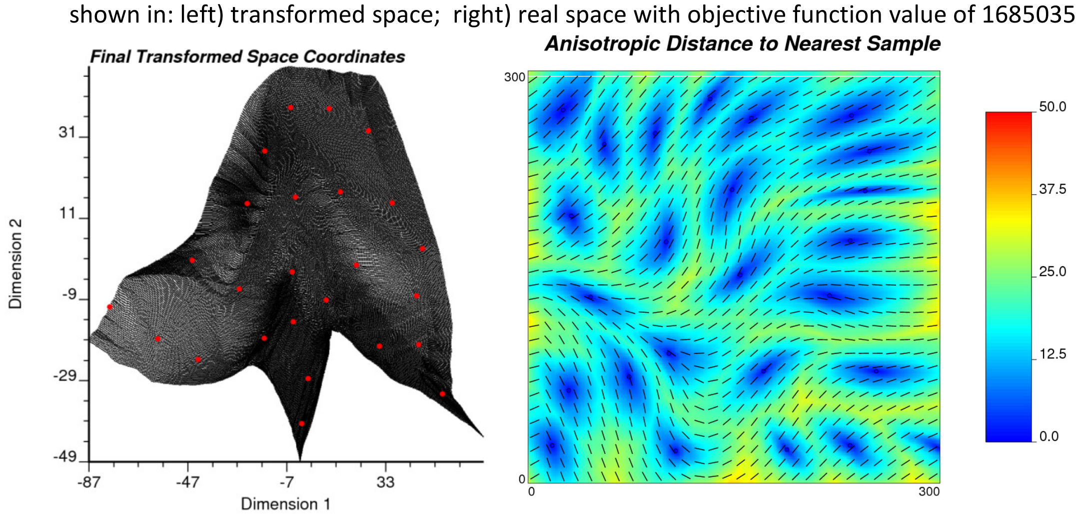

Figure 10: Final data location coordinates for the smooth LVA field shown in: left) transformed space; right) real space with objective function value of 1542587.

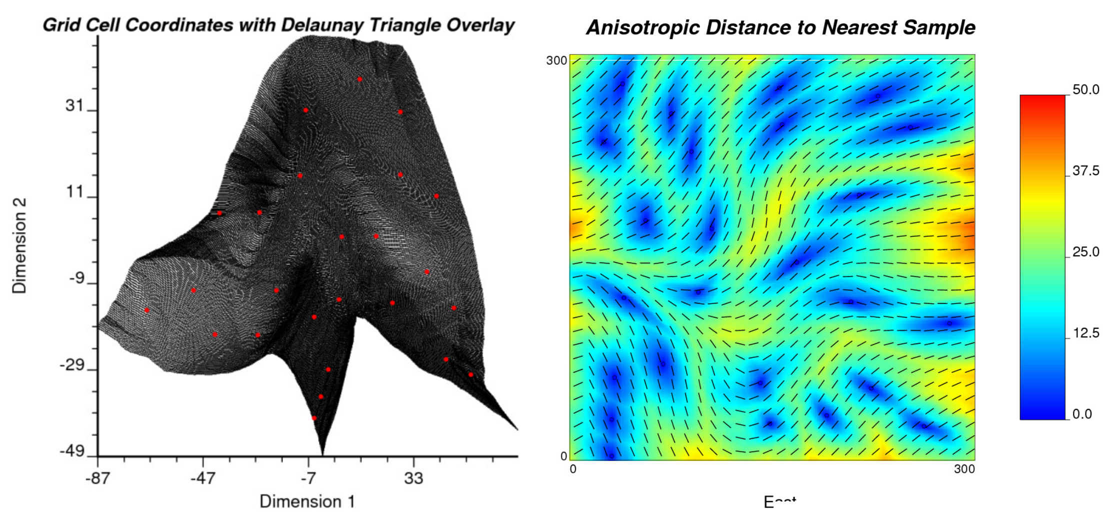

Figure 11: Data location coordinates for the smooth LVA field with Delaunay triangulation used to locate data shown in: left) transformed space; right) real space with objective function value of 1713923.