Assessing Geospatial Aleatory Uncertainty for Performance Assessment Modeling – 11075

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ABSTRACT

The aleatory (measurement) uncertainty introduced into Performance Assessment modeling has always been of concern. The incomplete knowledge of the physical make-up of the materials through which contaminants can be transported looms large when assessing the potential risk of a disposal facility. This paper presents a Best Linear Uncertainty Estimate (BLUE) methodology, "kriging", which allows the uncertainty to be quantified. This uncertainty quantification can be useful not only in its application to contaminant transport modeling, but it can also be extremely useful in determining where, in terms of modeling uncertainty reduction, the most useful, additional data can be obtained.

Many low level radioactive waste disposal sites and their surrounding areas are sparsely characterized due to the inherent costs of drilling and boring, sample preparation, etc. Material properties important to contaminant transport, such as porosity and clay/sand distribution, might be known at relatively few locations spread over a large area. The way in which these properties change can have a dramatic affect on the contaminant transport. It becomes incumbent on the analyst to not only be able to better describe the spatial distribution of these properties, but to be able to assess the uncertainties which will exist due to the discrete nature of the sample.

Two different examples of the application of kriging to uncertainty quantification will be discussed. The first will look at the distribution of water table elevations. This example was chosen because it is a physical property which is essentially continuous and therefore has the "stationarity" attribute. Stationarity refers to the mean and variance of a property not being a function of location. The second example will look at the distribution of clay. Clay can occur in lenses or facies, so its distribution does not necessarily meet the stationarity condition.

The water table distribution demonstrates the creation of a complete interpolated response surface (elevation). It further shows means for selecting different parameters in kriging to reduce the associated uncertainty. The clay data shows the effect of extremely sparse data on the uncertainty, discusses possibilities to reduce this particular effect, and serves as an exercise in determining optimal placement for new measurements to reduce uncertainty. The clay data example demonstrates that while the kriging shows areas of high uncertainty, if one were to look at additional information, such as flow streams from the waste form, an even more informed decision about sample location can be made.

INTRODUCTION

The Radiological Performance Assessment (RPA) group at the Savannah River National Laboratory would like to further its understanding of the on-site clay distribution through the use of kriging. Kriging is a well known statistical method that can be used to assess sparse spatially distributed data. Kriging creates a continuous distribution of the physical characteristic under study while also describing the uncertainties associated with that distribution. The uncertainty of the physical characteristics is referred to as aleatory uncertainty. While the variation in the clay distribution is of interest, the errors associated with the predictions those distributions are of particular interest for use in the stochastic modeling done for performance assessments.

The area of interest is clay measurements taken in the General Separations Area (GSA) on the Savannah River Site with the majority of the locations coming from near the E-Area Low Level Waste (LLW) disposal facilities. More specifically, we are interested in the clay composition of the earth above the water table. This is of interest as the clay/sand proportion can greatly affect contaminant transport. Originally, there was to be a series of 2D clay surfaces that would correspond to different, associated depths (i.e. a clay surface at 15 m, using all of the 15 m data, another at 30 m, using all of the 30 m data, etc.). Unfortunately, the data was extremely sparse, and the only depth that had enough data that it could tolerate kriging was at 3 m, so only a single clay surface was generated. This 3 m clay surface will be referred to as the clay surface, and all measurements and clay distributions will be from the data at 3m.

The recorded data for the clay distributions was from borings performed onsite. The approach of this paper will be to predict the clay distribution of unmeasured locations through interpolation. The method of interpolation will be kriging. The kriging process will be handled by the SAS software package. SAS is a statistical analysis suite which includes kriging. The application to performance assessment has several different uses: the kriging can provide a better image of areas with weak or missing data, and, more importantly, it can provide exact locations where new measurements would have the greatest positive impact.

METHODOLOGY

Kriging was used to generate clay and water surfaces from the clay and water data, respectively, shown below. Kriging is a group of geostatistical techniques used to interpolate the value of a random field. In this case, the locations contain a measurement of percent clay, and these measurements are used to create a surface of percent clay near, around, and especially between the points.

Essentially, for a point of interest, where one wishes to find a value based on those previously recorded values nearby, a neighborhood or bin is created with the point of interest at its center. This bin captures a certain number of measured locations and uses only the values at those locations to interpolate a value for the point of interest. Figure 1 shows the locations at GSA, and it is, of itself, a fairly good example of how the kriging process works. If you pick a location somewhere on the map, suppose a location somewhere in the middle of all of the other points, you would then use the other points (i.e. the points with actual measurements) to interpolate the value for the location you have selected. Both the distance to the arbitrarily chosen location from each of the measured locations and each of the measured location's clay percentages are taken into account in order to calculate the value of the clay percentage for the location you have selected.

Figure 1: Well Boring Locations in GSA

Now, for a point nearby, another bin is created. This second bin may or may not include the same previously recorded locations. In most cases, the second bin includes a slightly different set of previously recorded locations, and the second point of interest has a different value from the previous point of interest. For a brief demonstration, we will consider the following water table example: the recorded water table information for E Area was gathered from the Environmental Restoration Data Management System (ERDMS) database. The purpose will be to predict the water table elevations within E Area at certain unmeasured locations. The method of interpolation will be kriging.

The underlying assumption of the kriging methodology is that of stationarity. This assumption, more correctly called second-order (or weak) stationarity (or statistical homogeneity), requires the mean and the variance to be constant in space and the covariance to be only dependent on the separation vector [2] This is one of the reasons why water table elevation was chosen. Water table elevation is a continuous function and should be dependent on the separation vector. Some things, such permeability, could be non-stationary due to the geological layers, zones, or facies which have varying properties. However, in order to krige, specifically in geostatistical arenas, a valid variogram must be supplied (sometimes referred to in literature as a semivariogram). In these cases, the variogram can be approximated by the model function that ensures validity. The three variogram types of interest are spherical, Gaussian, and exponential.

Again, the most useful software package for kriging was the SAS System for Windows as it provides an easy mechanism for graphing uncertainty. Additionally, the particular function used can handle anisotropy which is useful in part of the analysis. In order to properly krige, there must be a variogram for the desired data set which generates two of the parameters used in the actual kriging. Therefore, the 'proc variogram' statement in SAS was used to create a variogram from the GSA clay data. Typically, one tests the three main variogram types (spherical, Gaussian, and exponential) against one another, but in this case, there was no pragmatic difference in the resulting surface, thus the outcome was not dependent on the model selected. The spherical model was chosen arbitrarily.

Additionally, the kriging process refers to a process for interpolating a spatial distribution in a method similar to the least squares approach where an unknown location x_0 has a corresponding value calculated from observations $z_i = Z(x_i), i = 1, \ldots, n$ of the field at nearby locations $x_1, \ldots, x_i$. It computes the best linear unbiased estimator (BLUE) $\hat{Z}(x_0)$ of $Z(x_0)$ based on the semivariogram $\gamma(x,y)$. The kriging estimator is $\hat{Z}(x_0) = \sum_{i=1}^{n} w_i(x_0) Z(x_i)$, where w_i is the weight for $i = 1, \ldots, n$ such that the variance is minimized [1].

As a result, the kriging interpolation is a system of linear equations:

$$\hat{Z}(x_0) = \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix}' \begin{pmatrix} c(x_1,x_1) & \cdots & c(x_1,x_n) \\ \vdots & \ddots & \vdots \\ c(x_n,x_1) & \cdots & c(x_n,x_n) \end{pmatrix}^{-1} \begin{pmatrix} c(x_1,x_0) \\ \vdots \\ c(x_n,x_0) \end{pmatrix}$$

and the associated error is:

$$Var\left(\hat{Z}(x_0) - Z(x_0)\right) = \underbrace{c(x_0,x_0)}_{Var(Z(x_0))} - \begin{pmatrix} z_1 \\ \vdots \\ z_n \end{pmatrix}' \begin{pmatrix} c(x_1,x_1) & \cdots & c(x_1,x_n) \\ \vdots & \ddots & \vdots \\ c(x_n,x_1) & \cdots & c(x_n,x_n) \end{pmatrix}^{-1} \begin{pmatrix} c(x_1,x_0) \\ \vdots \\ c(x_n,x_0) \end{pmatrix}$$

where c is the covariance function $c(x,y)=Cov(Z(x),Z(y))$ [1]

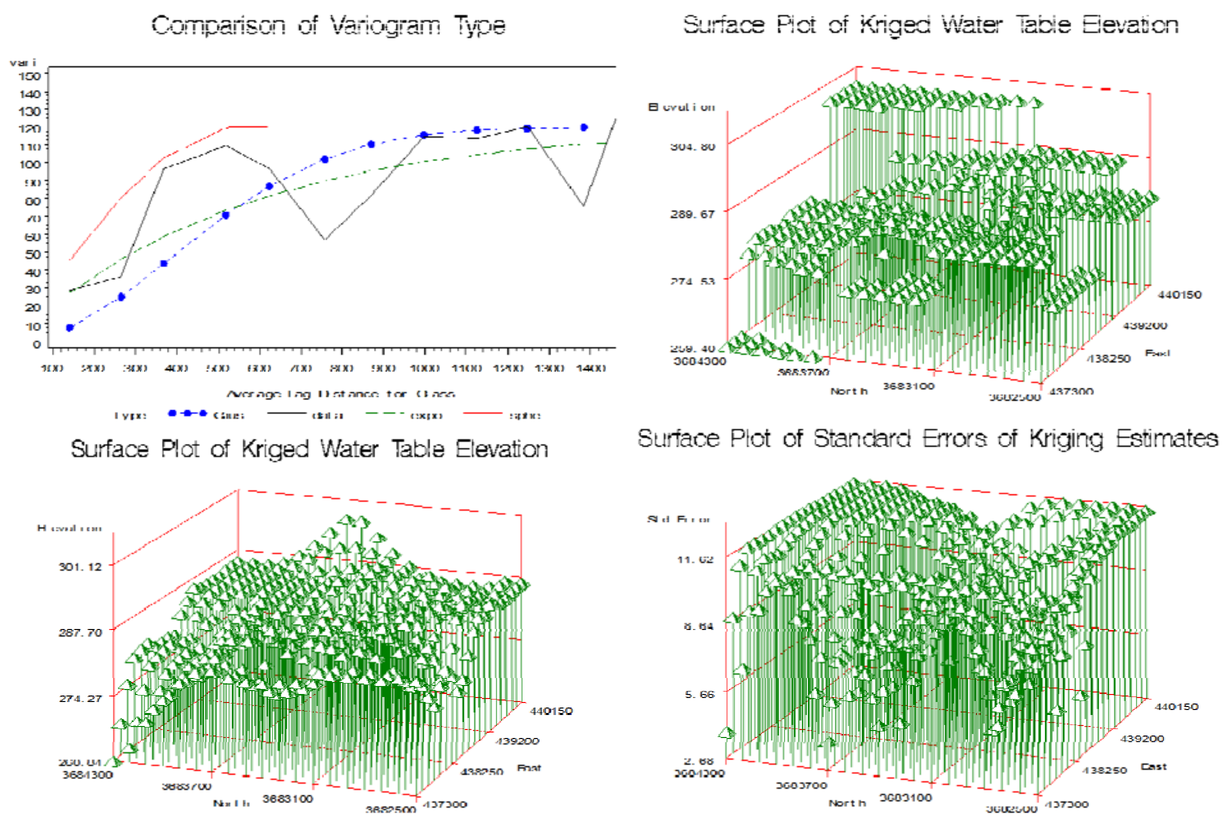

Figure 2: Variogram comparison and resulting kriges with associated error

Figure 1Figure 2 demonstrates the results of the variogram types. From this, one can see that the spherical variogram reaches the horizontal asymptote the most quickly, and thus is the best choice for the kriging of the data. The bottom two plots contain the kriged water table surface elevation and the error associated with this. Particularly for performance assessment, this is a very integral part in the analysis as the changes in data that affect the uncertainty can easily and graphically be depicted. The top right plot of Figure 2 is particularly of interest as it foreshadows the results from the clay study. The stepped plot result is due to decreasing the size of the bins for the water table so, for each stepped area, the bins are only capturing several measurement points. As a result of this the interpolation is much less comprehensive, and it is typical of responses surfaces with very limited data.

The clay distribution has very limited data. Due to the sparse data, this analysis tends to be an exercise in mapping uncertainty. However, this actually is useful as there is a need for uncertainty to be addressed in Performance Assessment settings. In any event, only eleven suitable locations provided data, albeit at several different depths each. Most authorities insist on thirty points at a minimum to krige properly. Obviously, this was evident from the outset and should be taken with a grain of salt. In terms of the uncertainty, the sparse data is actually more beneficial as the average value of the uncertainty is significantly greater than would be from a more robust data set. This serves to highlight differences in the uncertainty both in surface itself as well as in comparisons with similar but different methods.

To a certain extent, the clay surface that results is only a very broad one. As expected, the uncertainty tends to be highest furthest from the high density of location data. As a result, there is a corresponding area in the middle of the surface as well as at every edge where the predicted surface is nonsensical. In these cases, the estimates of percentages go above 100 and negative, respectively. Certainly, this is hardly appropriate. Thus, the only relevant surface data that can be discerned is near the groups of points, particularly in two main groups.

RESULTS

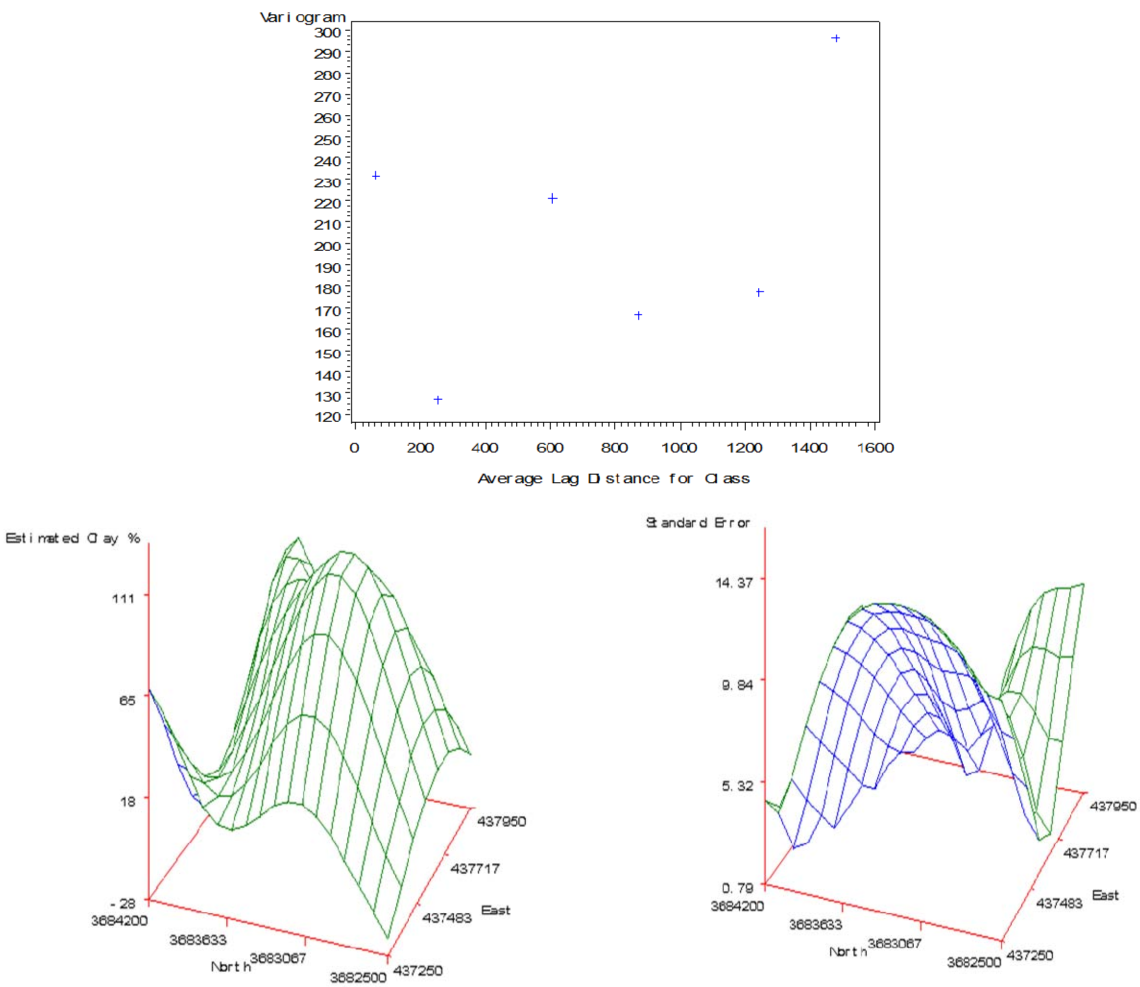

Figure 3: 11 point Krige-Variogram, Surface, Error Surface

In the top part of Figure 3, there is no distinct trend that is apparent for this variogram. In terms of 'fitting' a model to the data, there is no model that fits this particular arrangement with any great degree of accuracy. However, through trial and error, it was demonstrated that all three of the main model forms seem to have approximately the same surface regardless of variogram fit.

The surface from this particular example demonstrates the cautions that must be used in a kriging approach. Obviously, there is no realistic meaning for a percentage of over 100% or for a negative percentage, yet the surface in the bottom left of Figure 3 includes both. This demonstrates the danger of extrapolation in kriging.

Kriging is mostly an intrinsic method that excels at interpolating, but it is very weak at extrapolating. Once out of the data set, in this case, outside the location clusters where the borings are, the kriging values are much less reliable. What kriging does is find a trend from the outlying few points that are collected in bins on the edge of the data set. This trend or trends is continued, so when the data indicate that there is a rapid rise in clay percentage, kriging continues this trend into areas with no or very sparse data. This results in a bin with few, single, or no measurements in it where the trend is assumed to continue. The underlying assumption of isotropy in kriging tends toward this overall indication as this assumes that there would not be a deviation from this apparent trend.

In Figure 3, the interpolated values are reasonable. However, in the sections that are further from data, the hill of values of over 100 and the drop to below 0% appear. The hill appears in the gap that is apparent in Figure 1 between the more northern cluster and the more southern cluster and associated locations. As a result, the only useful output from the clay surface is in the immediate vicinity of each of these clusters separately.

For the extrapolation between the clusters, there is apparently a trend upwards of the clay percentages, and this trend is continued into the void of available data. When it peaks, it has become meaningless; also the peak indicates the intersection of the upward trend coming south from the northern group and north from the southern group rather than an actual petering out of the trend.

As shown in the bottom right of Figure 3, the error associated with the kriging varies spatially in a drastic manner. The error is smaller near the areas where the points are more closely concentrated and higher in areas where the points are more spaced. The increased error is a result of the increased distance between the points which introduced error into the variogram.

The error in the clay distribution is high from using kriging in this instance. In places, it is about half of the value of the actual clay percentage. However, as previously mentioned, it is highest in the areas of the map that have few to no points. It is somewhat difficult to discern the graph, but the blue grid is intended to be the underside of the surface while the green is the top of the surface. Also, it is not entirely visible, but there is a hump in the middle, corresponding to the peak of over 100% in the bottom left of Figure 3. Once past this hump, the error is uniformly lower, in the range of 2.5-4.2%, which is a much better estimate, as well as being appropriate to the northern cluster.

Addition of a Data Point to Reduce Uncertainty

In a departure from the previous methodology, we hope to demonstrate that a dramatic and vast reduction in uncertainty can be obtained from a strategically placed newly obtained measurement. This is not to say that this has been optimized for the greatest reduction in uncertainty that could exist, but merely to serve as an example of the kind of reduction that results from such an attempt. The methodology here is that we added a single data point with a value that seemed reasonable in a spot of particular influence. The manner in which selection or the location is made is very simple: choose the location with the highest uncertainty.

In this attempt, the point was added into the gap between the northern and southern groups of points. To better enable comparison, we again used the spherical form to calculate the kriging and variogram. The only difference in the calculations is the addition of the added point.

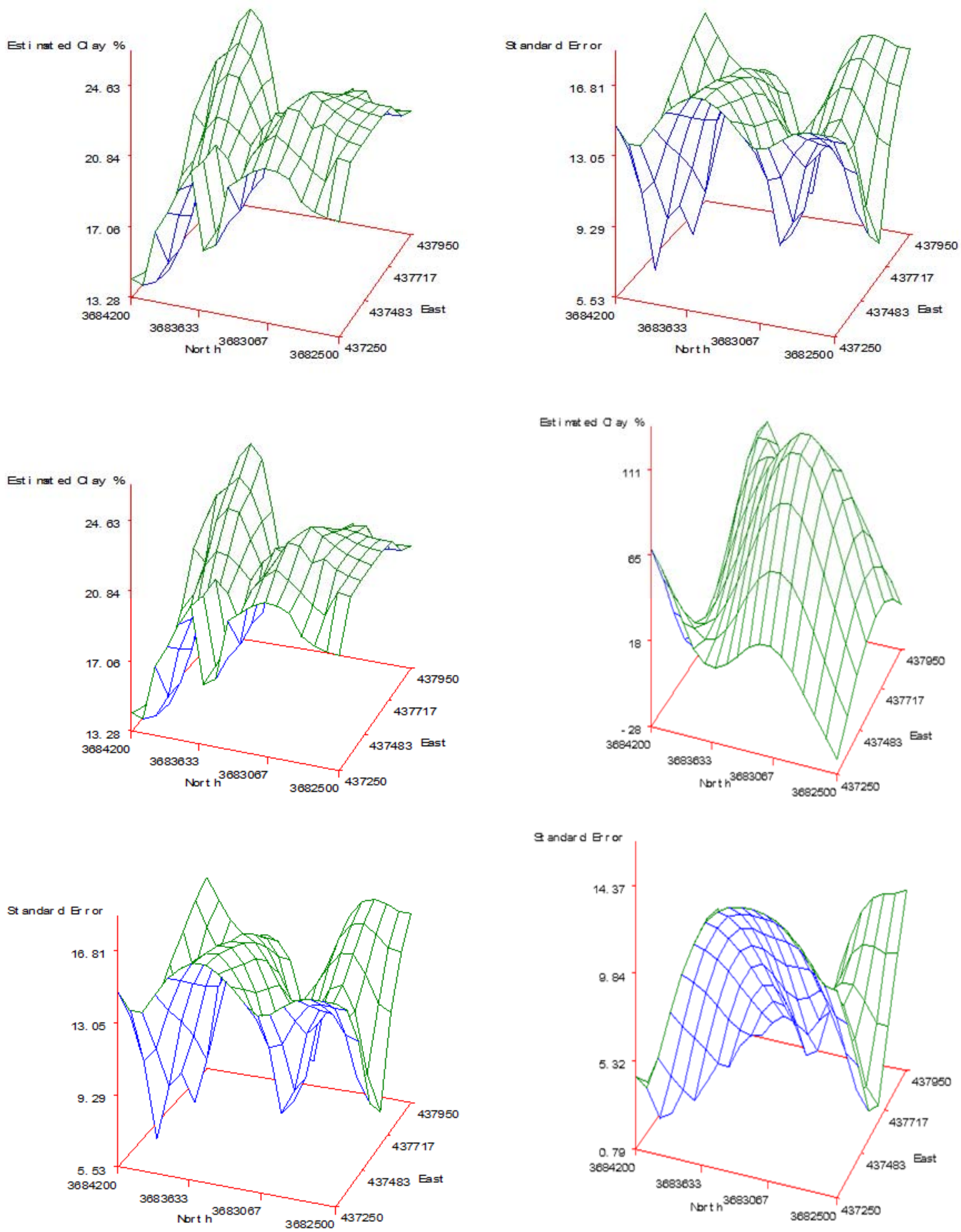

Figure 4: Adding a data point

Figure 4 shows the results of adding a data point in a region of high uncertainty. The top plots show the added point kriged surface (left) and its associated uncertainty (right). The middle plots show a comparison of the add point kriged surface (left) and the original kriged surface (right). The bottom plots show a comparison of the standard error of the added point (left) and original (right). In the comparison of the middle left of Figure 4 and the middle right, one can see the dramatic difference that a single well-placed point can make. Compared to original kriged clay surface, for the added point kriged surface there is a substantially more reasonable response surface. In fact, this surface is entirely plausible throughout its range in both north-south and east-west directions. The standard error, interestingly enough, is not reduced substantially. This is due to the fact that there is less extrapolation area now that there is a point in what used to be the great hole in the middle of the data set locations.

From the comparison of the bottom left and right of Figure 4, one can see that the standard error has not shrunk an appreciable margin. The fact that the standard error is still relatively high results from the fact that, even with a well-placed point, there has only been one point added. The data set is still very sparse, and the location of the point, while affecting the predictive abilities of the process, cannot overcome the severe lack of data. However, the importance of adding points, even a single point, when placed correctly, cannot be overestimated. Following the process of selection a location where the uncertainty is high **or** selecting a place where there is obvious extrapolation is of great benefit in terms of building a working knowledge of an area's actual composition. To build a greater and more accurate clay surface, at least one, but even several more points should be taken into consideration for bore sites.

CONCLUSION

Being a somewhat short research project, this has a remarkably simple conclusion. We have used the clay data to determine to what extent we could reduce an uncertainty based on a bore hole location. As seen in Figure 3, choosing a point (in Universal Transverse Mercator (UTM) coordinates, North: 368067, East: 437500, Clay Percentage: 24), based on a suspicion of extrapolation as well as being an area with a high uncertainty, greatly increased the applicability of our clay response surface. It greatly mediated the extrapolation that caused the middle of the graph to summit at over 100% clay. Additionally, contrary to expectations, it did not substantially reduce the uncertainty. This seemingly opposing trend indicates that there are several factors to account for during the review of the data, not merely the uncertainty. It does reduce the uncertainty, but not nearly to the extent that adding 5 or 10 more poorly placed points would. The existence of trending in the kriging is very important to notice. In many cases, it would not be as obvious as this (going above 100% or below 0%), and it would be more affecting of outcomes. Oftentimes, doing something as simple as adding a point in an area that appears to be trending can reveal that there may, in fact, be a trend due to a variety of reasons, not the least of which is lack of data.

The main way in which the analysis and predictive abilities can be improved is to get more data. For spatially distributed data, there can be different ways to approach this, but for those concerned with uncertainty, kriging appears to be best, certainly the easiest, manner in which to analyze the associated error.

According to surfaces generated by existing data, we can be more certain as to the best and most influential location of the additional data. Specifically, these points would be most beneficial in areas of either very high uncertainty or in an area of the kriged surface with a distinct and clear trend of extrapolation.

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