CHAPTER 2

JACKKNIFING & LATIN-HYPERCUBE SAMPLING

Uncertainty is associated with interpretation of the subsurface, and stochastic simulation techniques are incapable of accounting for all the uncertainty, if only a single deterministic semivariogram model is utilized. Jackknifing the sample data bounds the limits of model semivariograms, but typically indicates that a large number of simulations must be conducted to consider the full distribution of possible semivariograms. Latin-Hypercube sampling, particularly when combined with expert opinion reduces the number of simulations that must be created and evaluated. For small data sets, where there is significant uncertainty, this process provides for a more complete assessment of the potential variability of the subsurface and of flow paths for contaminants, given the available data. Such assessment can be used to guide the data collection program and decision making process.

2.1: Introduction

Hydrogeologists recognize that heterogeneity of hydraulic parameters has a major influence on groundwater flow and contaminant migration. Inaccurate description of the subsurface when modeling contaminant transport in groundwater systems can result in selection of inappropriate remedial actions. Identification and characterization of continuous high hydraulic conductivity units of complex geometry, which can dominate contaminant transport, is difficult because the amount of drilling that can be undertaken to characterize the site is less than desired, either due to expense, inaccessibility, or potential for creating pathways for contaminant migration. Thus, the modeler must settle for estimating the range of possible solutions, i.e. the modeler must evaluate the uncertainty in the site definition, and determine how each alternative subsurface interpretation may affect contaminant migration.

At this time, the best approach is to integrate all available data from a site into a range of possible subsurface interpretations and then consider the probability of satisfactory performance of alternative remedial actions. Multiple indicator conditional simulation (MCIS) blends indicator kriging and stochastic simulation to statistically evaluate the range of possible subsurface geologic configurations. Knowledge of the range of possible subsurface conditions aids the modeler in defining best, worst, and most likely case scenarios as well as the probability of occurrence of particular scenarios given the available data. To date, such simulations have been carried out at the level where the kriging matrix is solved, without incorporation of the uncertainty associated with definition of the semivariogram. Such an approach is based on the assumption that the specified semivariogram models are absolutely correct, but this is often not true, particularly when one considers the limited data usually available at a typical hazardous waste site. In such a situation use of the estimation error to evaluate the accuracy of the kriging is misleading because it appears to characterize uncertainty associated with the result but ignores the uncertainty associated with selection of the semivariogram. The result of a kriging process is based on the definition of the semivariogram. By evaluating the uncertainty in the semivariogram, the greater range of uncertainty associated with the simulated results becomes apparent. Uncertainty in the simulation process can be more completely evaluated by using methods such as jackknifing , latin-hypercube sampling , and expert opinion in defining the semivariogram models to be used for stochastic simulation. These methods are discussed in this chapter.

Data collection is time consuming and expensive. Data collection can be performed more efficiently by examining data as they are collected, preparing experimental semivariograms, plotting estimation errors, and using the results to select subsequent data types and locations. Some projects have used estimation errors to identify areas of greater uncertainty which can be targeted for further data collection, thus optimizing dollars spent in site characterization . Similarly, evaluation of experimental semivariograms as data are collected can guide the data collection program.

Because data are usually limited, the results of kriging can be misleading; depending on the parameters used to define the semivariogram, the same data can yield different results. Although kriging will produce results that honor the data, the estimated values at locations between sample sites are non-unique. The simple examples shown in Figure 2.1 demonstrate this point. These hypothetical, two-dimensional models represent two distinctly different geologic settings that are indistinguishable by examination of only the well data. The sample data in Figure 2.1a and 2.1b are identical. Of the eleven well borings, six are in fine-grained sediments of relatively low hydraulic conductivity (low K) and five are in coarse-grained sediments of generally high hydraulic conductivity (high K). Ideally more data should be collected, but because of cost constraints or constraints on drilling locations, this may be the only data set that can be used. Because different geologic configurations can yield distinctly different contaminant plumes (Figure 2.2), incorrect modeling of the site, or failure to recognize the uncertainty associated with subsurface interpretation, can result in remedial action that does not accommodate conditions at the site.

It is not sufficient to utilize a program that calculates an experimental semivariogram and selects a suitable model. For good results, the modeler must evaluate the uncertainty of the data. In many, if not most cases, there is not enough data available to clearly and absolutely define the semivarigram, but by incorporating the modeler's knowledge or expert opinion about the site, uncertainty may be reduced, possibilities limited, and reasonable results may be identified.

a).

b).

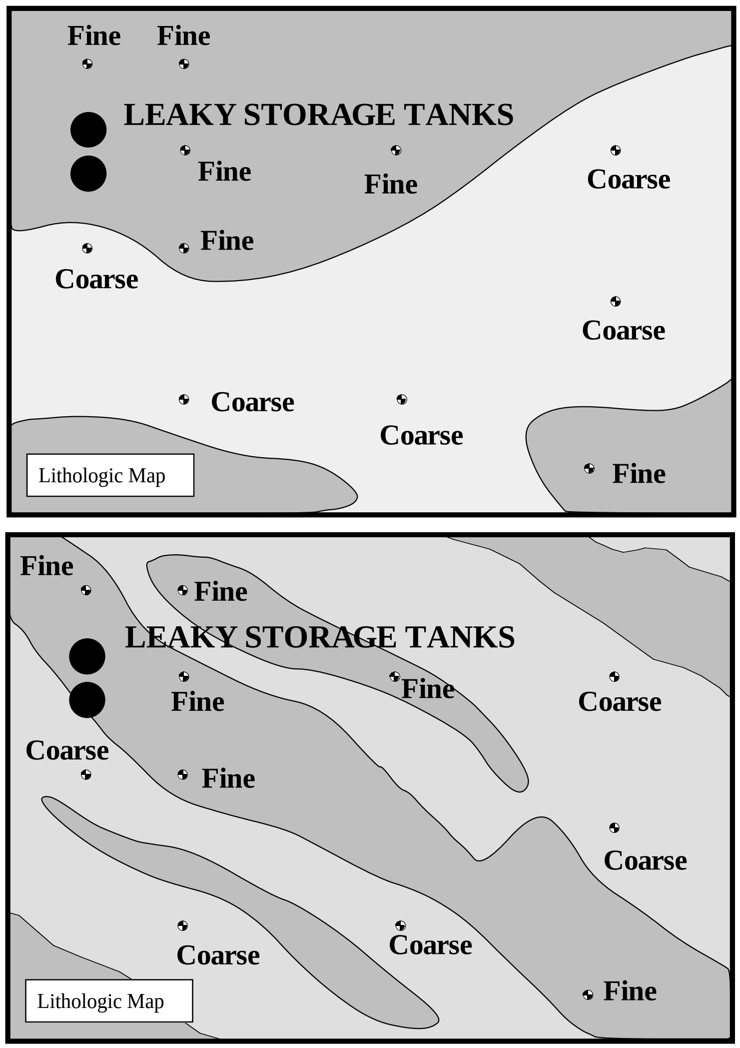
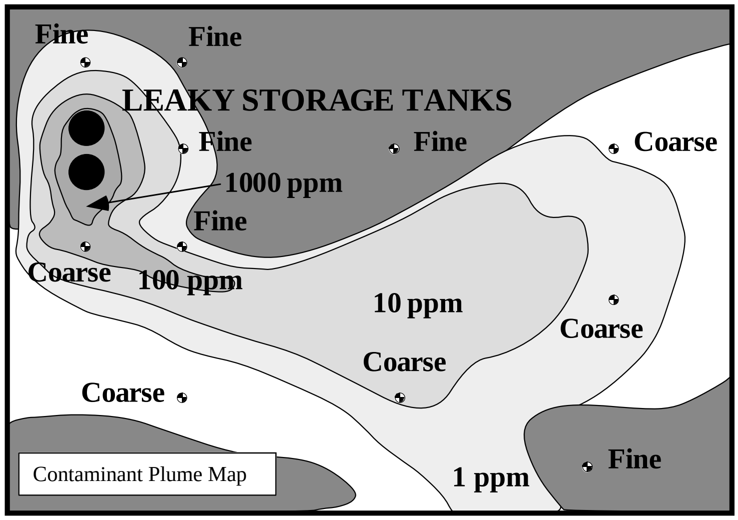


FIGURE 2-1. Borehole data used to interpret the subsurface may not provide a unique solution. In this case, there are eleven data samples; six of fine-grained sediments with low hydraulic conductivity, and five of coarse-grained sediments with high hydraulic conductivity. Although data for each map is identical, the nature of the geology in each map is substantially different. This illustrates that there is uncertainty associated with the interpretation of the character of subsurface at locations that have not been sampled.

a).



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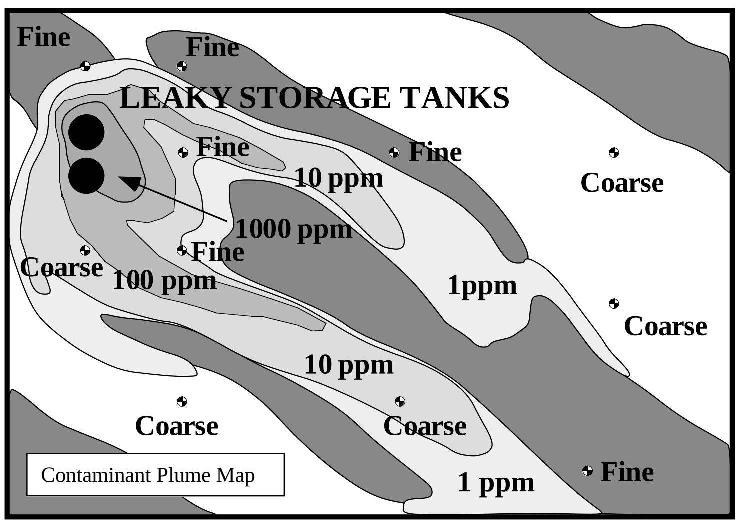

FIGURE 2-2. Contaminants will migrate in different patterns within the two geologic models presented in Figure 2.1. It is important to evaluate the probable alternative scenarios when designing a remediation plan.

2.2: Semivariograms

A semivariogram is a measure of the spatial correlation of a parameter. Samples taken close together are typically more similar than samples separated by larger distances. The semivariogram represents this change in variance with increasing separation distance. The experimental semivariogram ($\gamma^*(h)$) is defined as:

$$\gamma^*(h) = \frac{1}{2N}\sum_{i=1}^{N}\left[z(x_i) - z(x_i + h)\right]^2 \tag{2.1}$$

for a particular lag distance (h), where N = number of data pairs in the search area, and $z(x_i)$ and $z(x_i + h)$ are all the pairs of the N samples within the lag range, h. The search area is defined using a search direction and half angle. The search direction is measured clockwise from North (or the horizontal axis for a cross section) and defines parallel lines along which data of the given lag distance must fall in order to be used in the calculation of the semivariogram (Figure 2.3a). Often data exhibit anisotropy, consequently the experimental semivariogram is calculated in a number of directions. The major axis of the anisotropy is indicated by the search direction of the semivariogram with the longest range (range is the separation distance at which the semivariogram value reaches the population variance and is discussed later). Generally, few data will lie directly along a search direction line, therefore a tolerance angle (defined as the search half angle) is used to include data that are offset from the line (Figure 2.3a). The maximum bandwidth also excludes points that lie well to the side of the search direction. It is useful to note that any search direction accompanied by a search half angle of 90° includes all combinations of orientations of points at each spacing, thus is appropriate when evaluating data with an isotropic distribution.

The model semivariogram, $\gamma(h)$, is a function representing the experimental semivariogram. The distance at which the model semivariogram meets the data set variance is defined as the range (Figure 2.3b). The variance of the sample at a separation distance of zero is called the nugget (Figure 2.3b). This terminology arose in the mining industry where two assays from the same gold sample would sometimes yield markedly different results due to the presence of a gold nugget in one portion of the sample while another portion includes only disseminated gold. The variance of the entire data set is referred to as the sill (Figure 2.3b).

2.3: Indicator Kriging And Stochastic Simulation

One approach for generating alternative subsurface interpretations is indicator kriging combined with stochastic simulation . Indicator kriging differs from simple or ordinary kriging in that a range of parameter values are reduced to discrete indicators (integer values) by defining threshold values.

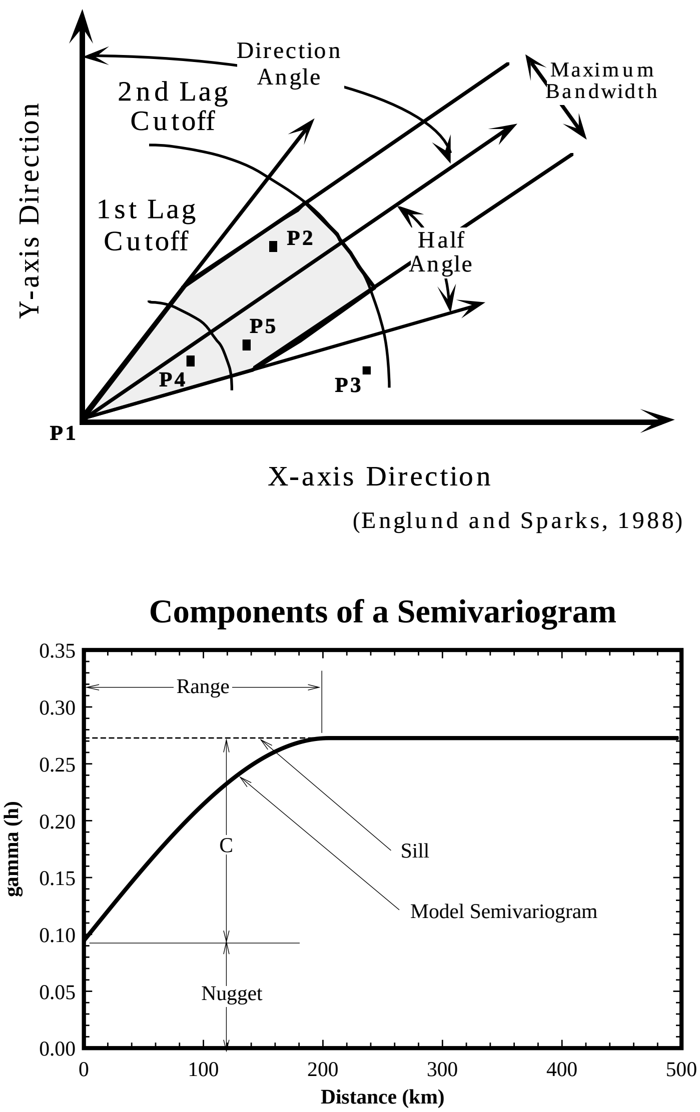

FIGURE 2-3. Features of a semivariogram and parameters defining the search area (after Englund and Sparks, 1988).

For example, materials with hydraulic conductivity less than or equal to $1x10^{-3}$ may be defined as indicator 1, materials with hydraulic conductivity greater than $1x10^{-3}$ and less than or equal to $1x10^{-1}$ may be defined as indicator 2, and materials with hydraulic conductivity greater than $1x10^{-1}$ may be defined as indicator 3. Indicator description makes it possible to krige qualitative parameters such as lithology which could be defined as indicator 1 for silt, indicator 2 for silty-sand, and indicator 3 for fine sand. Suffice it to say, that MCIS allows the modeler to generate multiple interpretations of the subsurface which are distinctly different, but honor all the original data and honor the nature of the model semivariogram . The modeler can use these simulations to assess the uncertainty associated with the subsurface interpretation and to evaluate the affects of the different possible geologic settings on contaminant migration. However, if it is assumed that the range of uncertainty of subsurface interpretations is completely defined by the process, then it is assumed that the model semivariogram accurately represents spatial variation at the site. This assumption is not necessarily correct.

An experimental semivariogram based on the well data from Figure 2.1 is presented as Figure 2.4.

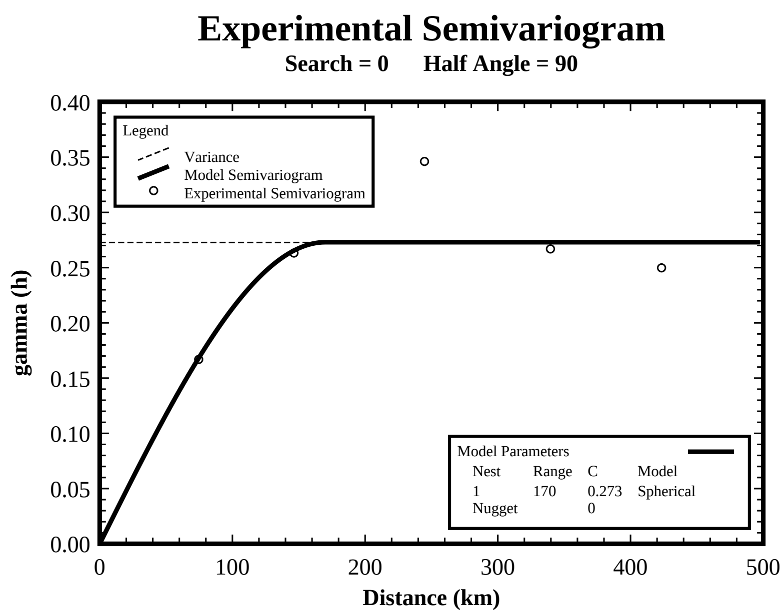

FIGURE 2-4. Experimental and modeled semivariograms developed from the eleven labeled data points in Figure 2.1. A great deal of uncertainty is associated with the modeled semivariogram because of the limited number of data.

For simplicity in demonstrating concepts, only two indicators were employed, one for low hydraulic conductivity materials and another for high hydraulic conductivity materials. Although both models in Figure 2.1 share the same experimental data, semivariograms generated using many data points selected from the two models (1750 points vs. 11 points) are substantially different (Figure 2.5). These semivariograms developed from the extensive data sets illustrate that use of only one experimental semivariogram of the raw data may lead to inaccurate simulations. The actual experimental semivariogram (Figure 2.4) is based on very few points, and arbitrary, simple

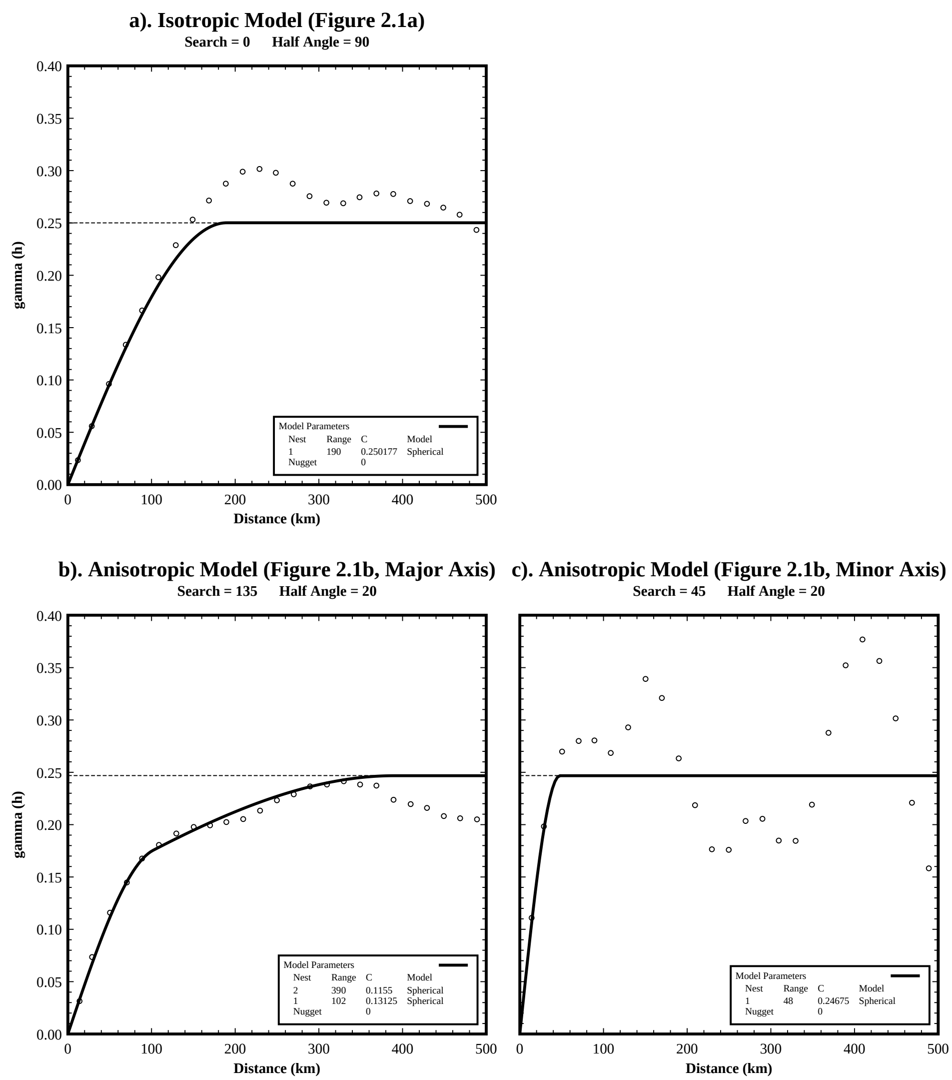

FIGURE 2-5. These experimental semivariograms based on 315 data points from the models in Figure 2.1 were determined by overlaying a regular grid (25’ x 25’) on each model. The distribution of high and low conductivity materials in Figure 2.1a was determined to be isotropic and is described by the model semivariogram in 2.5a. In Figure 2.1b, the distribution is anisotropic and the major and minor axes of the model semivariogram ellipsoid are shown in 2.5b and 2.5c respectively.

assumptions (in this case, a search direction of 0° with a 90° half-angle). When more restrictive searches were analyzed (i.e. searches with different directions and smaller half-angles), it was not possible to define anisotropy in the data. That is, there are not enough data to develop convincing statistics to indicate a distinctly longer range is obtained by orienting the semivariogram in a particular direction. Based on the sample data only, using isotropic assumptions, a spherical model was defined for the experimental semivariogram shown in Figure 2.4. The model parameters are:

Spherical Model: 0° search direction, 90° half-angle

range = 170 feet
C_1 = 0.273
C_0 = 0.00

where C_0 equals the nugget, and C_1 equals the portion on the data set variance, not due to the nugget. This semivariogram, developed from the 11 data points, contrasts to the semivariograms developed from the extensive data sets in Figure 2.5. An extensive data set taken from the model presented in Figure 2.1a yields a model semivariogram (Figure 2.5a) with the following characteristics:

Spherical Model: 0° search direction, 90° half-angle

range = 190 feet
C_1 = 0.251
C_0 = 0.00

This model is similar to the semivariogram model determined using the field data and simple assumptions, and though they are not identical, the simulated results would be similar. Semivariograms developed from the extensive data set for the model shown in Figure 2.1b exhibit a distinctly longer range for an orientation of 135°, yielding a selected model as follows:

(Major-axis) Two-Nested Spherical Model:

135° search direction, 20° half-angle
a_1 = 102 feet
a_2 = 390 feet
C_1 = 0.131
C_2 = 0.116
C_0 = 0.0.

(Minor-axis) Spherical Model: 45° search direction, 20° half-angle

a_1 = 48 feet
C_1 = 0.247
C_0 = 0.0.

where a_i represents the range of each model nest, and C_1 and C_2 represent the non-nugget portion of the data set variance for each nest. Considering the character of the experimental semivariograms developed from the extensive data set taken from the model in Figure 2.1b, the validity of the semivariogram model based on the limited field data and simple assumptions comes into question. These semivariograms suggest that there may be an anisotropic structure in the model. This anisotropy cannot be identified based on the field data alone, and as a result, a multiple indicator conditional simulation using the semivariogram of Figure 2.4 would not properly represent this alternative interpretation.

The purpose of this example is to illustrate that much of the uncertainty in the kriging process is directly accountable to the definition of the modeled semivariogram. The difficulty, however is that, at an actual site, sparse data often result in unsatisfactory experimental semivariograms . Two techniques, jackknifing and latin-hypercube sampling, can be used to address the uncertainty associated with the semivariograms. In some cases, it may also be reasonable to bias the results with expert opinion. Use of expert opinion in formulating semivariograms may lack statistical rigor, but may be necessary to limit the possibilities. Ground water hydrologists are hired for their expertise; exercising it, as opposed to blindly following a statistical method which we know has limitations, can improve results. Of course, hydrologists must remember to keep an open mind about the nature of the subsurface at a site and not assume the presence of trends nor assume a simple pattern (such as that of Figure 2.1a as opposed to that of Figure 2.1b) without sufficient observation.

2.4: Jackknifing

A method for directly measuring uncertainty, error, or confidence limits associated with an experimental semivariogram is not available, because for each lag, there is only a single calculable $\gamma^*(h)$ value. $\gamma^*(h)$ is calculated as the mean of squared differences for a given lag. Therefore, it is not a mean, but a variance of the data for that lag. Initially it may be thought that $\gamma^*(h)$ could be bounded by estimating the variance of the squared differences about $\gamma^*(h)$. However this is not appropriate because this is the variance about a variance which is calculated, using exactly the same data. Not only is such an approach circular and inappropriate, but as should be expected, the variance about $\gamma^*(h)$ increases with separation distance, yielding no useful information.

To circumvent this problem, a process called jackknifing is used . Jackknifing is a procedure where the experimental semivariogram is calculated with one (or more) data point(s) removed from the data set. By repeating this procedure for every point in the data set, a series of n (n = number of samples) experimental semivariograms is calculated. For each lag distance there are now n $\gamma^*(h)$ values. Using these values, confidence limits can be approximately determined, for the mean $\gamma^*(h)$ at a particular lag. When these are plotted, the error bars define the possible range of the modeled semivariogram (given a specific confidence level; 95% is used in this example). The problem with this method is that each mean value ($\gamma^*(h)$) is correlated with the other mean values ($\gamma^*(h)$) calculated at each specific lag (the same data, except for one point, is being used), therefore the variance calculations are not strictly correct . However, this technique is not being used to select the best semivariogram model, which it cannot do . Rather it is used to guide the modeler in optimizing further data collection or identifying a likely range of reasonable model semivariograms.

A semivariogram developed by jackknifing the eleven data points from the models in Figure 2.1 (using a 0° search direction with a 90° half-angle) is presented in Figure 2.6. By examining the

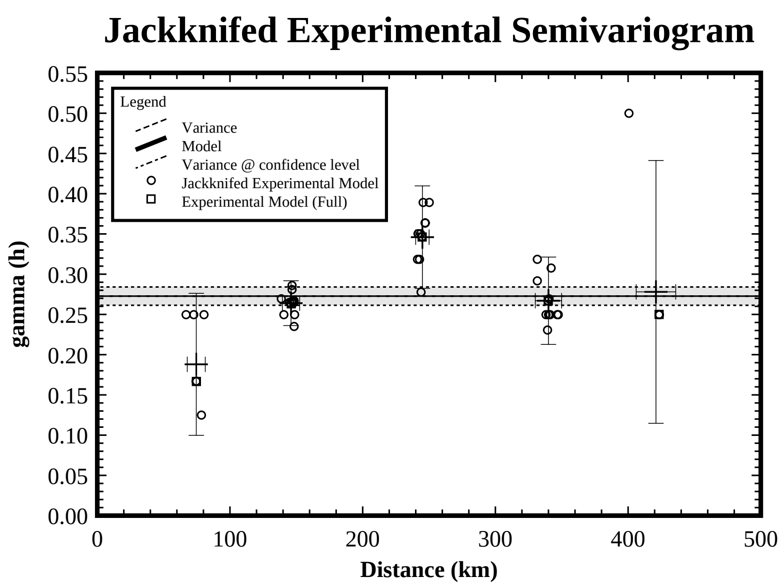

FIGURE 2-6. Jackknifing the eleven data points indicated in Figure 2.1 allows evaluation of uncertainty associated with the semivariogram. The vertical error-bars define the 95% confidence intervals for the mean $\gamma^*(h)$ of each lag. The variance around the mean lag is represented by the horizontal error bars. Each data point represents 1 instance of a jackknifed experimental semivariogram. This experimental semivariogram is based on the assumption of an isotropic material distribution.

error-bars, it can be seen that the modeled spherical range could vary from less than 70 feet to more than 155 feet, but is probably less than 220 feet (error-bars are set at 95% confidence). This compares favorably with the experimental semivariogram shown in Figure 2.5a.

The jackknifed semivariogram does not include the range exhibited in Figure 2.5b where the range of the nested structures, 390 feet, is much greater than 220 feet. This discrepancy occurs because the jackknifed experimental semivariogram in Figure 2.6 is evaluated using all points separated by a given lag distance regardless of their orientation (isotropic conditions were assumed). When the same search windows used to develop the semivariograms of Figures 2.5a and 2.5b are used to develop the jackknifed semivariogram from the limited data set, there is a hint of the character of Figures 2.5b and 2.5c (Figure 2.7). A semivariogram developed using a search direction of 135°

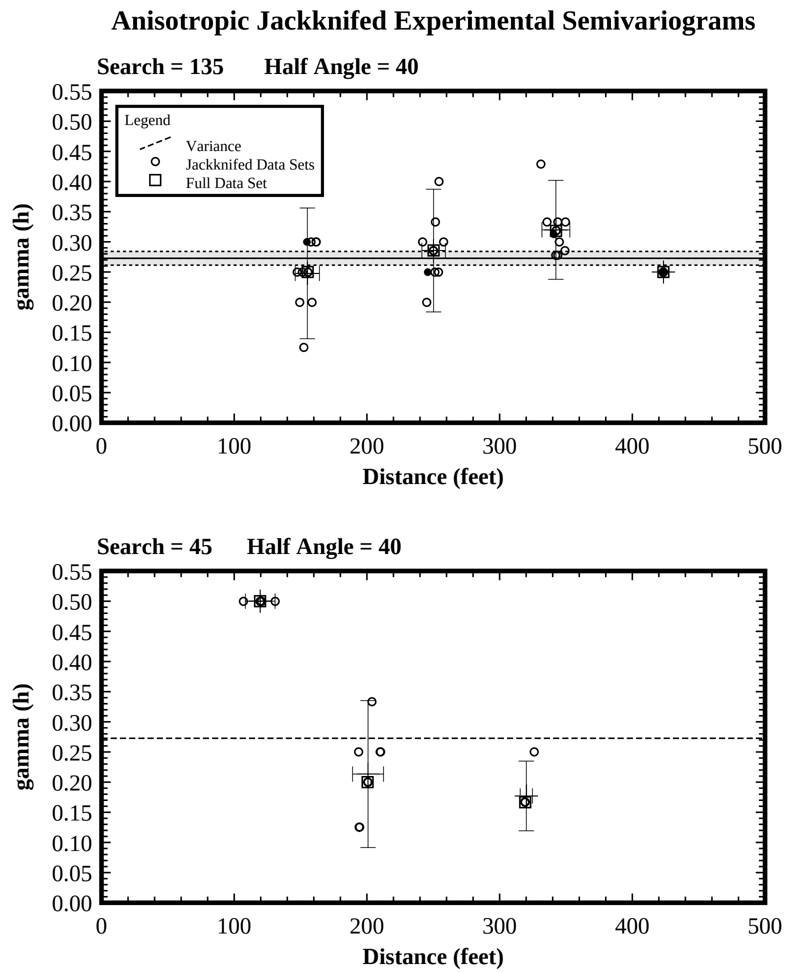

FIGURE 2-7. Although anisotropy cannot be identified by evaluating single semivariograms of the eleven data points, anisotropic character is hinted at when the same data are jackknifed along specified search directions. For a search direction of 45°, the range is likely to be less than 100 feet. In the 135° search direction, the range is likely to be greater than 150 feet, and possibly more than 500 feet. The anisotropy defined in Figure 2.5b-2.5c cannot be determined from the eleven data points, but its possibility is indicated by the data. Symbols are described in the caption of Figure 2.6.

and a 40° half-angle (the initial search used 20° half-angle, but too few pairs were found to be useful) is presented in Figure 2.7a. The range of this semivariogram cannot be determined from the data, but it is likely to be less than 500 feet (use of the extensive data set suggests the range is on the order of 390 feet). A semivariogram developed using the perpendicular search direction of 45° with a 40° half-angle (the initial search used 20° half-angle, but again too few pairs were found to be useful) indicates that the range in this direction is probably less than 120 feet (use of the extensive data set suggests the range is approximately 48 feet). It would be difficult to justify these last two experimental semivariograms, or to identify them without first knowing the exhaustive data set, but the fact that even limited data contain a hint of the underlying structure is important.

The jackknifed experimental semivariogram (Figure 2.6) also suggests that eleven data points are not enough to correctly define the model semivariogram. The data are not even sufficient to determine if the drilling pattern is tight enough to be within the range of the local variance, as indicated by the fact that the upper limit of the uncertainty bars associated with the smallest sample separation falls above the total (population) variance (the sill). This suggests that further drilling (data collection) is required. Given an increasing number of samples, the jackknifed lag variances will decline (Figure 2.8), and ideally, a jackknifed semivariogram will appear more like that shown in Figure 2.8c. Unfortunately, uncertain semivariograms are the norm rather than the exception as indicated by the work of Shafer and Varljen (1990), and the erratic nature of published indicator semivariograms of lithology . The lack of variation in the experimental jackknifed semivariogram illustrated in Figure 2.8c allows the modeler to clearly define the model semivariogram. If the experimental jackknifed semivariogram of lithology at a site had the character of Figure 2.8c, it could be argued that, too much money was expended collecting data; the semivariogram could have been modeled adequately with fewer data (Figure 2.8b). In this case, if jackknifed semivariograms had been calculated while data were being collected, the characterization program could have been terminated sooner or redirected to focus on collecting data to reduce uncertainty in poorly characterized areas of the site (as indicated by areas of high kriging estimation error), as opposed to collecting data that would further define the semivariogram, thus saving time and money.

2.4.1: Additional Comments About Jackknifing

Several other concepts should be considered when using jackknifing in a semivariogram analysis. First, because data points are being removed from the data set to calculate the experimental semivariogram, the variance, and therefore the sill, will generally increase slightly. Second, when a single experimental semivariogram based on all the data is calculated, the results may appear to be easily modeled. However it is difficult to differentiate an experimental semivariogram that represents the true nature of the site, from one that is the product of a fortunate lag selection. Jackknifing provides error-bars which give the modeler insight on the level of confidence which can be attributed to the modeled semivariogram. Finally, jackknifing should not be considered for every data set where the experimental semivariogram is poorly behaved. Jackknifing computationally is very expensive. For N data samples, N + 1 semivariograms must be calculated. As N increases by one, the computational effort to calculate a single semivariogram doubles. As N gets into the hundreds, particularly thousands, the time to compute the uncertainty for a single experimental semivariogram could take days, weeks, or even longer.

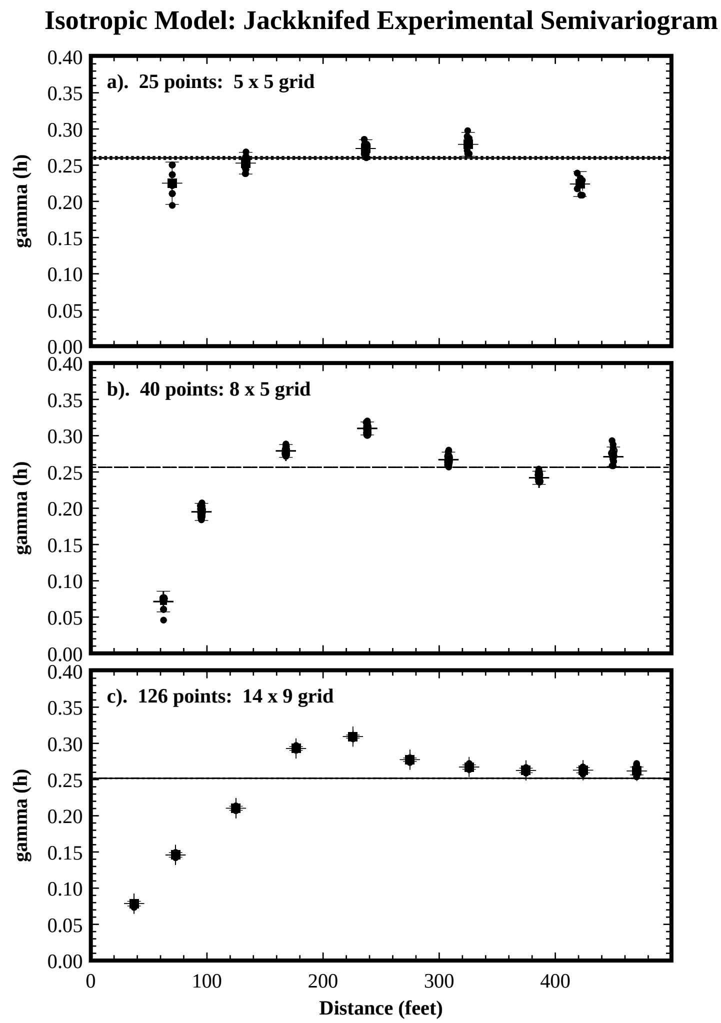

FIGURE 2-8. When a substantial amount of data are collected, the experimental semivariogram may be clearly defined. In this jackknifed simulation, there is little uncertainty in the lag means, and there would be little uncertainty in defining the model semivariogram.

2.5: Latin-Hypercube Sampling

Once the statistical distribution of experimental semivariograms has been calculated, semivariograms can be fit through the zone defined by the error-bars. The objective is not to make a single best estimate of the character of the subsurface (i.e. a single semivariogram), rather the objective is to select model semivariograms representative of the range of possible conditions at the site. This range of semivariograms is used with the original data to conduct indicator kriging and stochastic simulation to generate multiple interpretations of the subsurface. One approach is to use Monte-Carlo techniques and randomly select, for example, 100 model semivariograms that fall within the range of reasonable solutions (Figure 2.9a). This might appear reasonable, but, for

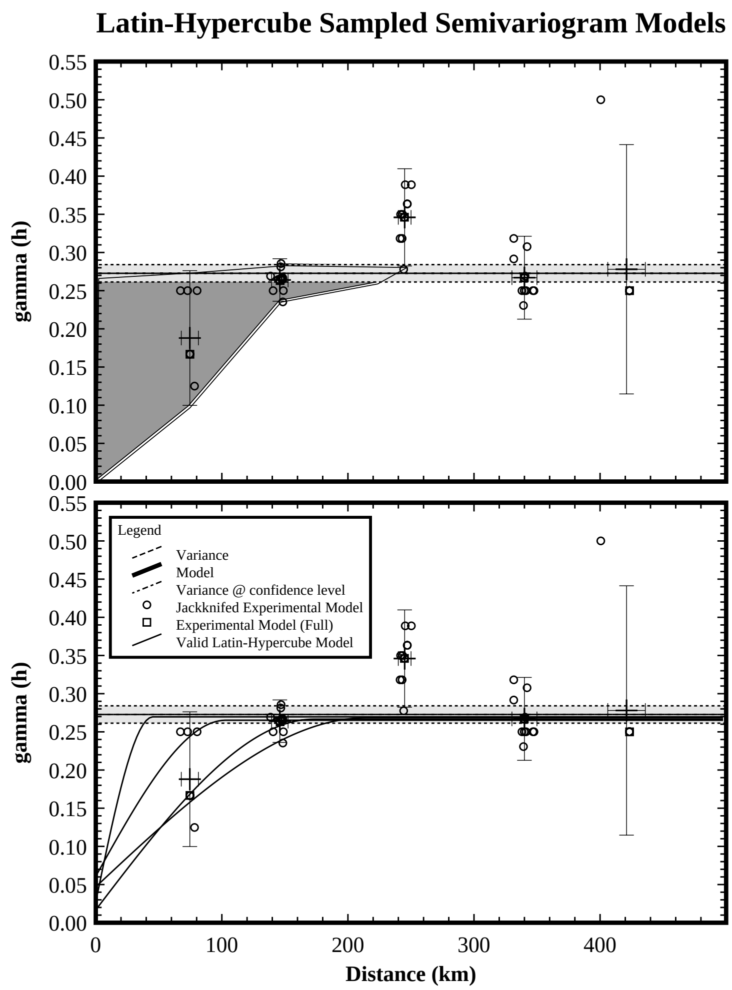

FIGURE 2-9. Reasonable models must be selected from the shaded region in 2.8a to represent the "flavor" of the alternative interpretations of the data. Four model semivariograms with a nugget selected from the lower quartile of possible nugget values are shown in 2.8b. The ranges of the four semivariograms are selected to represent each of the quartiles of possible ranges. Sixteen models would be used to represent the distribution of semivariogram models for the isotropic case. Symbols are described in the caption of Figure 2.6.

example, expert opinion of conditions at the site may indicate that models generated with nuggets approximately equal to the sill or ranges near zero are unreasonable or unrealistic, even though the jackknifed experimental semivariogram in Figure 2.6 indicates such semivariogram models of the site are possible interpretations.

An alternative approach to random selection of a large number of possible semivariogram models is to use latin-hypercube sampling. This reduces the number of simulations required to insure that the ”flavor” of all alternatives is addressed . For this example, one might suggest the nugget must fall within one of four equiprobable regions, and the range also must fall within one of four equiprobable regions. The actual nugget, or range within each region is then randomly calculated (Figure 2.9b). This allows sixteen model semivariograms to be calculated for an isotropic model. For an anisotropic model, the direction and magnitude of the anisotropy can be restricted similarly. This, however requires many more simulations. If the anisotropy factor between the major and minor axis is evaluated at four ratios (e.g. 1.0, 0.5 0.25, and 0.125 or some other ratios as determined from jackknifing the data to obtain a semivariogram in the direction of the minor axis of anisotropy), the number of semivariograms is increases to 64. If the search directions, 0° to 180°, are divided into four directions (0°, 45°, 90°, and 135°), the number of semivariograms is increases to 256.

This approach can yield a daunting number of simulations, many of which will bear little resemblance to one another if the data set is small. Such a situation results in the obvious conclusion that some data sets provide so little information about a site that more data should be collected before further assessment is undertaken. If the data are more abundant, the range of possible models will be constrained, and the simulated models may represent a modest range of possible subsurface interpretations. If the jackknifed semivariogram has small error-bars, as in Figures 2.8b and 2.8c, the entire process of using a variety of semivariograms for simulation of one site can be omitted because the process is not likely to indicate a larger uncertainty associated with the interpretation of such well characterized sites.

Recall that the objective of this approach is not to make a single best estimate of the subsurface interpretation, but to evaluate the possible range of subsurface character based on available data. From a purely mathematical approach this may be computationally intractable, however incorporation of expert opinion into the process makes it possible to limit the reasonable alternatives.

2.6: Expert Opinion

Thus far, only mathematical techniques for describing the subsurface have been discussed, and only field data from wells at the site have been used for interpretation of the subsurface configuration. Two points are important to consider; 1) these mathematical techniques do not necessarily honor geologic laws, and 2) hydrogeologists often know more about the site than the borehole data suggest.

The process of stochastic simulation uses probabilities to estimate a value at a grid location. Unfortunately, these probabilities are based on measured values near that location and, consequently, geologically impossible configurations can be simulated. For example, the "law of original horizontality" and the "principal of stratigraphic superposition" are readily broken. Eventually techniques that incorporate these concepts into stochastic simulation will be developed . Until that time, such simulations must be identified, deemed unreasonable, and discarded.

Although creation of such geologic fallacies cannot be prevented with the current simulation process, the simulations can be improved by incorporation of geologic knowledge from analog sites. An expert can infer more information about the site than is evident in the borehole data. For example, and expert may know that sand lenses in the area tend to be between 10 and 25 feet thick. The borehole data at the site may be too sparse to determine this range of thickness, but knowledge from analog sites in the area may render it reasonable to assign a range of 10 to 25 feet to the vertical modeled semivariogram. Although such action is not based on data from the site, knowledge of analogs adds information to (decreases uncertainty associated with) the simulation process. If the site is made of horizontally bedded alluvial deposits, there is no reason to run simulations which assume the material distribution is isotropic. In such settings, units are generally continuous for greater distances horizontally than vertically. The modeler may be able to confirm the presence of layered anisotropy by demonstrating that semivariograms with different search directions and limited half-angle and bandwidths have the potential to have different ranges. Even if the indications are sketchy, due to scarcity of data, the modeler can limit the simulations to produce only reasonable interpretations given the local geology. Similarly, anisotropy may be present in lateral directions and geologic knowledge of directional trends of lenses or channels may be used to limit the number of orientations considered for semivariograms which will, in turn, limit the number of simulations that must be undertaken.

There is little reason to evaluate solutions that are mathematically possible, but geologically improbable. Discarding geologically improbable solutions adds "bias" to the results that may have to be defended later. However omission of the bias means that we do not use all the information available to us. When expert opinion is used wisely, the bias is likely appropriate, and will speed the site evaluation, thus limiting exploration and analysis costs.

2.7: Results

Four examples are presented to illustrate the process of multiple indicator conditional simulation using latin-hypercube sampling of a jackknifed experimental semivariogram. The differences in these simulations demonstrate the variability of subsurface interpretation that is obtained using the limited data given in the example in Figure 2.1.

These simulations were created using the MCIS code ISIM3D . The map area was modeled in two-dimensions using a 50x35 grid, with ten foot square grid cells.

Simulations resulting from use of the modeled semivariogram using the extensive data set (Figure 2.5a) are presented in Figure 2.10. These simulations differ significantly from the model because

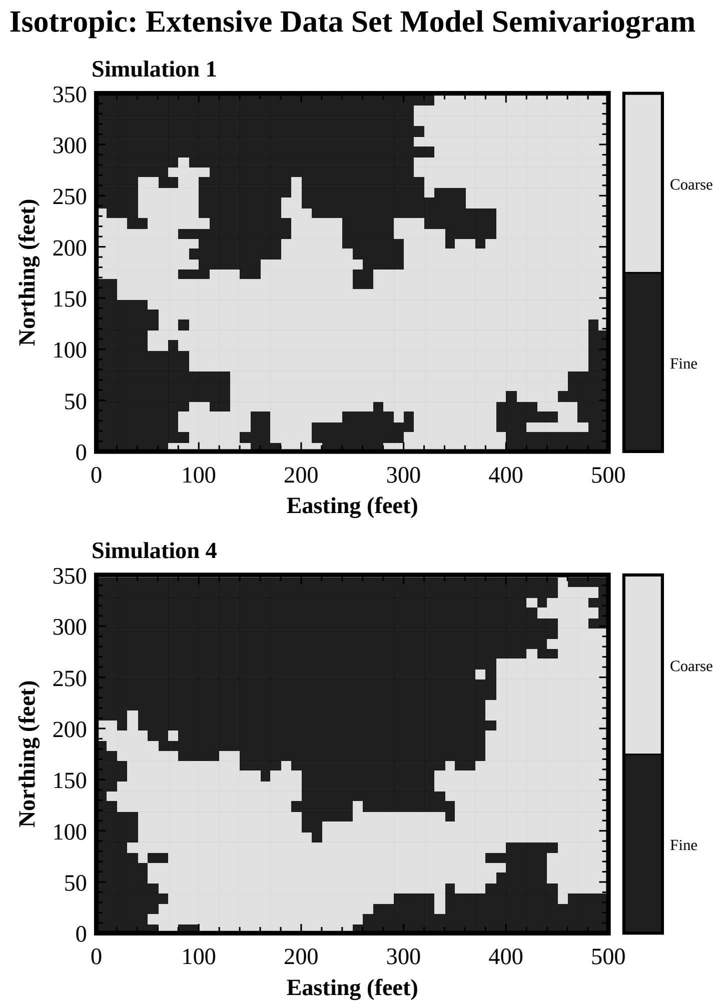

FIGURE 2-10. These two simulations were generated assuming isotropy and using the model semivariogram developed from the extensive data set and illustrated in Figure 2.5a. The solutions are a reasonable approximation of the map in Figure 2.1a.

only the 11 data points were used to condition the simulation. Simulations presented in Figure 2.11 are based on a model semivariogram (a_1 = 115’, C_1 = 0.25, C_0 = 0.0) sampled from the jackknifed experimental semivariogram shown in Figure 2.6. Although neither simulation (Figure 2.11a or 2.11b) is identical to the model in Figure 2.1a, they are reasonable approximations considering the limited data. The simulation in Figure 2.11b is particularly close to the model of Figure 2.1a. The

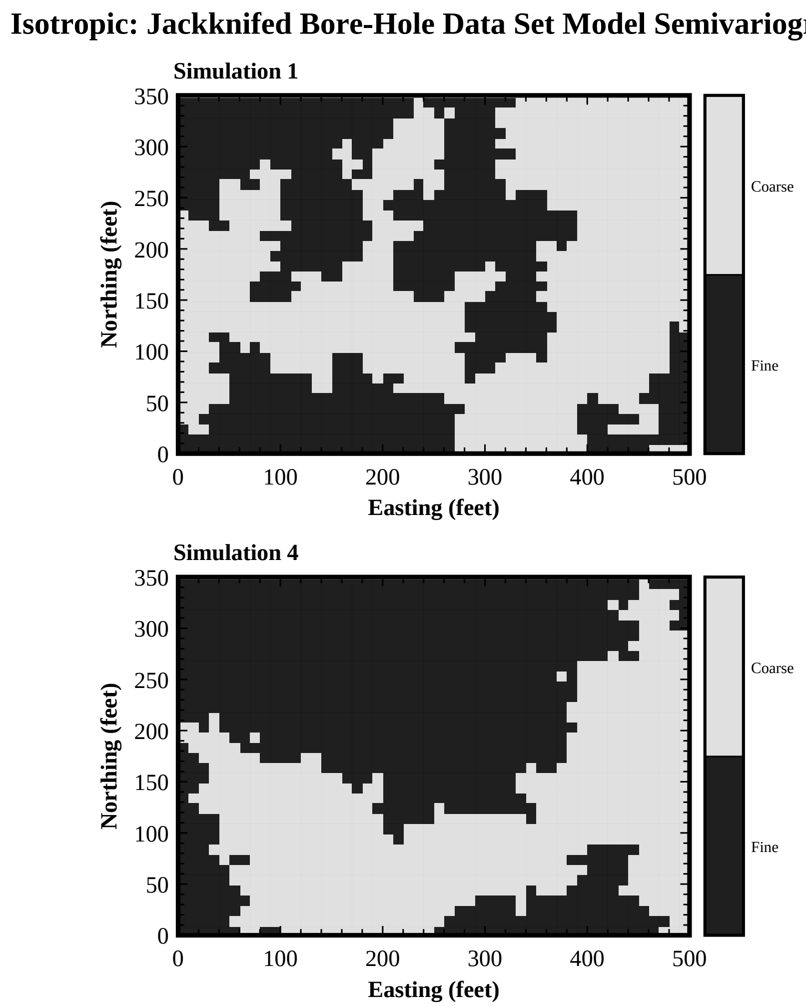

FIGURE 2-11. These two simulations were generated assuming isotropy and using a latin-hypercube sample from the jackknifed model semivariogram (C_0=0.0, C_1=0.25, a_1=115') developed from the eleven data points and illustrated in Figure 2.6. The solutions are a reasonable approximation of the map in Figure 2.1a, and are very similar to those generated in Figure 2.10. Much of the reason that the simulations in Figure 2.10 and 2.11 are similar is that the same random path through the grid was used to simulate 2.10a and 2.11a and another path was used to simulate 2.10b and 2.11b.

appearance of the resulting simulation is rather insensitive to the choice of range (compare Figure 2.11 with Figure 2.10 which was generated using a range of 190’ vs. 170’). Both the experimental semivariograms (Figure 2.5a and Figure 2.6) were developed based on an assumption of isotropic material distribution. The simulations in Figure 2.10a and Figure 2.11a are also similar because the same random path (same random number seed) was used to generate all of the ’(a)’ simulations in Figures 2.10-2.13. A different path was used to generate the ’(b)’ simulations. These isotropic

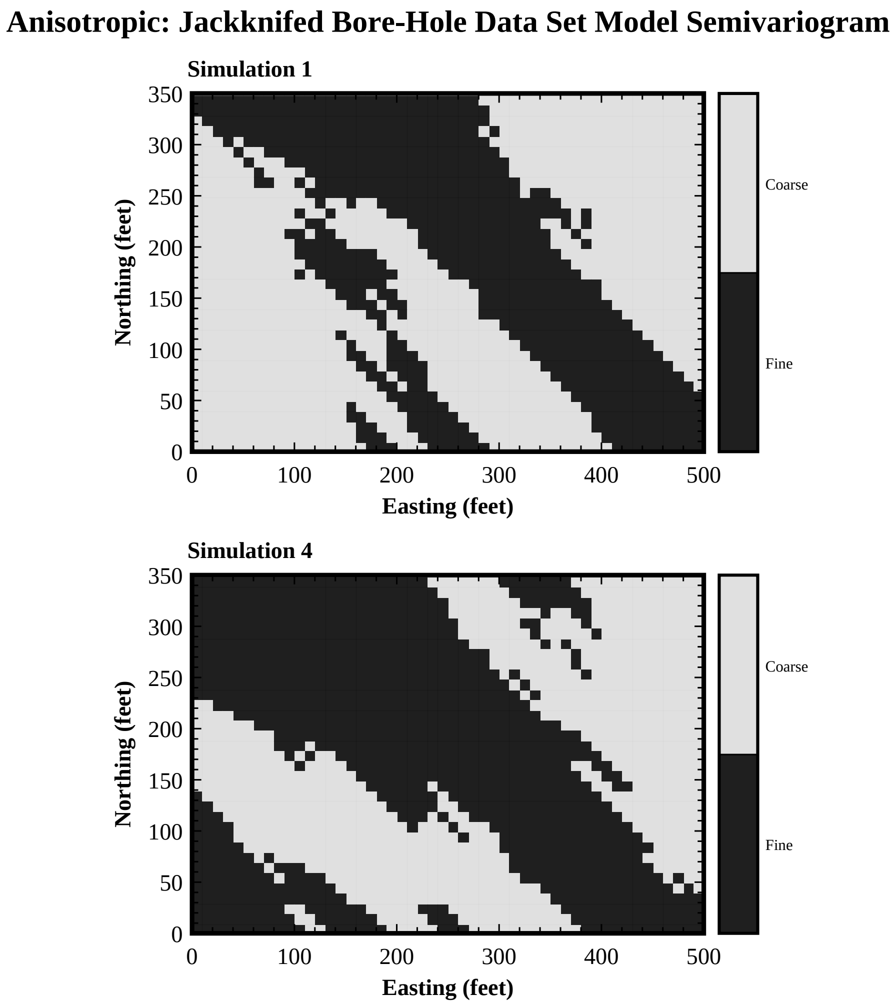

FIGURE 2-12. These two stochastic simulations were generated assuming anisotropy using the jackknifed model semivariogram based on the eleven data points and illustrated in Figure 2.6. The latin-hypercube technique was applied and these are two simulations of a potential 256, as described in the text. Even though the geologic models presented in Figure 2.1 are different, use of jackknifing and Latin Hypercube sampling can produce both configurations from limited data. These solutions are a reasonable approximation of the map in Figure 2.1b. Unfortunately, the method will not indicate whether these simulations or the simulations in Figures 2.10 and 2.11 are the most likely because the data are not sufficient to draw such a conclusion.

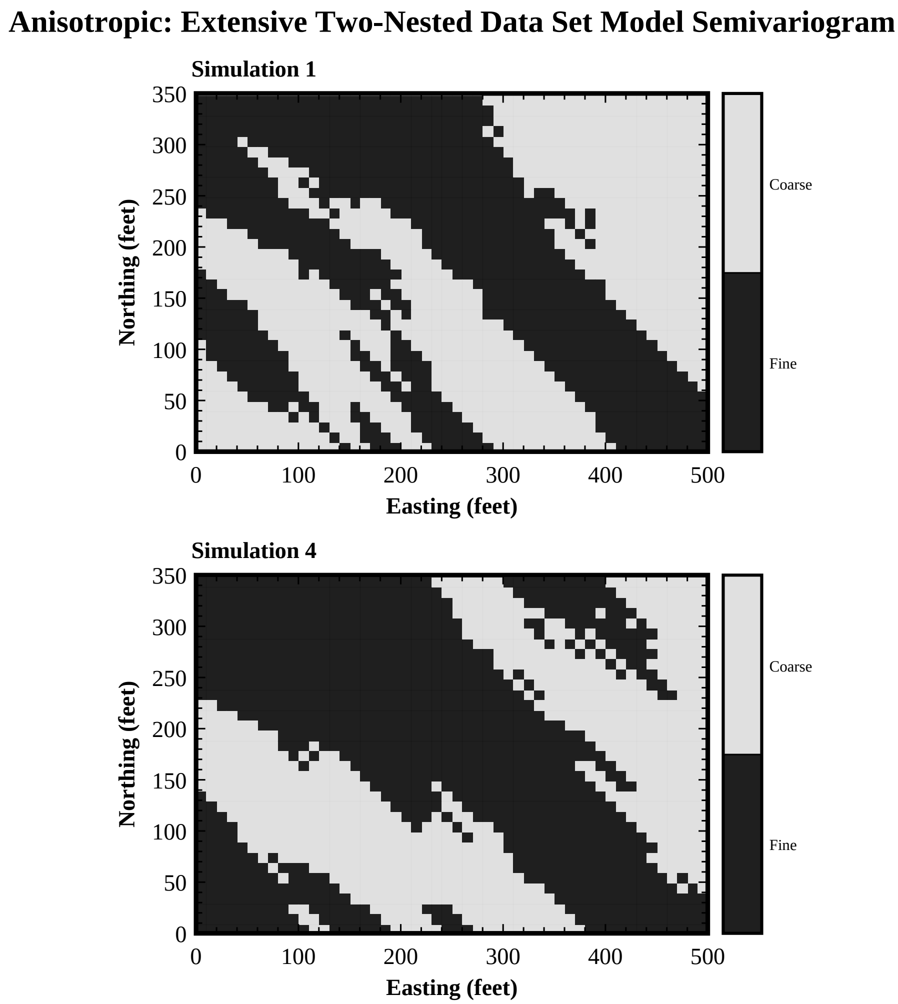

FIGURE 2-13. These two simulations were generated assuming anisotropy using the extensive model semivariogram based on the extensive data set and illustrated in Figures 2.5b-2.5c. The solutions are a reasonable approximation of the map in Figure 2.1b, and are very similar to those generated in Figure 2.12, indicating that extensive data are more important to determining the character of the semivariogram than they are to conditioning the simulation.

simulations bear little resemblance to the model in Figure 2.1b which is a viable interpretation of the data from the 11 field measurements. This inability to represent the full range of possible interpretations is not unexpected.

If expert opinion indicated that the site would be expected to exhibit the locally observed NW-SE trend of high and low hydraulic conductivity deposits, then the simulations presented in Figures 2.10 and 2.11 could be assumed to be less probable. They would be superseded by the probability of occurrence of anisotropic representations of the site. If such expert opinion were not available the two alternative configurations would have to be considered equally likely to occur. The two simulations in Figure 2.12 were generated in the latin-hypercube sampling process, using one of the semivariograms that would fall in the shaded area in Figure 2.9a with a range between 120 and 180 feet (third quartile estimate of range), a nugget between 0.0 and 0.061 (first quartile estimate of the nugget), an anisotropy factor of (minor to major axis) 0.125, a major axis orientation of 135°, and using different random paths through the grid. Although they are not identical to the model in Figure 2.1b, they mimic its nature. When using the range, sill and nugget terms identified by the semivariogram developed from the extensive data set (Figures 2.5b and 2.5c), the simulation results (Figure 2.13) are not significantly different from the simulation results (Figure 2.12) obtained using the jackknifed semivariogram (Figure 2.7), indicating that an extensive field sampling would not improve the character of these simulations but might improve the certainty of occurrence of units with a 135° orientation. That is, more data will improve the certainty of the semivariogram having a given orientation whereas the jackknife approach only indicates the possibility of units having that orientation. Of course, a larger data set improves conditioning of the simulations.

The simulations presented in Figures 2.10-2.13 demonstrate that correct definition of anisotropy is important in order to capture the character of the site. Similar results in paired simulations also suggest that the differences in model ranges are less important than the assumption of isotropy.

2.8: Conclusions

A great deal of uncertainty is associated with interpretation of the subsurface, and simulation techniques are incapable of accounting for all the uncertainty if only a single deterministic semivariogram model is utilized. Typically there are not enough data available at hazardous waste sites to adequately define a single model semivariogram in a rigorous statistical basis.

By jackknifing the data to determine a reasonable range of model semivariograms, and using latin-hypercube sampling and incorporating expert opinion to limit the required simulations, the uncertainty associated with the subsurface interpretation can be more completely assessed utilizing a reasonable amount of simulations. Unfortunately the uncertainty may be so great that little can be concluded about site. However, this is important information because it indicates that more data must be collected before conclusions are made about the site. Given one data sample, one can begin to make interpretations of the site, but quantifying the uncertainty associated with those interpretations is important.

The method presented herein is useful when a significant amount of uncertainty is associated with the experimental semivariogram. If the uncertainty is small, the process only adds unnecessary work. For small data sets, where there is significant uncertainty, this process may be the only way to correctly assess the potential variability of the subsurface, and evaluate potential flow paths for contaminants.

Although the application considered herein pertains to indicator conditional simulation, evaluation of the uncertainty associated with a semivariogram is important whenever a semivariogram is used. Jackknifing is a practical tool for relatively small data sets, but for large data sets, the computational intensity of the jackknifing process may make the process unmanageable.