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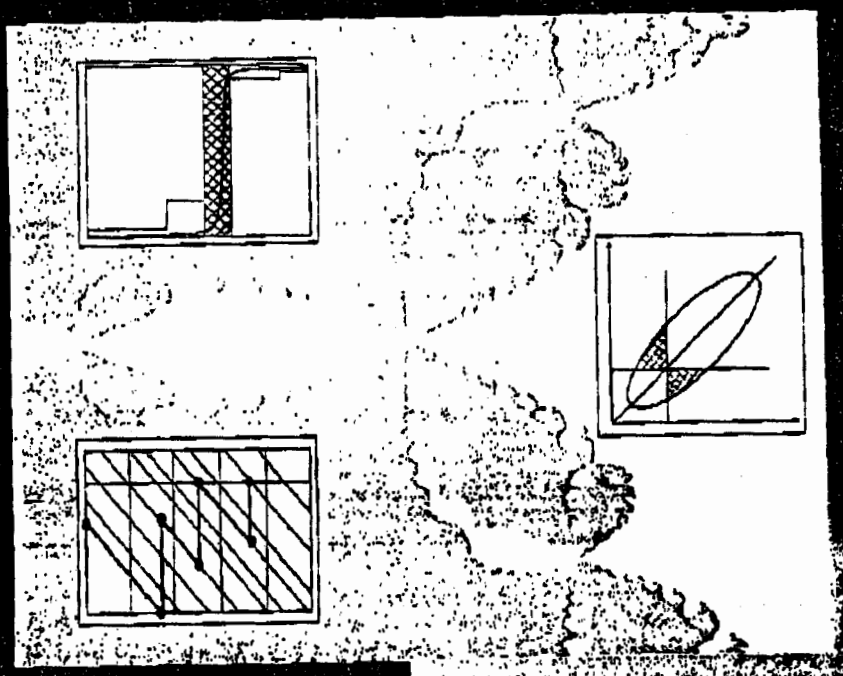
# GEOSTATISTICAL ERROR MANAGEMENT

## Quantifying Uncertainty for Environmental Sampling and Mapping



Jeffrey C. Myers

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## *Quantifying Uncertainty for Environmental Sampling and Mapping*

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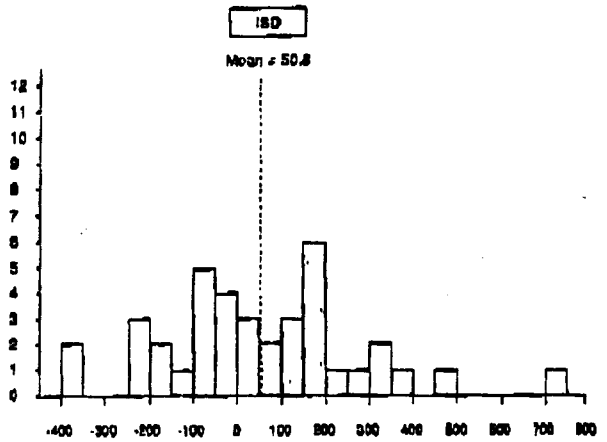



**Figure 3-19.** Histogram of error values resulting from estimation using inverse squared distance.

but the distribution for the kriged estimates is more tightly centered around zero; that is, it has a preferable smaller variance.

## 3.7 Misclassification Errors

Precision, accuracy, and unbiasedness are not the only criteria by which we may wish to select an estimator. In many cases, the statistics of the two distributions will be closer to one another than the two presented here. Equivalent performance makes the selection of an optimal estimator more difficult. In this situation and in situations in which only one threshold concentration is of concern, another procedure may be utilized.

Often, maintaining small errors and unbiasedness will be superseded by classification issues. For example, if an unsampled area has a concentration of 1000 ppm, an estimator will seldom estimate the value of the area to be 1000 ppm exactly. An estimate of 980 ppm might be considered a "good" estimate or a "good" approximation based on the accuracy. Similarly, an estimate of 1010 ppm might also be considered accurate. Note that, in each case (980 ppm and 1010 ppm), the percent error is 2% or less. For spatial estimation, this level of accuracy is considered very good.

For remedial activities, critical threshold concentrations are established for each contaminant of concern. Areas estimated to have concentrations above this

threshold will receive treatment, but areas estimated to be below the threshold will not. Given a strict threshold level, "small" estimation errors or inaccuracies may be quite significant. In the following discussion, the difference between a quantitative error (real minus estimated) will be contrasted with a qualitative error (misclassification).

### 3.7.1 Type I Error: False Positives

Consider another situation in which the true soil PCB concentration of a block area is 22 ppm and the established threshold for remediation is equal to 25 ppm. Any soils estimated to be 25 ppm or above will be excavated and treated. If the block is estimated to have a PCB concentration greater than or equal to 25 ppm (29 perhaps), two errors have been made. The first is the *error of estimation* (29 ppm minus 22 ppm or 7 ppm). The second is the *misclassification* error, so named because the block has been incorrectly classified above the 25 ppm threshold.

Despite a relatively "small" error of estimation, the misclassification error in this case (as well as generally) will have a greater impact on the remedial consequences than will the estimation error. The reason for this is that a treatment decision is being made based on the classification of the estimate. An area whose estimated concentration is above 25 ppm that truly has a concentration less than 25 ppm will be remediated. This remediation is inappropriate and increases the remedial expense to those who are funding the cleanup. This form of misclassification is called Type I Error (Rendu 1980). It is also referred to as *overestimation* or, as discussed in Chapter 1, a *false positive*.

If the estimated concentration had been 15 ppm, the error of estimation would have been of exactly the same magnitude as before (7 ppm vs. 7 ppm). Although the magnitude of the error is equal in both cases, an estimate of 15 ppm places the block in a different material classification. More important, this time it is a correct classification. Despite the 7 ppm error of estimation, this block will not incur inappropriate remedial costs.

### 3.7.2 Type II Error: False Negatives

Type II Error is the counterpart of Type I Error in terms of misclassification. If the estimated concentration of the block described above does not exceed the threshold (21 ppm, for example), the block goes untreated based on the 25 ppm action threshold. If the true concentration of the block is really above 25 ppm, a decision will be made to forgo treatment. This incorrect decision is known as Type II Error, also known as *underestimation* or *false negatives*. In this case, potential future health risk liabilities (of unknown magnitude) arise as opposed to the direct, immediate cost of unnecessary remediation. Even though the long-term liability

may indeed prove to have a cost, it is very difficult to estimate and is beyond the scope of this book.

If the estimation had been 62 ppm, the error of estimation would have been much greater than that for the estimate of 21 ppm. However, an estimate of 62 ppm will cause a correct classification decision to be made despite a large estimation error. Estimation errors for areas with concentrations above the threshold limit are often very large. For example, it is not uncommon for soils PCB concentrations to reach 25,000 ppm or more although the threshold limit may be closer to 25 ppm. Also, in the case of PCBs, the contaminant distribution is often highly erratic, with concentrations exhibiting steep gradients over short distances. Therefore, an area could be estimated to have a PCB concentration of 1000 to 5000 ppm when its actual concentration may be closer to 500 ppm. Nevertheless, the correct classification will be made.

Figure 3-20 shows a generalized visual representation of the correct and incorrect classifications described above. This graph is known as a *misclassification ellipse*. To develop the ellipse, the estimated concentrations are plotted on the $X$ axis, and the true concentrations are plotted on the $Y$ axis. If an estimation method were perfect, the estimated concentration would always equal the true concentration. Plotting true vs. estimated in this situation would result in a graph with a 45° line emanating from the origin of the graph.

Unfortunately, perfect estimation is seldom achieved and the estimated concentrations fall off the 45° line. As repeated estimation experiments are performed

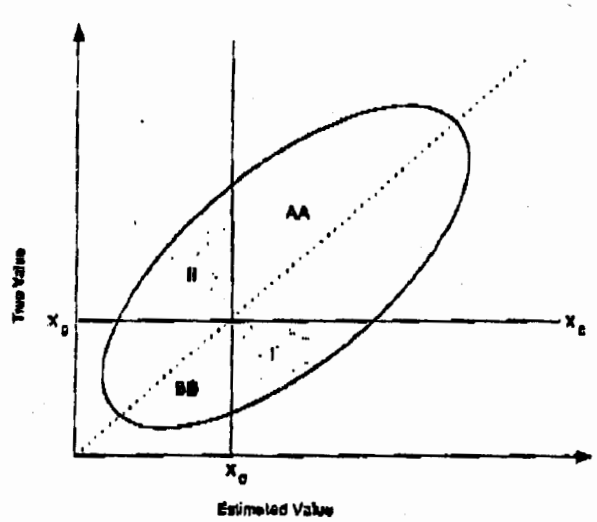



**Figure 3-20.** The misclassification ellipse. (From *Optimization of Sampling Policies: A Geostatistical Approach*, by J-M. Rendu, MMIJ-AIME, 1980, with permission.)

and the true vs. estimated values plotted, a scatter of points forms. This scatter plot often takes on a roughly elliptical shape; hence the name misclassification ellipse.

To ascertain the quantities and types of misclassifications present, the threshold concentration is also plotted on the graph (Fig. 3-20), perpendicular to axes for both the true and estimated values. By means of this process, four distinct quadrants of classification emerge. These correspond to the error and correct classification types, with each representing a different decision category.

The lower left quadrant of Figure 3-20 (labeled BB) contains concentration values for which both the estimated and the true values are below the threshold. In this case, correct classification has been made, so that the area will appropriately avoid treatment. Similarly, in the upper right quadrant (labeled AA), both the estimated and true values fall above the threshold. Again, correct classification decisions result, this time with the material being scheduled for appropriate treatment.

The remaining quadrants, labeled I and II, present situations of problematic classification. These correspond to Type I and Type II Errors. The lower right quadrant, labeled I, shows the estimated concentrations above the threshold limit, although the true concentrations are below the threshold. This is Type I Error. In the upper left quadrant, labeled II, the estimated values are below the threshold but the actual values fall above the threshold. This situation is Type II Error.

Table 3-2 presents the kriging and ISD data in a misclassification format. Instead of listing the actual error, the type of classification is presented. For this approach, the magnitude of the error takes a back seat to the decision made on the classification. Differences in classification between the two methods are highlighted with an asterisk.

As with the statistical comparison, the kriging estimates again emerge the winners since kriging produces fewer misclassification errors. Kriging produced three Type I Errors and one Type II Error, whereas ISD produced six Type I Errors and two Type II Errors.

Scatter plots for the kriged and ISD data can be seen in Figure 3-21. The kriged values cluster around the 45° line much more tightly than the ISD estimates do. This "slimmer" ellipse is generally an indication of better estimation and more accurate classification.

The term *Typecasting of Error* has been applied to the technique of analyzing misclassification error (Myers 1991). This approach is highly useful in conjunction with the method of cross validation. This approach can be used to determine optimal variogram and optimal kriging parameters employing performance-based goals.

The Typecasting of Error approach may not always point to kriging as the best interpolation method for a particular data set. For different data, a spline or other interpolation method may be more appropriate. This can assist greatly in problems discussed in Chapter 2. Typecasting techniques will be discussed in detail in later chapters.

Table 3-2. Comparison of number of misclassification errors produced by two estimation techniques (Kriging vs. Inverse Squared Distance).

| | *Value* | | | *Class* | |
|---|---|---|---|---|---|
| Sample Number | Real | Kriged | ISD | Kriged | ISD |
| 1 | 1671 | 1536.0 | 1304.1 | AA | AA |
| 2 | 993 | 1146.2 | 1219.0 | I | I |
| 3 | 1630 | 1647.8 | 1546.8 | AA | AA |
| 4 | 1439 | 1509.3 | 1559.0 | AA | AA |
| 5 | 746 | 738.5 | 766.1 | BB | BB |
| 6 | 667 | 757.4 | 787.0 | BB | BB |
| 7 | 1254 | 1284.1 | 1447.2 | AA | AA |
| 8 | 1318 | 1267.9 | 1368.3 | AA | AA |
| 9 | 1154 | 1143.6 | 991.9 | AA | II[a] |
| 10 | 1012 | 1012.6 | 1172.3 | AA | AA |
| 11 | 827 | 1017.3 | 1206.0 | I | I |
| 12 | 1726 | 1736.9 | 1807.6 | AA | AA |
| 13 | 1105 | 933.7 | 913.8 | II | II |
| 14 | 1239 | 1209.3 | 1218.9 | AA | AA |
| 15 | 921 | 919.2 | 808.0 | BB | BB |
| 16 | 644 | 689.8 | 674.4 | BB | BB |
| 17 | 1452 | 1410.8 | 1512.7 | AA | AA |
| 18 | 1220 | 1176.1 | 1169.6 | AA | AA |
| 19 | 1954 | 1803.0 | 1713.0 | AA | AA |
| 20 | 1389 | 1588.3 | 1850.6 | AA | AA |
| 21 | 976 | 996.7 | 1131.1 | BB | |
| 22 | 1330 | 1208.6 | 1087.5 | AA | [illegible] |
| 23 | 863 | 893.5 | 1053.5 | BB | I |
| 24 | 2034 | 1850.4 | 1813.2 | AA | AA |
| 25 | 1587 | 1717.1 | 1838.1 | AA | AA |
| 26 | 956 | 936.9 | 938.7 | BB | BB |
| 27 | 1131 | 1106.0 | 1080.7 | AA | AA |
| 28 | 1338 | 1227.5 | 1320.2 | AA | AA |
| 29 | 2267 | 1973.5 | 1868.8 | AA | AA |
| 30 | 1541 | 1365.3 | 1450.9 | AA | AA |
| 31 | 792 | 1071.6 | 1132.0 | I | I |
| 32 | 974 | 962.6 | 994.3 | BB | BB |
| 33 | 1275 | 1244.4 | 1254.9 | AA | AA |
| 34 | 1553 | 1302.5 | 1362.6 | AA | AA |
| 35 | 1076 | 1453.1 | 1813.3 | AA | AA |
| 36 | 588 | 738.0 | 908.0 | BB | BB |
| 37 | 964 | 984.1 | 1145.1 | BB | I[a] |
| 38 | 1298 | 1349.1 | 1459.3 | AA | AA |

[a]Estimates where ISD produces a misclassification while Kriging produces the correct classification.

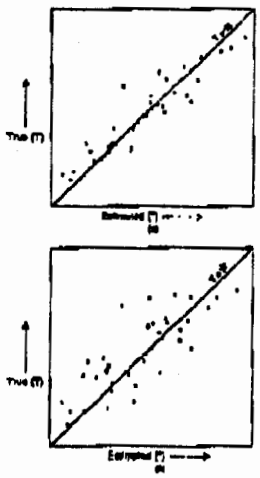


Figure 3-21. Scatter plot of estimated vs. true values: (a) Kriged estimates are used; (b) e squared distance estimates are used.

## CONCLUSION

Prediction is a risky game as one tries to generalize from specific sample data to the surrounding area. Estimation is an unfortunate necessity as time and resource constraints limit other options. Risk and uncertainty are a priori entities as they describe potential problems. Error is a posteriori in that one can measure or define a specific result. A number of techniques for estimating spatial data have been presented, with varying levels of complexity. Although not comprehensive, this sample of techniques is sufficient to demonstrate that any estimation technique has a degree of associated error. It is important to realize that the difference between a deterministic algorithm and a statistical model is that the statistical algorithm provides an error of estimation. Within the realm of error, different types exist that must be managed in different ways, depending on the DQO and other needs of a project. Chapter 3 has defined some general conditions and considerations; subsequent GEM chapters will set out specific techniques for addressing, solving, and managing the errors and uncertainty surrounding estimates and maps through statistics, STP, and GA.

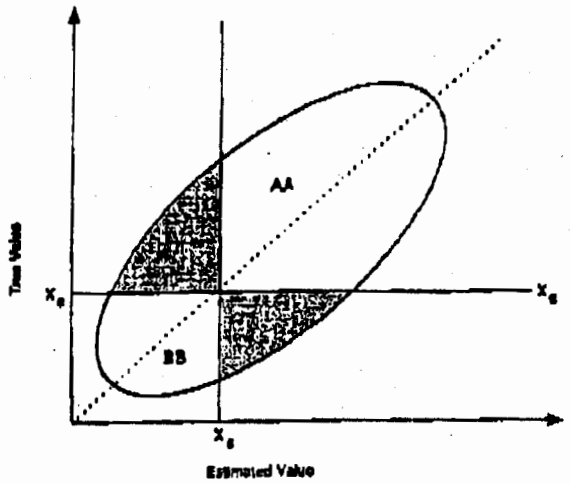
In Figure 14-23a, there is little deviation of the conditional expectation curve the 45° line over any range of concentrations. No conditional bias is present is case, and the estimates are also globally unbiased.

## 5.4 Assessing Performance: Typecasting Error

mary statistics of estimates and errors, along with distribution analysis of nates and errors derived from the cross validation process, provide a general for decision making. However, as Figure 14-20 demonstrates, the results of rent statistical criteria used to measure performance may be in conflict, once n relegating decisions regarding preferred estimators and appropriate ogram parameters to the subjective realm. Modified approaches have been osed (Clark 1986, David 1988), but the conclusions again indicated that ectivity could not be eliminated from the cross validation process.

The simplified decision rules applicable to environmental remediation offer pportunity to remove the subjectivity from cross validation studies. Once an on level has been selected for remediation, all soil estimated to contain con- rations equal to or greater than this value will be subject to remediation. For lial purposes, it does not matter whether the concentration of lead (Pb) in soil 01 or 50,000 ppm; both will be treated when the action level is 500 ppm. If a k concentration is incorrectly estimated, the magnitude of the error is far less ortant than the classification of clean or dirty. One possible exception is PCBs, which incineration may be required at levels above 500 ppm in soil.

In Chapter 3, the misclassification ellipse was introduced, along with the ess of typecasting error. Figure 14-24 shows a diagram of the misclassifica-




ure 14-24. Misclassification ellipse.

Table 14-1. Typecasting of error cross-validation results for a PCB project.

| | | |
|---|---|---|
| Threshold concentration, ppm: | 25 | |
| Total number of estimates: | 665 | |
| | *Number* | *Percent* |
| Occurrences of Type I error: | 86 | 12.93 |
| Occurrences of Type II error: | 63 | 9.47 |
| Occurrences below threshold: | 318 | 47.82 |
| Occurrences above threshold: | 198 | 29.77 |
| Total misclassifications: | 149 | 22.41 |
| Total correct decisions: | 516 | 77.59 |

tion ellipse. Two general categories are illustrated by the ellipse: (1) correct classification in the lower left and upper right quadrants (BB and AA), and (2) incorrect classification (Types I and II) in the lower right and upper left quadrants, respectively.

By plotting the action threshold limit on a scatter plot of true concentrations vs. concentrations estimated by cross validation, the misclassification ellipse is formed. Then, either by counting points on a scatter plot or by computer-generated summary, the number of correct classifications and the number of errors for each category may be tabulated. This comparison of correct vs. erroneous decisions called *typecasting of error* (Myers 1991).

Using this process, a cross validation estimate falls into only one of four possible classes. The results of the classification are then totaled and summarized. An example result of a typecasting cross validation for a PCB project is presented in Table 14-1.

The objective of the typecasting approach is to minimize the misclassification errors associated with a given estimator or given set of estimation parameters. This will help minimize decision errors during remediation. Goals can be set during the DQO process according to the needs of the stakeholders. PRPs will benefit by reducing the occurrences of Type I errors, and thus minimizing false positive results and costly overremediation. Regulatory agencies will benefit by minimizing Type II errors, thereby helping to assure health and safety.

## *14.5.5 Typecasting Error as a Decision Tool*

### *14.5.5.1 Selecting An Estimator*

Many computerized interpolation methods are available for gridding data or creating block models. Among the commonly available routines are inverse power distance, triangulation, radial basis functions, Shepard's method, minimum curv

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ture, polynomial regression, splines, trend surface analysis, and, of course kriging. Kriging also comes in many "flavors": ordinary, simple, disjunctive, multi-gaussian, universal, indicator, probability, and so on.

It is unlikely that a single estimator will be optimal for all situations. Therefore, we may wish to test various interpolation methods in order to determine which method performs best for a particular data set or a particular COC. The typecasting error approach allows us to compare estimators based on environmentally relevant objectives.

### *14.5.5.2 Selecting Sample Locations*

The results from a typecasting cross validation lend themselves to informative visual display. Figure 14-25 shows one level of the ReSolve site, a multilevel

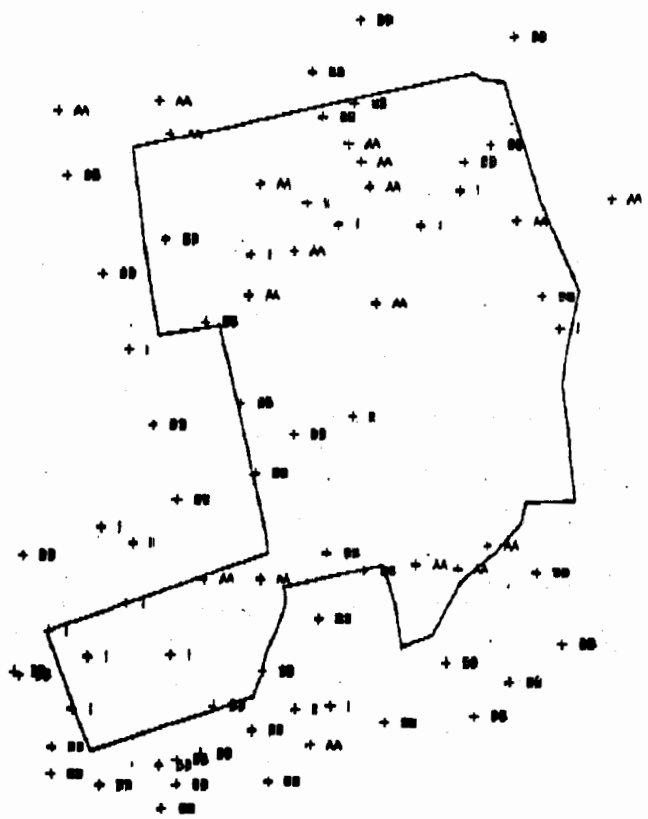


**Figure 14-25.** Typecasting of error location map for one level of the ReSolve PCB site. (From A geostatistical analysis of PCB concentrations in soils at the ReSolve site, by J.C. Myers, 1992.)

site contaminated with PCBs. As a group, the classification results show roughly the same classification percentages as those listed in Table 14-1.

The spatial configuration of the results is also of interest. BB (below/below) results (from locations where both the true and estimated concentrations are below the threshold, or Below/Below) tend to be at the margins of the site, as might be expected. Similarly, AA (above/above) results tend toward the interior portions of the site. Type I errors occur in both interior and exterior locations. They also cluster in the southwest portion of the map, indicating a consistent difficulty in appropriate estimation. Type II errors are few and widely dispersed, showing no consistent pattern.

Once the original sample data are returned to the data set, we would expect local estimation to improve, eliminating some of the misclassifications. The next step, however, is to estimate block concentrations instead of sample locations. It is reasonable to assume that the areas that were correctly classified without the benefit of the removed sample will continue to be correctly classified. Whether the estimates given to the transition areas between the Type I and II errors and AA and BB classifications will result in correct classifications is still in doubt.

Transition areas provide good targets for additional samples. This may be possible if the site is in the early stages of investigation or if additional sampling programs are already planned. PRPs wishing to reduce the cost of remediating clean soil classified as dirty may wish to invest some money in attempts to reduce the remedial cost associated with Type I error. If no additional characterization sampling is planned, transition Type II areas provide good targets for postremedial excavation sampling. These areas are known to be difficult to classify and have the highest probability of false negative classifications.

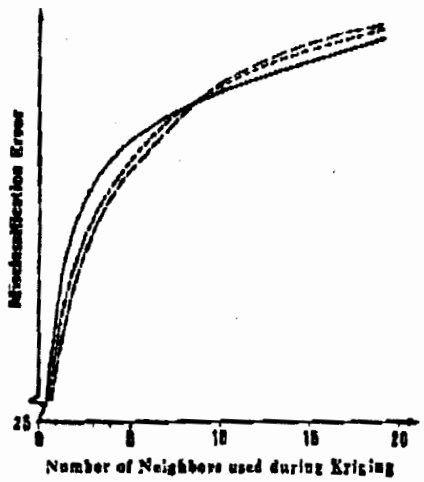
### *14.5.6 Optimizing Interpolation Parameters*

Cross validation and typecasting error techniques may be used for more than simply distinguishing between different estimation techniques. They may also be used to optimize the parameters used for a particular estimator, some of which are extremely sensitive. For simplicity, only kriging parameters will be discussed in this section; the same or similar methods may be used for other interpolators.

#### *14.5.6.1 Number of Neighbors*

Experience has shown that the parameter most sensitive to typecasting error for kriging is the number of neighboring samples used in the cross validation process (Myers 1991). One reason for this is that environmental data often span several orders of magnitude. An extreme concentration can dramatically influence the estimated concentration, even at great distances.

Figure 14-26 shows a plot of the misclassification error as a function of the




ure 14-26. Plot of the total misclassification error vs. the number of neighbors used ·pecasting of error cross validation (sample concentrations) for the ReSolve PCB
From A geostatistical analysis of PCB concentrations in soils at the ReSolve site, J.C. Myers, 1992.)

mber of neighbors for a soil PCB site using three different sets of spherical riogram parameters. The graph depicts a steady and rapid increase in total isclassifications from one sample to approximately 10, with a slower rate of cline beyond. Based on this curve, the optimum number of neighbors for cross lidation is one. This implies that, for the actual kriging, two samples will be ed because the original sample will be replaced in the data set.

Note that all three variogram models performed in a surprisingly similar shion. This does not imply that they are not important. It does, however, suggest reasonable approach to optimizing the kriging parameters. A preliminary riogram analysis should be run and a reasonable model fit to the experimental ta. This preliminary model may then be used to determine the optimal number neighbors. Once that number has been determined, it can be held constant while e sensitivity of other kriging parameters is investigated.

The results presented in Figure 14-26 suggest an almost polygonal approach estimation. Such results are not necessarily typical. Figure 14-27 shows another aph of the same type as Figure 14-26, this time for the indicator values of the me data. Instead of a continuous rise with increasing neighbors, the graph shows consistent drop in error until a minimum is reached for 15 neighbors. Beyond is minimum, errors begin a slow but fluctuating rise.

Figure 14-28 shows another example of misclassification error behavior. ror values fall sharply at first, reaching a minimum at four. Error then begins a

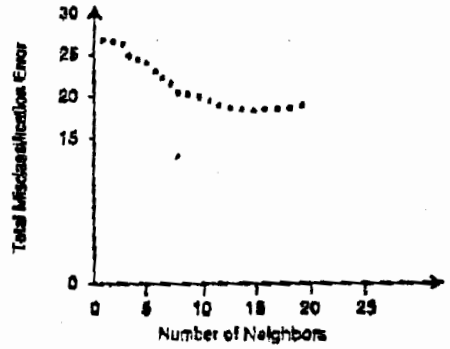



Figure 14-27. Plot of the total misclassification error vs. the number of neighbors used in typecasting of error cross validation (indicator values) for the ReSolve PCB site. (From A geostatistical analysis of PCB concentrations in soils at the ReSolve site, by J.C. Myers, 1992.)

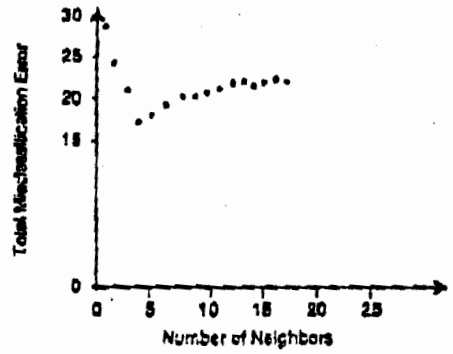



Figure 14-28. Plot of the total misclassification error vs. the number of neighbors used in typecasting of error cross validation of sample concentrations for a VOC in groundwater. (From A geostatistical analysis of PCB concentrations in soils at the ReSolve site, by J.C. Myers, 1992.)

slow but mostly consistent rise beyond the minimum. As a reminder, five sampl should be used during kriging as it is appropriate to include the original samp and all four optimal neighbors.

### *14.5.6.2 Search Radius*

As discussed earlier in this chapter, the final estimate is influenced by search parameters used. Cross validation results are also influenced by the se parameters and are somewhat related to the number of neighbors.

In order to obtain a large number of neighbors, a reasonably large search adius will be needed in many instances. One must remember that, whereas 15 eighbors may be specified as a maximum, an insufficient radius may never apture this many sample points. This must be balanced by the fact that samples t extreme distances may not be appropriate for local estimation.

#### 14.5.6.3 Variogram Range

The kriging example in Chapter 13 demonstrated that the range of the variogram model has an effect on the kriging weights and, consequently, the final estimate. While typecasting error results are not as sensitive to the range as to the number of neighbors, different variogram ranges and anisotropies (both ratios and orientations) should be investigated. The model that provides the best fit to the experimental variogram may not, in fact, be the most reliable estimator.

#### 14.5.6.4 Nugget Effect

Typecasting error results are quite sensitive to the influence of a nugget effect. s the nugget effect increases, sample weights become more alike and estimates raw closer to a simple average. In general, the addition of a nugget effect has a detrimental effect on the typecasting error results. The effect of various nugget-to-sill ratios should be investigated during a cross validation study.

#### 14.5.6.5 Variogram Sill

As discussed in Chapter 13, the height of the sill does not affect the kriging weights nor the block or point estimate. Therefore, it is not necessary to investigate different sills during cross validation.

### 14.5.7 Caveats for Cross Validation

#### 14.5.7.1 Problems in Two Dimensions

Figure 14-29a shows a regular unit grid of samples at distance $d$ ($d = 1$), with an unsampled point $P$ to be estimated. In this case, for any unsampled point,

$$\text{Maximum distance} = \frac{d}{\sqrt{2}} \tag{14.5}$$

or approximately 0.7.

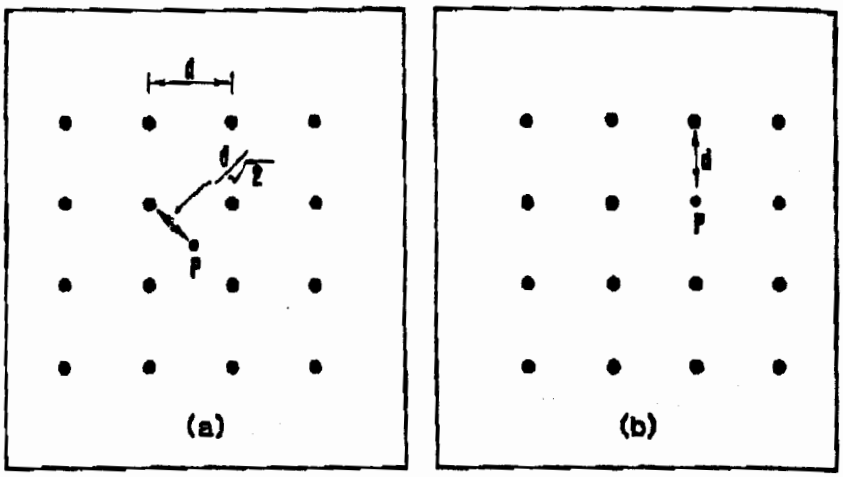



Figure 14-29. Problems in cross validation: the two-dimensional case. (From *Handbook of Applied Advanced Geostatistical Ore Reserve Estimation*, by M. David, Elsevier, 1988. Courtesy of Michel David.)

Figure 14-30. Problems in cross validation: the three-dimensional case. (From *Handbook of Applied Advanced Geostatistical Ore Reserve Estimation*, by M. David, Elsevier, 1988. Courtesy of Michel David.)

The geometry changes when a point is removed for cross validation. Figure 14-29b shows that the closest distance from point $P$ to a sample is now $d$ or 1. With all samples at a greater distance, it will be more difficult for any estimator to produce an accurate estimate or classification of the unsampled point.

### 14.5.7.2 Problems in Three Dimensions

Figure 14-30 shows the reverse problem from two dimensions. A vertical boring is shown with a central interval removed in anticipation of estimation by cross validation. Now, the nearest neighbors are directly above and below the point to be estimated. Regardless of the estimator of variogram model selected, the point estimate will be very close to the average of the two samples surrounding the interval.

Without additional sampling, the problem in two dimensions is not easily solved. In three dimensions, however, we may remove samples within a certain distance of the point to be estimated. This should be done with caution so as to avoid recreating the two-dimensional problem.

## CONCLUSION

Successful implementation of kriging depends not only on a computer program that respects the equations developed in Chapter 13 but also on a practical understanding of the interactions between the various kriging parameters and block model constraints. These include topographic constraints, correct search procedures, and appropriate cross validation where typecasting error may be valuable. Computer kriging and contouring can often be accomplished with the push of a button, but the practitioner is responsible for determining whether the resultant map should be classified as "gospel" or "garbage."