Kriging Analysis Applied to Ecological Risk Assessment of Harbor Sediments

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Abstract

This study applies the spatial statistical technique, kriging, to the estimation of benthic invertebrate community ecological parameters associated with ecological risks from hazardous contamination in harbor sediments. The types of ecological risk assessment used in the US Navy's Installation Restoration program for cleaning up sites contaminated with hazardous substances are described. Benthic invertebrate community data from contaminated harbor sediments at a California Navy base are presented as an example of ecological community data being used in ecological risk assessment of harbor sediments. The ecological community parameters in the dataset include abundance, diversity, number of species, dominance, evenness, and biomass. The kriging of the benthic ecological community data from the example harbor shows that the total number of sampling stations initially planned may be reduced by 10% without compromising the characterization of the benthic ecological community. Kriging can be a very effective statistical method for limiting the number of samples needed to spatially characterize hotspots while still insuring adequate data quality. Maps of the spatial error variance of a parameter's sample data—the error of estimation—may be used to place additional sampling points or to minimize the number of additional samples needed at a site.

Keywords: kriging, ecological, risk

Introduction

Kriging is a geostatistical method of spatial data interpolation that can be used to limit the number of samples in eco-risk assessments. In 1963 G Matheron named kriging after DG Krige, a South African mining engineer who used the technique to more accurately predict the extent of gold deposits. Kriging is an interpolation method that optimally predicts data values by using data taken at known nearby locations. It can be either two- or three-dimensional. For this paper, ecological data from harbor surface sediments, considered a two-dimensional surface, were kriged.

Kriging is a set of linear regression routines that minimizes estimation variance from a predefined covariance model (1). It is based on the assumption that the parameter being interpolated at a site is a *regionalized* variable. A regionalized variable varies in a continuous manner spatially so that data values from points nearer to one another are better correlated. Data values from widely separated points are statistically independent in kriging.

Estimates of chemical or biological parameters and their associated variances can be predicted at each node of a grid by a kriging model. New proposed sampling

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locations can be added to a dataset and the reduction in kriging variance can be estimated at each location. The resulting maps of kriging variance with the proposed additional sampling locations can then be used to limit the number of suggested new sampling sites. Only those resulting in significant variance reduction would qualify as actual sampling locations. Alternative new sampling designs can also be assessed with kriging to determine the greatest benefit for the cost of additional sampling sites.

The data from the example harbor in this paper were kriged using the US Department of Defense's Groundwater Modeling System (GMS) package (1). Kriging software is also available in other geostatistics packages, such as Surfer for Windows: Contour and 3-D Surface Mapping (Golden Software, Inc., Golden, CO) and MGE Kriging Modeler (Intergraph Corporation, Huntsville, AL).

Steps in Ecological Risk Assessment

Ecological and human health risk assessments are integral to the scientific investigation of sites contaminated by toxic chemicals. The US Navy conducts cleanups of toxic chemicals found at sites on Navy or Marine bases through its Installation Restoration (IR) program, the Navy's version of Superfund. Evaluation of an IR site includes five steps: scoping, screening, baseline, effectiveness (confirmation sampling), and monitoring eco-risk assessments. Resampling or taking additional spatial samples for hotspot delineation can be very expensive; at Navy and Marine bases, for example, each sampling event of harbor sediments for eco-risk assessments can cost over $1 million. Kriging can reduce the need for resampling if it is used to systematically organize all stages of the assessment effort to reduce spatial error variance at a site. Kriging can also be used to limit the number of sampling stations needed to delineate hotspots.

Data Quality Objectives

Ecological risk assessment follows the seven-step Data Quality Objectives (DQOs) process, as do all sampling investigations in the Navy's IR program. The seven steps in the DQO process are:

1. State the problem
2. Identify the decision
3. Identify inputs to the decision
4. Define the study boundaries
5. Develop a decision rule
6. Specify tolerable limits on decision errors
7. Optimize the design

Kriging should be used to plan the tolerable limits on decision errors in step 6 of the DQO process. The use of error variance maps generated by the kriging of data can reduce the error of spatial estimation in studies such as the one profiled here. The project team has to agree upon the amount of tolerable spatial error of estimation in step 6 before the investigation proceeds to step 7, where the sampling design is optimized. A major consideration in this decision is the cost of sampling. Although kriging may indicate that a certain number of locations should be sampled, it may not be possible to pay for the optimal number of samples in a project. In addition to error from the spatial variation in data values, other sources of error variance in studies of ecological data are the regular variance about the mean value of the data itself, temporal variation, and error in the reported data from lab tests. In the case of harbor sediments, the temporal variation in the ecological data is due to the movement of sediment and biological changes in response to changing site conditions.

DQO step 7 includes four substeps (2):

1. Review DQO outputs and existing environmental data.
2. Develop general data design alternatives.
3. Formulate the mathematical expressions needed to solve the design problem for each data collection design alternative.
4. Develop and document the sampling strategy.

Kriging can be used in substeps 2, 3, and 4. In substep 2, kriging is useful as a statistical method to determine the appropriate number of samples. In substep 3, it can be used as a statistical model and, in substep 4, to decide on the locations of the sampling stations delineated.

Data and Example Study Areas

The study area for this application of kriging to an eco-risk assessment was a 0.738 acre harbor at a California Navy base. The harbor is approximately 4,500 feet by a maximum of 8,200 feet across (0.85 by 1.55 miles), with an average water depth of 45 feet. The sediments contained a wide range of grain sizes, but they were about 65% fines, meaning the particles were smaller than 62.5 μm in diameter. The sediment in the area near the basin entrance on the east side contained a high percentage of sand-sized particles.

The study included 32 open harbor sampling sites. Only open water sampling stations were included in this analysis. Although samples were also collected from underneath piers around the sides of the example basin, these areas are considered a different ecosystem than the open harbor and the samples were not included in the analysis. Sample volumes of 0.006 m^3 were obtained using a Teflon corer inserted into a box core surface sediment sample from the harbor bottom.

This study used a triad approach to eco-risk assessment of the harbor sediments. The first two components of the triad were chemical contaminant concentrations and bioassay results, including bioaccumulation tests from sediment samples. Some of the hazardous contaminant chemicals found above background concentrations in the example harbor included the metals arsenic, beryllium, cadmium, total chromium, copper, lead, mercury, nickel, silver, and zinc; sulfide; polynuclear aromatic hydrocarbons (PAHs); polychlorinated biphenyls (PCBs) such as Arochlor 1260; and total 4,4'-dichloro-diphenyl-trichloroethane (DDT).

Benthic community data was the third major component of the triad approach. The benthic community found in the open areas of the harbor was dominated by five polychaetes: *Monticellina tesselata, Cossura sp. A, Aphelochaeta multifilis* Type 2, *Chaetozone corona,* and *Paraprionospio pinnata.* The polychaete, *Pseudopolydora paucibranchiata,* and the crustacean, *Amphideutopus oculatus,* were also abundant at several sampling sites in the open harbor.

The benthic invertebrate ecological community parameters calculated from the sediment samples included abundance, the Shannon-Weiner diversity index, evenness, Margalef species richness, dominance, and biomass. Abundance was reported as the total number of individual specimens collected in each sample. The Shannon-Weiner species diversity index was calculated as:

$$H = -\sum_{i=1}^{s} (p_i)(\ln p_i) \quad (1)$$

where H is the Shannon-Weiner diversity index, s is the number of species, and pi is the proportion of the total sample belonging to the i^{th} species, the abundance of species i/total abundance. Evenness was computed as:

Evenness = (Shannon-Weiner species diversity index H)/ln(number of species) (2)

Margalef's species richness was defined as:

Margalef's species richness = (number of species – 1)/ln(total abundance) (3)

Dominance was calculated as the number of species accounting for 75% of the total abundance. Biomass was the wet weight in grams of all organisms found in a sample (g/[0.006 m^3]).

Variograms

In ordinary kriging, a variogram is first constructed using the dataset from a site. A variogram consists of two parts: an experimental variogram based on the data, and a model variogram. An experimental variogram is constructed by first calculating the variance of each point in a dataset with respect to each of the other points. The experimental variogram consists of the plotted variances versus the distance between each data point at the site. The variance is typically computed as one-half the difference in a data value squared. Several types of experimental variograms can be selected in the GMS software (1).

The following semivariogram equation was used to calculate the variance, γ(h), as a function of the distance, h, between data points, for the experimental variogram for this study:

$$\gamma(h) = (1/2n) \sum_{i=1}^{n} (f_{1i} - f_{2i})^2 \quad (4)$$

where n is the number of pairs of points whose separation distance falls within the lag interval and f_{1i} and f_{2i} are the data values at the head and tail of each pair of points (1). In computing the experimental variogram, it is impractical to plot a variance for each data point with respect to every other value in the dataset. Therefore, the variances are averaged for all the data points in donut-shaped areas around each data point called *lags* and plotted on the experimental variogram. The distance between the edges of each adjacent lag area is called the *unit separation distance* (1). Ten lags, the number normally used, was chosen as the number of lags for the kriging of the ecological data in this study. Thus, only ten points are shown on the experimental variogram (Figure 1), corresponding to the average variances in ten lag areas.

The model variogram is a curved line through the experimental variogram points. It represents a simple mathematical function modeling the trend in the points of the experimental variogram. In the GMS package, spherical, exponential, Gaussian, and power model equations can be used to fit a model variogram line to the experimental variogram points. A spherical model equation resulted in a line closely matching that

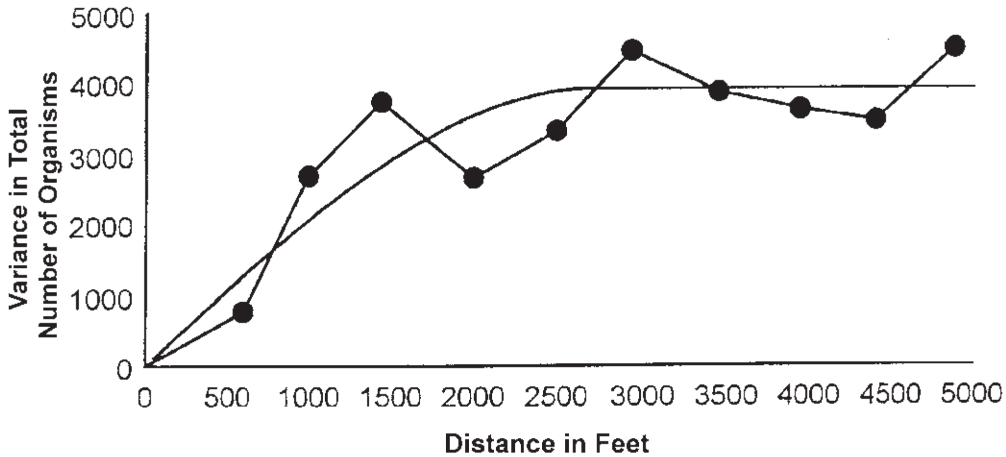

Figure 1 Variogram for benthic invertebrate total abundance in the example harbor.

of the benthic community variance data points on the experimental variogram, and it was used for the model variogram in this study:

$$\gamma(h) = c\,[1.5(h/a) - 0.5(h/a)^3]$$
$$\text{if } h/a \leq a \tag{5}$$

where $\gamma(h)$ is the variance as a function of distance h, a is the *range,* and c is the *contribution* or *sill.*

On a model variogram, a *nugget* is a minimum variance—the point where the model variogram line intercepts the y axis. The sill is the upper flat part of the model variogram line where the variances of far data points have no correlation to the distance from the other data points. The range represents the distance at which there is no longer a correlation between data points (1).

Some datasets exhibit *anisotropy,* meaning the correlation between data points changes with the direction set through the dataset. For isotropic data, the azimuth angle has little effect on the resulting experimental variogram. The benthic ecological community dataset used for this paper was assumed to be isotropic and the azimuth angle was set at zero degrees.

Estimation Error Variance Maps

The variogram in kriging can be used to calculate the expected error of estimation at each target interpolation point because the estimation error is a function of the distance to surrounding data points. The estimation variance can be represented as:

$$s^2_\varepsilon = w_1\,(S(d_{1p}) + w_2S(d_{2p}) + w_3S(d_{3p}) + \lambda \tag{6}$$

An estimation standard deviation can also be calculated by taking the square root of the estimation variance. In the kriging module of GMS, a contour map of estimation variance can be generated for a mesh or grid at a site by selecting a simple option button in kriging options.

Data Interpolation

The basic equation used in ordinary kriging is:

$$F(x,y) = \sum_{i=1}^{n} w_i f_i \tag{7}$$

where n is the number of data points in the set, f_i are the values of the data points, and w_i are weights assigned to each data point (1). The weights used in kriging are from the model variogram. To interpolate at a point P, for example, using surrounding points P_1, P_2, and P_3 , the weights w_1, w_2 , and w_3 must be found. The weights are found through the solution of the simultaneous equations:

$$w_1S(d_{11}) + w_2S(d_{12}) + w_3S(d_{13}) = S(d_{1p}) \tag{8}$$

$$w_1S(d_{12}) + w_2S(d_{22}) + w_3S(d_{23}) = S(d_{2p}) \tag{9}$$

$$w_1S(d_{13}) + w_2S(d_{23}) + w_3S(d_{33}) = S(d_{3p}) \tag{10}$$

where $S(d_{ij})$ would be a value from the model variogram evaluated at a distance equal to the distance between points i and j. Because it is necessary that the weights sum to one, a fourth equation is added:

$$w_1 + w_2 + w_3 = 1.0 \tag{11}$$

Because there are now four equations and three unknowns, a slack variable, λ, is added to the equation set:

$$w_1S(d_{11}) + w_2S(d_{12}) + w_3S(d_{13}) + \lambda = S(d_{1p}) \tag{12}$$

$$w_1S(d_{12}) + w_2S(d_{22}) + w_3S(d_{23}) + \lambda = S(d_{2p}) \tag{13}$$

$$w_1S(d_{13}) + w_2S(d_{23}) + w_3S(d_{33}) + \lambda = S(d_{3p}) \tag{14}$$

$$w_1 + w_2 + w_3 = 1.0 \tag{15}$$

These equations are solved for the weights w_1, w_2, and w_3. The f value of the interpolation point is then calculated as:

$$f_p = w_1f_1 + w_2f_2 + w_3f_3 \tag{16}$$

The expected estimation error is minimized in a least squares sense in kriging by using the variogram to compute the weights (1). For this reason, kriging is said to produce the best linear unbiased estimate. In most mapping software manuals, kriging is recommended as the best interpolation method.

Results of Interpolated Data and Variance Mapping

Maps of isopleths for total abundance and other community parameters for benthic invertebrates were computed using the kriging interpolation equations. The maps were first computed and printed for all 32 original sampling stations in the harbor. Figure 2, for example, illustrates isopleths of benthic invertebrate total abundance for all the

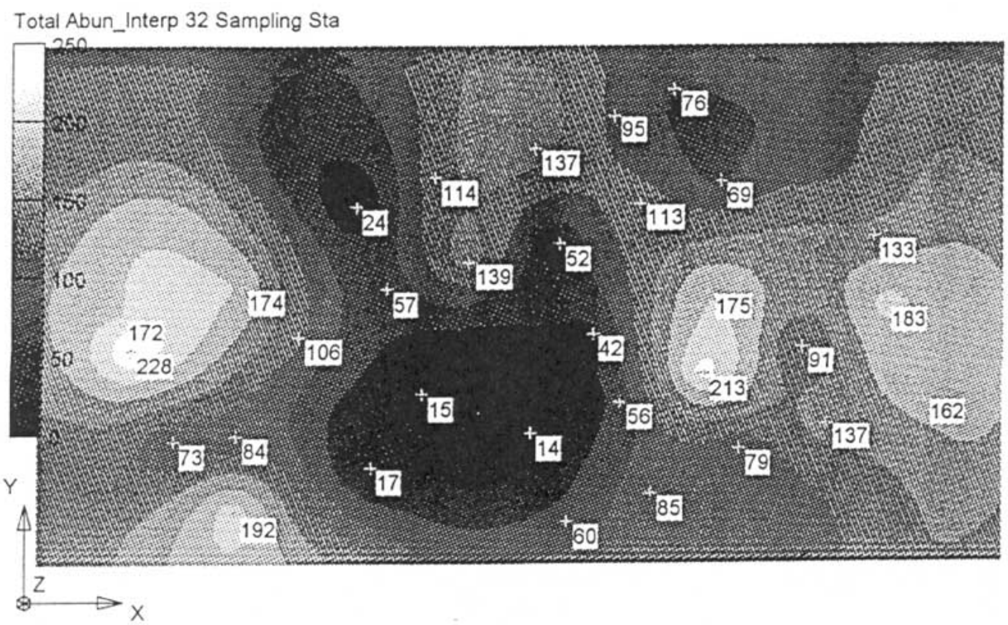

Figure 2 Kriged isopleths for benthic invertebrate total abundance for the original 32 sampling stations in the example harbor.

sampling stations. An estimation error variance map was also computed for each parameter at each station; Figure 3 shows the estimation error variance for total abundance.

Four, and later eight, sampling stations were then removed from the dataset. The eliminated sites were those located nearest to other stations. The purpose of computing interpolated isopleths and estimation error variance maps for datasets with reduced numbers of sampling stations was to see if the isopleths would stay the same or change with fewer sampling stations. Maps of isopleths for total abundance and the other ecological community parameters were then produced using kriging interpolation for reduced datasets with 28 and 24 sampling stations. Figure 4 shows the resulting interpolated isopleths for total abundance for 28 sampling stations. Estimation error variance maps were also computed using 28 and 24 sampling stations.

Conclusions

The positions of the isopleths of the predicted values of total abundance changed very little when four sampling stations were removed from the original dataset (Figures 2 and 4). The positions of the interpolated isopleths did change, however, when the number of stations was reduced from 32 to 24. The positions of the estimation error variance isopleths on maps changed very little when the number of sampling stations was reduced to either 28 or 24 stations. Because the number and position of original sampling stations were arrived at by the best collective judgement of the IR team, it is likely that 10% fewer sampling stations could be used to collect benthic ecological community data for eco-risk assessments of harbor sediments at this site. For a harbor the size of

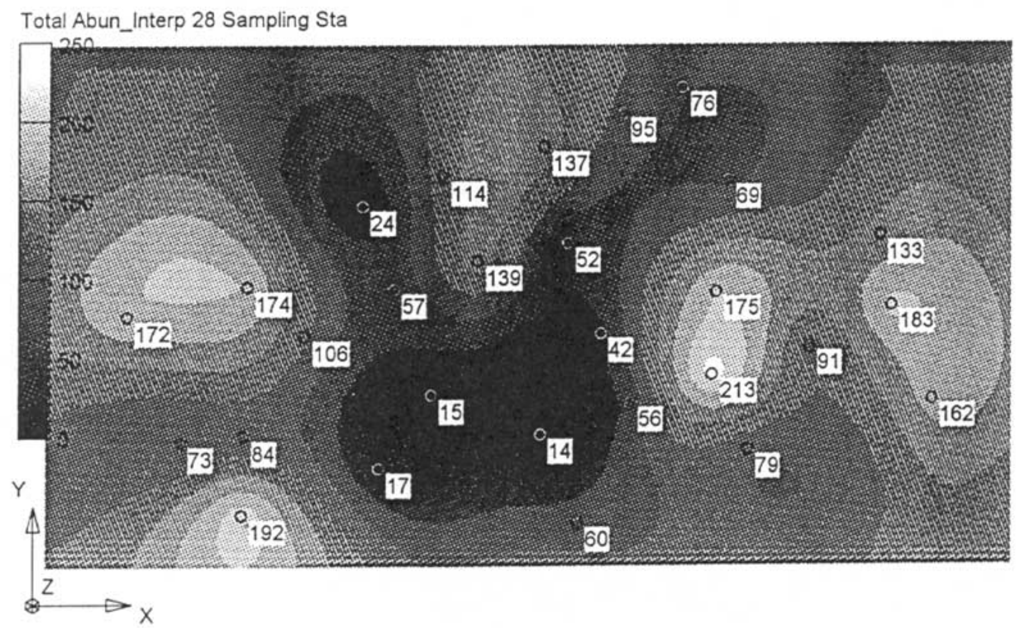

Figure 3 Kriged isopleths for benthic invertebrate total abundance with the number of sampling stations reduced to 28 in the example harbor.

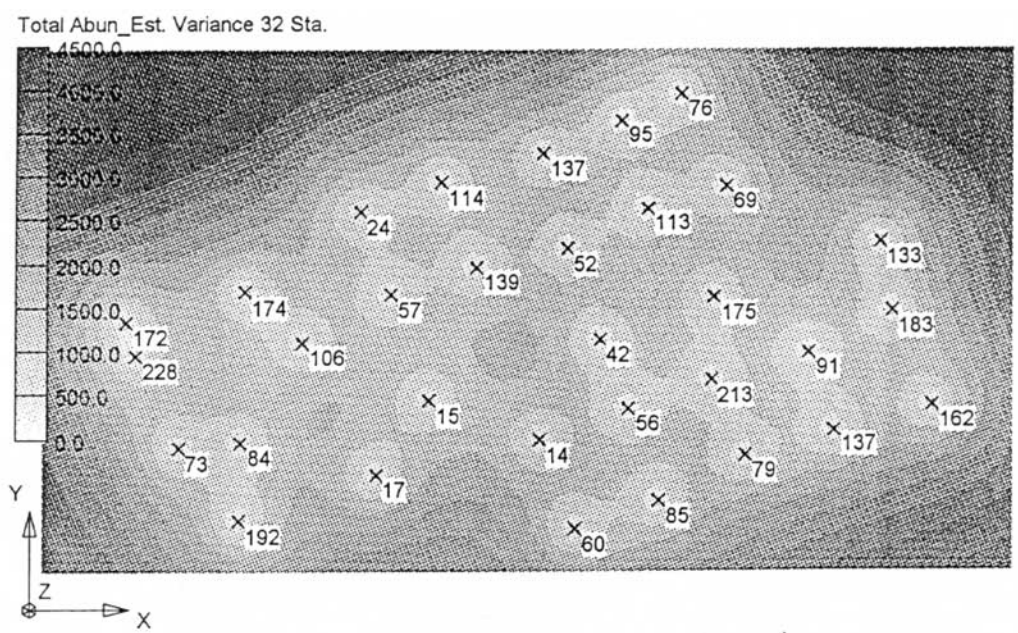

Figure 4 Estimation error variance map for benthic invertebrate total abundance for the original 32 sampling stations in the example harbor.

the one in this study, collecting 10% fewer benthic community samples could result in savings of between $100,000 and $250,000 in 1998 dollars through the three to five major stages of an eco-risk assessment.

Using 28 sampling stations as the number necessary to characterize the spatial distribution of benthic ecological community parameters in a harbor the size of the example harbor, one sampling station is needed per 1,147,995 square feet of sediment. This represents an area 1,071 feet on a side to adequately characterize benthic ecological community parameters. This is probably a larger area of harbor bottom per sampling station than was previously thought adequate to characterize benthic ecology.

Hotspot Definition

Kriging could save the government millions of dollars in sampling costs by reducing the number of samples collected to define the volumes of hotspots—small areas with high contaminate concentrations. Before remediating a hotspot, contractors have been intuitively collecting samples from hundreds of sampling stations to avoid remediating too much soil or sediment and to avoid missing contamination. Using kriging estimation error variance maps to plan the locations of sampling stations in areas with the most estimation variance could reduce the number of stations needed to characterize hotspots. Isopleths of contamination on maps of hotspots could be more accurately predicted by using kriging interpolation.

Recommendations

Kriging should be included in DQO planning for eco-risk assessments of harbor sediments. Through each successive stage of an eco-risk assessment, an effort should be made to build a database by placing sampling station locations in a consistent grid pattern. Kriging estimation error variance maps of preliminary data should be used to plan the size of the grid and optimally place sampling station locations in the areas with the most estimation error variance. The location of each sampling station should be placed randomly inside each grid cell. As additional sampling is planned through the stages of an eco-risk assessment, new stations should always be placed in the areas with the most estimation error variance. Kriging estimation error variance maps and interpolated isopleths of data should be used to plan sampling and define the shape of hotspots.

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References

1. US Department of Defense. 1998. *Groundwater modeling system, GMS v2.0, reference manual.* Washington, DC: US Department of Defense.

2. Bilyard GR, Beckert H, Bascietto JJ, Abrams CW, Dyer SA, Haselow LA. 1997. *Using the data quality process during the design and conduct of ecological risk assessments.* Washington, DC: US Department of Energy, Assistant Secretary for Environment, Safety, and Health, Office of Environment.