Kriging in Eco-Risk Assessments

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Abstract

The application of the spatial statistical technique, kriging, to the spatial estimation of benthic invertebrate bioassay data, associated with ecological risks from hazardous contamination in harbor sediments, is described in this position paper. The types of ecological risk assessments used in stages of the Navy's Installation Restoration program for cleaning up sites contaminated with hazardous substances are described. Benthic bioassay data from contaminated sediments in a large harbor at a California Navy base are presented as an examples of the bioassay data used in ecological risk assessments of harbor sediments. The kriging of the benthic bioassay data from the example harbor generally shows that the total number of sampling stations usually planned can be reduced by 10% and the benthic bioassay data can still be adequately characterized. The laboratory analyses of benthic bioassay samples collected for ecological risk assessments in harbors can be very expensive. 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 sample data of a parameter, the error of estimation, can be used to place additional sampling points or minimize the number of additional samples needed at a site.

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 D.G. Krige, a South African mining engineer, who used the technique to more accurately predict the extent of gold deposits in unsampled areas. Kriging is an interpolation method that optimally predicts data values by using data taken at known nearby locations. Kriging can be either two-dimensional or three-dimensional. For this paper, ecological data from the surface sediments, a two-dimensional surface, in a harbor was kriged.

Kriging is a set of linear regression routines which minimize estimation variance from a predefined covariance model (DoD, 1998). Kriging 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 each other are more correlated. Data values from widely separated points are statistically independent in kriging.

Estimates of the concentrations of chemical or biological parameters and an associated variance can be predicted at each node of a grid by a kriging model. New proposed sampling locations can be added to a data set and the reduction in kriging variance can be estimated at each location. The resulting maps of kriging variance with the new proposed

sampling locations can be used to limit the number of new proposed sampling locations. Only those new sampling locations resulting in significant variance reduction would qualify as new sampling locations.

The data from the example harbor in this paper was kriged using the kriging options in the Groundwater Modeling System (GMS) package (DoD, 1998).

The Steps in Ecological Risk Assessments

Ecological risk assessments, as well as human health risk assessments, are basic parts of the scientific investigation of sites contaminated by toxic chemicals. The 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 the Superfund. The main steps or tiers in the evaluation of the eco-risks at an IR site, according to the Navy Eco-risk Policy (DoN, 1999), are: Screening (including Scoping), Baseline, and Evaluation of Remedial Alternatives. Resampling or taking additional spatial samples for hotspot delineation for eco-risk assessments in harbor sediments can be very expensive, running to over a million dollars per sampling event for eco-risk assessments at Navy and Marine bases. Kriging can reduce resampling events if used to systematically organize the whole effort to reduce spatial error variance at a site through all the stages of an eco-risk assessment. Kriging can also be used to limit the number of sampling stations needed to delineate hotspots.

Data Quality Objectives

Ecological Risk Assessments follow the seven step Data Quality Objectives (DQO's) process like 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; and (7) Optimize the Design. Kriging should be used to plan the tolerable limits on decision errors in Step 6 of the DQO process before proceeding to Step 7.

DQO Step 7 includes four substeps: (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; and (4) Develop and Document the Sampling Strategy (Bilyard et al, 1997). Kriging can be used in Substeps 2, 3, and 4 in DQO Step 7. In Substep 2, kriging would be used as a statistical method to determine the appropriate number of samples. It would be used as a statistical model in Substep 3 and to decide on the locations of sampling stations in Substep 4 of DQO Step 7.

Data and Example Study Areas

The study area for this application of kriging to an eco-risk assessment is a harbor at a California Navy base with an area of 738 acres, roughly 4500 by 8200 feet in the longest distance across or 0.85 by 1.55 miles. Water depths average about 45 feet. The sediments

contained a wide range of grain sizes, but the sediments are 65% fines -- which are particles smaller than 62.5 µm in diameter. The sediment in the area near the basin entrance on the east side contains a high percentage of sand-sized particles.

Only open water sampling stations from the example harbor were included in this kriging analysis of benthic bioassay data. Samples were also collected from underneath piers around the sides of the example basin, but were not included in this analysis. The areas under the piers are considered a different ecosystem than the open harbor areas. The benthic bioassay data collected for the eco-risk assessment at the example harbor was the second major component of the triad approach to eco-risk assessments in harbor sediments. The other two components of the triad are chemical contaminant concentrations and benthic ecological community data 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 (PAH's), polychlorinated biphenyls (PCB's) such as Arochlor 1260, and total 4,4'-dichloro-diphenyl-trichloroethane (DDT). The benthic invertebrate community found in the open harbor areas of the example harbor was dominated by five polychaetes: Monticellina tesselata, Cossura sp. A, Aphelochaeta multifilis Type 2, Chaetozone corona, and Paraprionospio pinnata. The polychaete, Psuedopolydora paucibranchiata, was also abundant at several sampling sites in the open harbor. The crustacean, Amphideutopus oculatus, was also abundant.

The benthic invertebrate bioassay parameter calculated from lab tests on sediment samples taken from 33 open harbor sampling sites in the example harbor included amphipod survival and reburial, echinoderm survival and development, and polychaete survival and growth rates. The bioassay data kriged in this paper were the survival percentages for amphipods, echinoderms, and polychaetes.

Solid sediment was used in the amphipod bioassays. In the acute test, the percent survival for the standard test amphipod, Rhepoxynius abronius, was measured over a 10-day test period. The percent of the surviving amphipods capable of reburying in the sediment was also reported as a chronic bioassay parameter. The echinoderm survival test, the percent survival of the sand dollar larvae, Dendraster excentricus, was the pore water acute bioassay test. Pore water was extracted from the sediment samples for use in the tests. The percent of normally developed sand dollar larvae was also measured as a chronic parameter for a range of pore concentrations over a 72-hour test period. Solid sediment was used in the polychaete bioassay tests. The percent survival and growth rates of the polychaete, Neanthes arenaceodentata, were measured at the end of a 28-day exposure period.

Variograms

In ordinary kriging, a variogram is first constructed using a spatial set of soil or sediment data, for example, from a site. A variogram has two parts: an experimental data and a model variogram. In the GMS software, both the experimental and model variograms are

calculated by simply clicking on software options. 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.

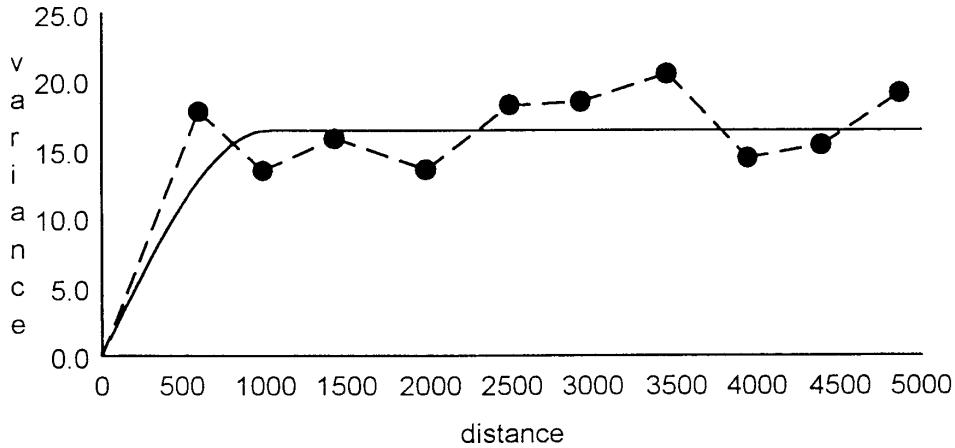

Figure 1. Variograms for Percent Amphipod Survival in the Example Harbor.

The model variogram is a curved line through the experimental variogram points. The model variogram represents a simple mathematical function modeling the trend in the points of the experimental variogram. The variogram in kriging can be used to calculate the expected error of estimation at each target interpolation point since the estimation error is a function of the distance to surrounding data points. In the kriging module of GMS (DoD, 1998), 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.

The expected estimation error is minimized in a least squares sense in kriging by using the variogram to compute weights in the kriging equations (DoD, 1998). 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

For percent amphipod, echinoderm, and polychaete survival in the example harbor, maps of isopleths of the values for these parameters were computed using the kriging interpolation equations. The isopleth maps were first computed and printed out for all 33 original sampling stations in the example harbor. Figure 2 is an example of one of these maps, showing isopleths of amphipod survival for all 33 sampling stations. An estimation error variance map was also computed for each parameter for the 33 original sampling stations. Figure 4 shows one of these maps, the estimation error variance for percent amphipod survival for 33 sampling stations.

Four and then eight sampling stations were then removed from the dataset. The sampling stations that were removed were the stations located nearest 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 interpolated isopleths and estimation error variance isopleths would stay the same or change with fewer sampling stations. Maps of isopleths of the values for percent amphipod, echinoderm, and polychaete survival were then produced using kriging interpolation for reduced datasets with 29 and then 25 sampling stations. Figure 3 shows the resulting interpolated isopleths for percent amphipod survival for 29 sampling stations. Estimation error variance maps were also computed for the reduced datasets with 29 and 25 sampling stations.

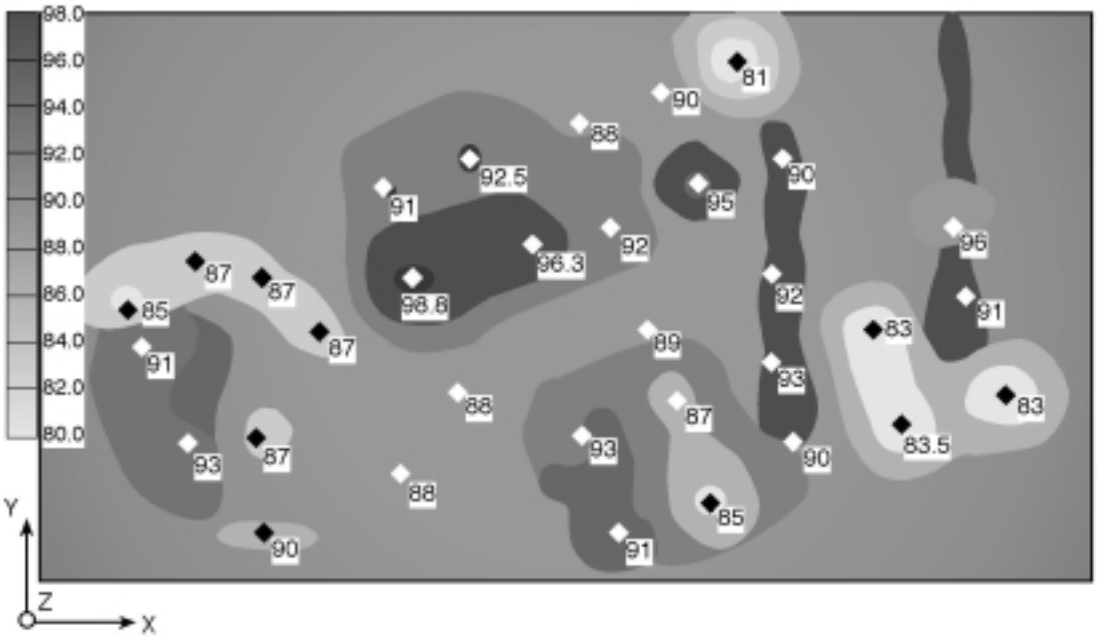

Figure 2. Kriged Isopleths For Percent Amphipod Survival for the Original 33 Sampling Stations in the Example Harbor.

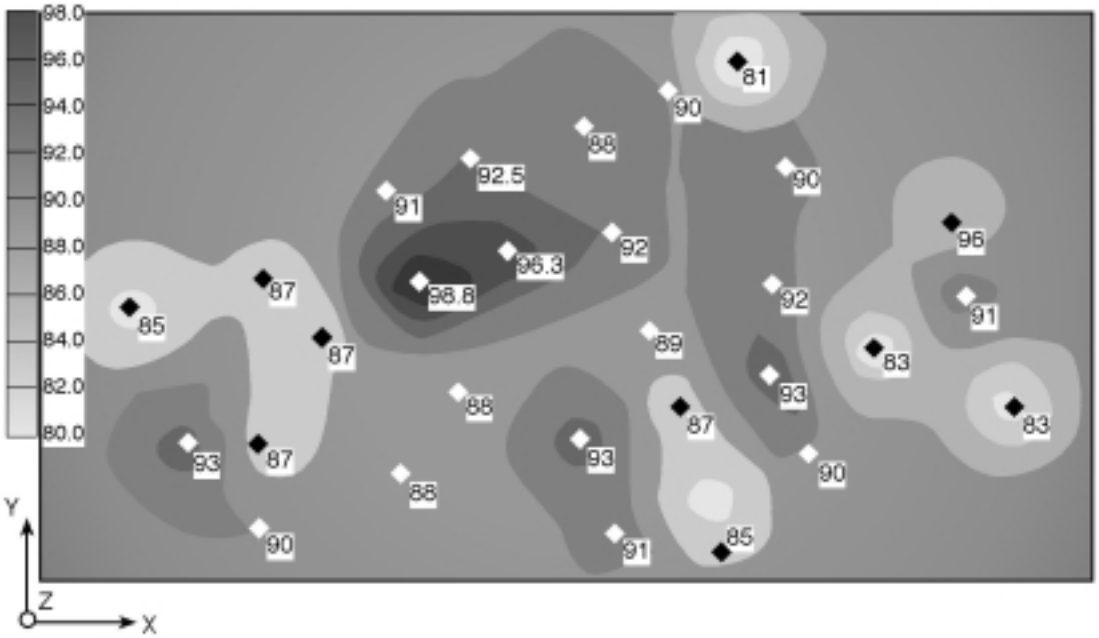

Figure 3. Kriged Isopleths For Percent Amphipod Survival for the Number of Sampling Stations Reduced to 29 in the Example Harbor.

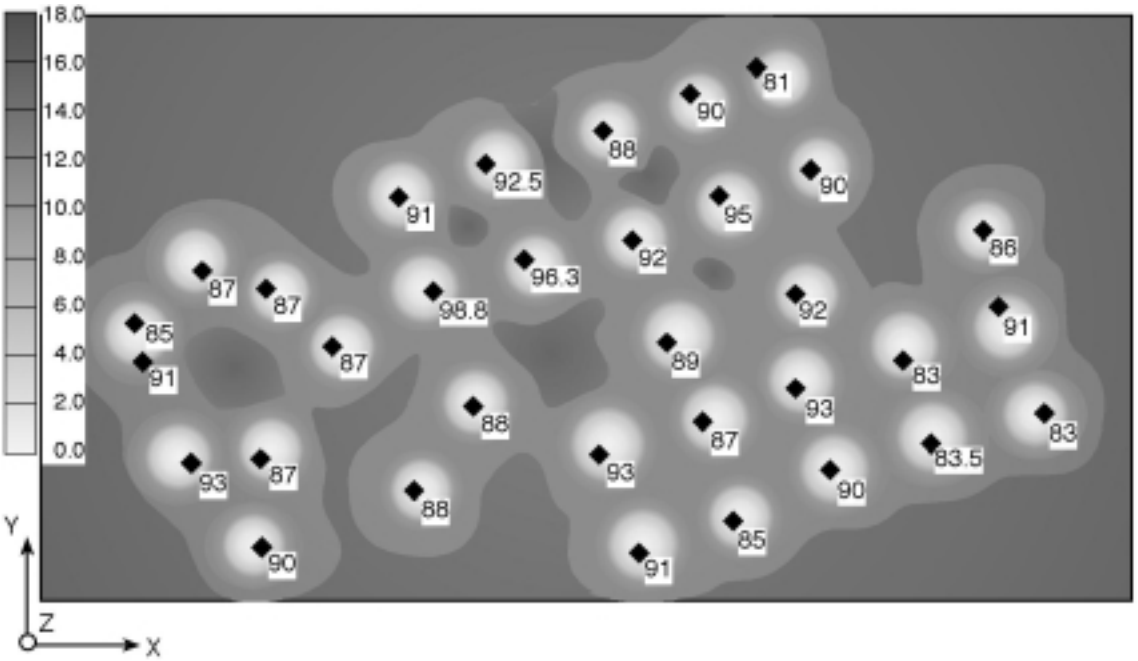

Figure 4. Estimation Error Variance Map for Percent Amphipod Survival for the Original 33 Sampling Stations in the Example Harbor.

Conclusions

The positions of the isopleths of the predicted values of percent amphipod survival changed very little when four sampling stations were removed from the 33 stations in the original dataset (Figures 2 and 3). The positions of the interpolated isopleths did change, however, when the number of stations were reduced by eight to 25 stations. The positions of the estimation error variance isopleths on maps changed very little when the number of sampling stations was reduced to either 29 or 25 stations. Since the number and position of original sampling stations, 33, in the example harbor were arrived at by the best collective judgement of the IR team for the harbor, this means that it is likely that 10% fewer sampling stations could be used to collect benthic bioassay data for eco-risk assessments of harbor sediments. For a harbor the size of the example harbor, collecting 10% fewer benthic bioassay samples could save the federal government $100,000 to $250,000 in 1998 dollars through the three to five major stages of an eco-risk assessment.

Using 29 sampling stations as the number necessary to characterize the spatial distribution of benthic bioassay parameters in a harbor the size of the example harbor, it appears that one sampling station is needed per 1,108,409 $ft.^2$ of harbor sediment. This is an area 1053 feet on a side. Only one sampling station is needed for an area of sediment 1053 feet on a side to adequately characterize benthic bioassay parameters. This is probably a larger area of harbor bottom per sampling station than was previously thought adequate to characterize benthic bioassay data.

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. In terrestrial eco-risk assessments, isopleths around areas of soil with contaminant concentrations representing successively larger eco-Hazard Index (HI) levels could be more accurately interpolated using kriging. In the baseline eco-risk stage, kriging could be used to interpolate isopleths of toxicity or eco-risk, such as for delineating areas representing contaminant concentrations above Eco-Preliminary Remediation Goal (EPRG's) levels in terrestrial eco-risk assessments.

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 sampling 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. New sampling stations should always be placed in the areas with the most estimation error variance as new sampling is planned through the stages of an eco-risk assessment. Kriging estimation error variance maps and interpolated isopleths of data should be used to plan sampling and define the shape of hotspots.

Where to Find More Information

The Civil Engineer Corps Officers Naval School (CECOS) In Port Hueneme, CA. has a three day " Geostatistics " course that includes good explanations and working examples of Kriging. The telephone number for the CECOS Registrar is (805) 982-2895, FAX number (805) 982-2918 and their website is http://www.cecos.navy.mil. The website for the Groundwater Modeling System (GMS) is http://ripple.wes.army.mil/software/gms/.

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