Spatial analysis of grain size in Santa Monica Bay

Molly K. Leecaster[1]

ABSTRACT

Maps are useful scientific tools for presenting environmental information, but the statistical techniques necessary to prepare scientifically rigorous maps have primarily focused on terrestrial habitats. This study compares three popular techniques (triangulation, kriging, and co-kriging) to map sediment grain size in Santa Monica Bay, California. Two grain size data sets, one collected in 1994 (79 sites) and one collected in 1997 and 1998 (149 sites) were used for model development. A bathymetric data set collected in 1997 was used as a model covariate. A third grain size data set (40 sites) collected in 1996 from independent sites was used for model evaluation. Predictions were compared to validation data by average difference, prediction mean square error (PMSE), and a goodness-of-prediction measure, G. The average difference between prediction and truth was similar for all methods, but the PMSE for triangulation was more than twice that for kriging or co-kriging, which were similar. The G measure also shows triangulation to be a far worse predictor than kriging and co-kriging. Small-scale differences were observed between kriging and co-kriging at steep depth contours, where co-kriging predicted values commensurate with the expected depth-defined grain size.

INTRODUCTION

Maps are useful scientific tools for portraying information and facilitating communication between the scientific community and the public. Maps provide a geographic reference for information, making them more useful than tables or charts. Maps also aid in the interpretation of data, the identification of gradients and patterns, and the formulation of hypotheses. Modeling techniques provide the information required to produce maps. Modeling extrapolates information from discrete stations to create maps of values that cover the whole area of interest. Maps are produced by using the information at stations to predict the value or values between stations and then filling in the gaps with this information.

Numerous techniques are used for spatial modeling. These techniques are categorized as interpolators that reproduce sample values or non-interpolators that do not. Techniques are also categorized as global predictors that use all data or local predictors that use only data from neighboring sites. Non-interpolators and global predictors, such as kriging, generally produce a smoother surface over the area of interest, whereas interpolators and local predictors, such as triangulation, generally produce a jagged surface. Another discriminating aspect of modeling is the ability to utilize covariate information. For example, kriging can be extended to co-kriging to accommodate variables related to the variable of interest.

Many modeling techniques have been compared in the terrestrial setting (Gotway Crawford *et al.* 1996, Gotway and Hergert 1997, Laslett *et al.* 1987, Laslett and McBratney 1990, McBratney and Webster 1983). In these comparisons, kriging and co-kriging have resulted in the highest prediction accuracy and precision. The comparisons for terrestrial soils focus on soil texture and soil parameters, such as pH. The terrestrial soil techniques have demonstrated a limited spatial structure (between 1 and 200 m) (Bragato and Primavera 1998, Gotway Crawford *et al.* 1996, Gotway and Hergert 1997, Kabrick *et al.* 1997, Laslett *et al.* 1987, Laslett and McBratney 1990, McBratney and Webster 1983, Streck and Richter 1997).

This study compared similar modeling techniques for sediment samples from the marine environment. The terrestrial comparisons may not apply to the marine environment because the vast sea floor lacks the interference of roads, buildings, or other structures, and marine sediments

[1]*Present address: INEEL, Bechtel WBXT, Idaho, LLC, P.O. Box 1625, Idaho Falls, ID 83415-3779*

may exhibit a far-reaching spatial correlation. Sediment grain size was selected as the mapping parameter in the marine environment because it is an analog to the terrestrial soil parameters that have been mapped. Grain size is also an important parameter for marine scientists, who use it as a correlate for chemical and biological patterns. Chemists use sediment grain size as a normalizing factor in determining the concentration of contaminants in sediments (Butcher 1996, Maurer *et al*. 1996, Schiff and Weisberg 1997, Schiff and Gossett 1998). Biologists recognize that benthic organisms partition their chosen habitat, in part, based upon sediment grain size, making this parameter important for assessing benthic communities (Bergen *et al*. 1998, Dorsey et al. 1995, Wu and Shin 1997, and Zmarzly *et al*. 1994). Similarly, microbiologists acknowledge that bacterial concentrations correlate to sediment grain size (Irvine and Pettibone 1993). Generally, the percent of sediment less than 63 micrometers (percent fines) is used to describe sediment grain size.

FIGURE 1. Santa Monica Bay, California, with depth contour lines.

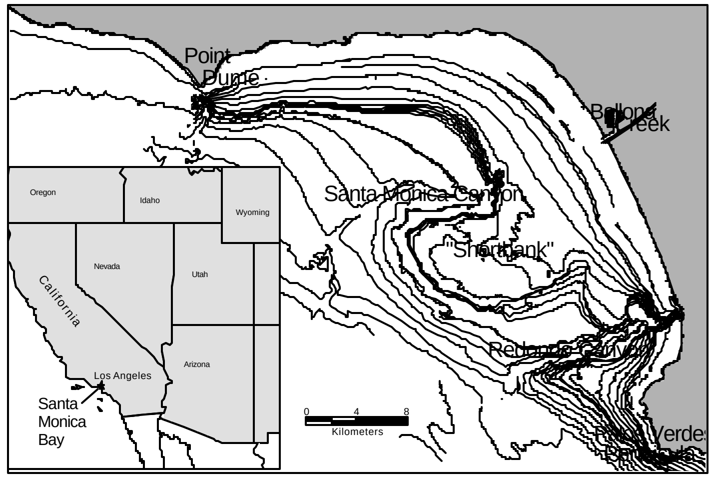
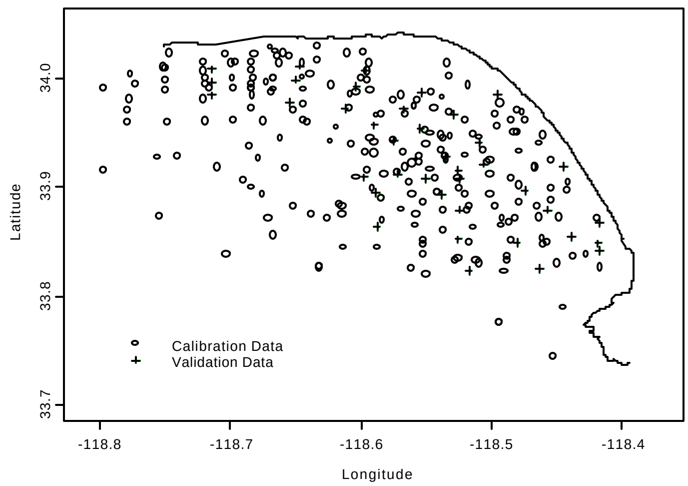


FIGURE 2. Sample site locations in Santa Monica Bay, California.



METHODS

Three modeling techniques—triangulation, kriging, and co-kriging—were compared by creating models with one data set and then testing those models with an independent data set. All data sets were derived from sediment samples collected from Santa Monica Bay, California (Figure1), which drains the watershed of the greater metropolitan Los Angeles area. The study area consisted of approximately 550 square km reaching a maximum depth of 800 m. The bay contains two canyons, Santa Monica and Redondo, which frame a large shallow shelf or shortbank.

Three data sets were combined to form a calibration data set (Figure 2). The first data set was collected in 1994 from 79 randomly selected sites, and was analyzed using a Horiba LA900 Laser (Schiff 2000). The second data set was collected in 1997 from 26 randomly selected sites, and was analyzed using a SediGraph 5100. The third data set was collected in 1998 from 123 subjectively chosen sites, and was also analyzed using a SediGraph 5100. The validation data set was collected in 1996 from 40 subjectively chosen sites, and was analyzed using a Horiba LA900. The data sets were obtained using two measurement methods whose results have been found to be comparable (Dalkey and Leecaster 2000).

The first modeling technique applied to these data was triangulation. Triangulation makes predictions for the triangles formed by connecting three sampling points. The prediction equations are bivariate fifth-degree polynomials. The connecting edges of the triangles are then smoothed by using partial derivatives of the prediction equations (Akima 1978).

The second modeling technique applied to these data was kriging, which makes predictions based upon a weighted mean of all sample values. Kriging makes two assumptions: (1) that there is a locally common expected value (stationarity) and (2) that spatial correlation is independent of direction (isotropy). Stationarity and isotropy of percent fines was verified by comparing the variograms (values of distance and variance between pairs of points at each distance) of the raw data and of the residuals from a polynomial regression on latitude and longitude. These two variograms were compared for six directions corresponding to north-south, east-west, northeast-southwest, northwest-southeast, along-shore, and cross-shore. The data set that displayed similar variograms for all directions was considered stationary and isotropic. The empirical variograms of the stationary and isotropic data were then modeled by specifying a spherical model with specified nugget (small-scale variation), sill (asymptotic variance between pairs of sites), and range (distance at which the sill is attained). Kriging predictions were calculated to minimize the error variance, which was accomplished by weighting station values in the prediction equation based upon the variogram model parameters. Those values closer to the prediction point received larger weight. Since these values are more highly correlated with the prediction site, this results in smaller variance.

The third modeling technique applied to these data was co-kriging. Co-kriging, which is kriging plus a covariate, was performed using depth as a covariate. Depth data were obtained from side-scan sonar in 1997. Kriging assumptions of stationarity and isotropy were checked for depth as well as percent fines. In addition to the kriging assumptions, a linear model of co-regionalization assumption was used. The model is necessary to ensure positive variance functions and is assured by specifying variogram and cross-variogram models with similar structure with respect to choice of nugget and range values. The variograms for percent fines and depth and their cross-variogram, values of distance and covariance between pairs of variables at that distance, were modeled using spherical models with specified nugget, sill, and range. Co-kriging predictions were calculated to minimize the error variance based upon both variogram model parameters and cross-variogram model parameters, similar to kriging.

All modeling techniques were performed on the residuals from the polynomial regression. Predictions of percent fines were calculated as the modeled residual predictions plus the polynomial regression fit. Predictions of percent fines were made over a 50-by-50 grid. This grid resulted in estimates made every 1.12 km east-west and every 0.89 km north-south. The prediction surface covered at most 56 km east-west and at most 44.5 km north-south.

All model results were compared to the validation data by calculating the average difference between the actual and predicted value, the prediction mean square error (PMSE), and an accuracy measure (G) introduced by Agterberg (1984). The PMSE is defined as:

$$\frac{\sum_{i=1}^{n}(z_i - \hat{z}_i)^2}{n}$$

where:

n = the number of validation stations

z_i = the validation value (truth) at station i

$\hat{z}_i$ is the predicted value at station .

G is defined as:

$$G = \left(1 - \frac{PMSE}{MSE_{\bar{z}}}\right) * 100\%$$

where:

$PMSE$ = prediction mean square error defined above

$MSE_{\bar{z}}$ = mean square error from on the overall mean (53.2)

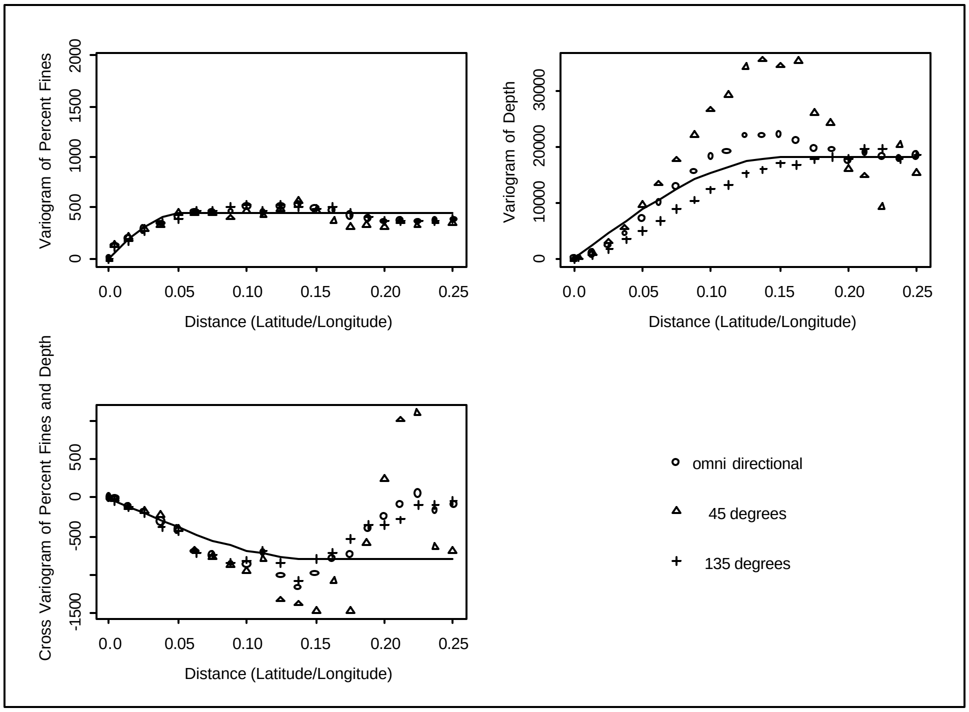
The average difference between actual and predicted values is small for a good model, as is the PMSE. For G, a value of zero would represent a model that performs equally as well as the overall mean. Larger numbers imply predictions better than the overall mean, while negative numbers imply predictions worse than the overall mean. The measure is used to compare models and has no inherent stand-alone numerical significance.

RESULTS

Percent fines and depth data were stationary and isotropic after regressing each variable on latitude, latitude squared, longitude, and longitude squared. All directional variograms had a similar structure for percent fines and depth, as did their cross-variograms (Figure 3). A spherical model with a range of 0.06 was used for variograms on percent fines and depth and for their cross-variograms. The range of 0.06 on coordinate scale corresponded to approximately 6 km. The sill of the percent fines variogram was estimated to be 400 and the nugget, 50. The sill of the depth variogram was estimated to be 12,000 and the nugget, 50. The sill of the cross-variogram was estimated to be -1000 and the nugget, 0.

The triangulation predictions were not as close to the validation data set as were the kriging and co-kriging predictions (Tables 1 and 2, Figure 4). The average difference between the truth and the predictions was approximately 7 percent fines, where the full range of predictions was between 3 and 92 percent fines. All models tended to over-predict percent fines, resulting in positive average differences. The PMSE was 2.5 times smaller for kriging

FIGURE 3. Empirical variograms of residuals from a polynomial regression and spherical model estimates (lines).



and co-kriging compared to triangulation. Although the average differences were the same among methods, some very large over- and under-predictions from the triangulation method were evident in the plot of measured-versus-predicted values (Figure 4). The G measure of validation accuracy was approximately the same for kriging and co-kriging, but was very small for triangulation.

DISCUSSION

Based upon numeric measures from the validation data, kriging and co-kriging techniques provided similarly accurate predictions. This finding is also evident in the correlation between model predictions (Table 3).

A more robust approach for comparing models is to consider the details in the final maps (Isaaks and Srivastava 1989). Using this approach, it was determined that co-kriging produced a better map of the Santa Monica Bay than the kriging method (Figures 5 and 6). The differences between these two methods are evident at the depth-defined canyons, canyon lips, and shortbank. The co-kriging map corresponds much better with these bathymetry-defined features. The kriging map shows a different shape for the shortbank and does not reflect Redondo Canyon at all. Deep canyons contain a much higher percentage of fine sediment while the shallow shelf area is generally rocky and contains a much lower percentage of fine sediment. The inclusion of depth in the model improves prediction in the depth-defined areas.

Triangulation performed poorly compared to the kriging techniques on all counts. The predictions were further from the validation set and were not highly correlated with the kriging or co-kriging predictions. Triangulation predictions were also sometimes less than 0 or greater than 100 percent fines near the edges of the data hull. Interpolators often suffer from poor predictions (Laslett *et al.* 1987). Since triangulation is an interpolator, fitting a model through two values, one larger and on the edge of the data hull, would result in an ever-increasing prediction slope. Limiting the prediction to the convex hull produced very tight isopleths at the boundary that still exceeded the range of possible values (0–100%). In practice, all values exceeding the range would be assigned the limiting value (0 or 100%), but this solution does not reduce concerns about the limitations inherent in interpolating methods.

The findings of this study correspond well to modeling method comparison studies conducted with terrestrial soils. When kriging was compared to techniques other than co-kriging in the terrestrial environment, it performed best (Gotway Crawford *et al.* 1996, Gotway Crawford and Hergert 1997, Laslett *et al.* 1987, and Laslett and McBratney 1990). Two comparison studies were conducted on terrestrial soils involving co-kriging. Co-kriging was found to be the best method in one study (McBratney and Webster 1983), and regression plus kriging was found to be the best method in the other study (Odeh *et al.* 1994).

While the modeling approach deemed best by this study had an average absolute difference of 11.3%, this value overstates the true modeling error because it includes inter-annual variability introduced by using a validation data set from a different year. To estimate the effect of inter-annual variability, City of Los Angeles data collected from 1987 to 1995 at the same 40 sites used in the validation data set were used to calculate the biennial average absolute difference of 6.8%. Biennial deviation was used since the validation data were collected two years later than one modeling data set and one or two years earlier than the

TABLE 1. True percent fines and predictions for validation stations. Bold values represent predictions that are larger than the true value.

Station Number	1996 Percent Fines	Triangulation Prediction	Kriging Prediction	Co-Kriging Prediction
1	10	3	**24**	**32**
2	11	10	7	10
3	8	**30**	**20**	**23**
4	67	55	**70**	**79**
5	73	50	**76**	**79**
6	54	34	52	46
7	42	34	**43**	38
8	43	**48**	**52**	43
9	43	**55**	**52**	42
10	50	**65**	**56**	50
11	26	**34**	**33**	**40**
12	33	32	29	**37**
13	39	**82**	**46**	**48**
14	68	65	**81**	**77**
15	65	**67**	**75**	**68**
16	37	18	**41**	**44**
17	20	15	**31**	**38**
18	53	35	35	36
19	32	**36**	**33**	**33**
20	18	**29**	**28**	**30**
21	28	**40**	**34**	**38**
22	24	**90**	**46**	**50**
23	50	36	42	44
24	24	**68**	**33**	**35**
25	33	18	25	24
26	35	27	33	31
27	26	**83**	**71**	**61**
28	40	**92**	**69**	**67**
29	47	**56**	**75**	**78**
30	51	42	**73**	**70**
31	62	62	**72**	**82**
32	55	**77**	**73**	**83**
33	48	40	**55**	**60**
34	50	**68**	**53**	**55**
35	48	40	**50**	37
36	33	**50**	**50**	**40**
37	77	**90**	**84**	73
38	45	43	42	**54**
39	35	**60**	**43**	35
40	49	**60**	43	32

other modeling data set. Thus, half of the variability associated with differences between prediction and validation data appears to be due to differences in years and not error in prediction.

Overall, the co-kriging map of percent fines corresponds to local knowledge of the system, but some shortcomings were observed in the predictions (Figure 6). The model fails to accurately describe the canyon lip areas that are very active, so that sediment grain size is spatially as well as temporally variable; in fact, all models fail to some degree in these areas. Limited data on the canyon lips and in the canyons made prediction difficult in this study. Other data sources might be used to adjust these predictions. Backscatter information, which portrays the hardness of the seafloor as shades of gray, and seafloor photographs at some calibration data sample sites might be used to adjust predictions a posteriori or be included a priori as a covariate in the co-kriging model. Another possible discrepancy was found in the northern shoreline, which is predicted to be quite muddy. This finding conflicts with the general belief that shorelines have sandy sediments, but is consistent with Allen (1982) who found that this area has finer sediments because the south-facing shore is largely protected from extreme currents.

In this study, several data sets were combined to achieve a higher sampling density than is typically available from most areas. This higher sampling density resulted in an improved level of confidence in the variogram upon which the kriging models were based. The resulting variogram provides information about the level of density necessary to achieve optimal kriging variance (McBratney *et al.* 1981, McBratney and Webster 1981), since kriging variance depends only upon sample station spacing and variogram parameters. The optimal grid spacing to map grain size in Santa Monica Bay is approximately 950 m on a triangular grid. This spacing corresponds to a density of approximately 1.4 samples per square km, which is 7 times as dense as the current routine monitoring effort being conducted in Santa Monica Bay (City of Los Angeles 2000) and 10 times as dense as the most recent regional survey of conditions throughout southern California (Schiff 2000). Although the kriging variance would be very large, the designs are useful for their intended purposes of trend analysis and inferential statistics.

TABLE 2. Three measures of prediction accuracy, with respect to the validation data, for the modeling methods.

	Triangulation	Kriging	Co-kriging
Average Difference	7.2	7.5	7.3
Prediction Mean Square Error	499	183	209
G	5	51	42

FIGURE 4. Measured values of percent fines for validation data versus predictions from triangulation, kriging, and co-kriging.

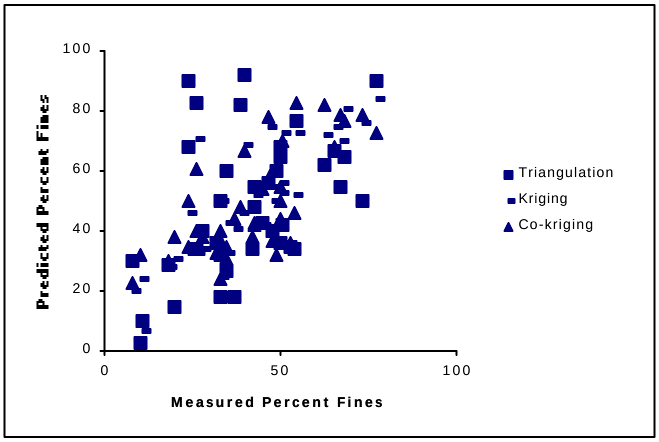
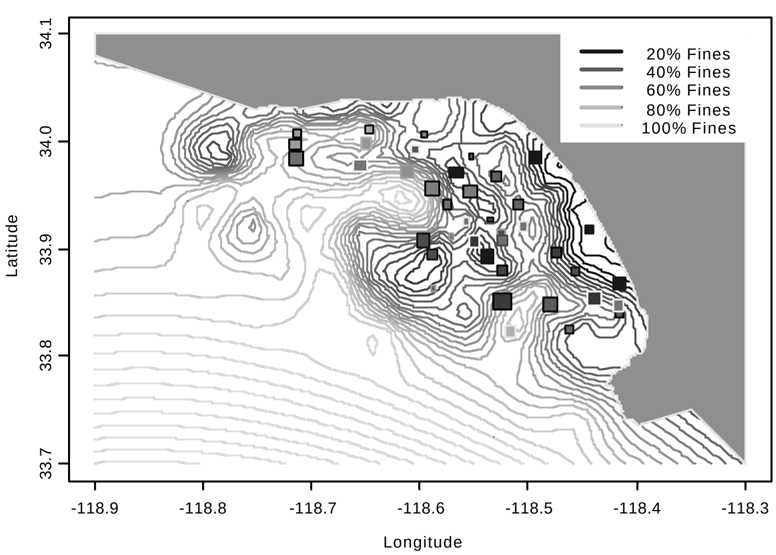


TABLE 3. Spearman rank correlation coefficient among model predictions.

	Kriging	Triangulation
Co-kriging	0.95	0.43
Kriging		0.48

FIGURE 5. Kriging prediction of percent fines for Santa Monica Bay. Squares represent validation data values and size signifies the deviation from prediction.



LITERATURE CITED

Agterberg, F.P. 1984. Trend surface analysis. pp. 147–171 *in:* G.L. Gaile and C.J. Willmott (eds.), Spatial Statistics and Models. Reidel, Dordrecht. The Netherlands.

Akima, H. 1978. A method of bivariate interpolation and smooth surface fitting for irregularly distributed data points. ACM *Transactions on Mathematical Software* 4:148-159.

Allen, M.J. 1982. Functional structure of soft-bottom fish communities of the southern California shelf. Ph.D. Dissertation. University of California, San Diego.

Bergen, M., S.B. Weisberg, D. Cadien, A. Dalkey, D. Montagne, R.W. Smith, J.K. Stull and R.G. Velarde. 1998. Southern California Bight 1994 Pilot Project: IV. Benthic infauna. Southern California Coastal Water Research Project. Westminster, CA.

Bragato, G. and F. Primavera. 1998. Manuring and soil type influence on spatial variation of soil organic matter properties. *Soil Science Society of America Journal* 62: 1313-1319.

Butcher, J.B. 1996. Co-kriging to incorporate screening data: Hudson River sediment PCBs. *Water Resources Bulletin* 32:349-356.

City of Los Angeles, Department of Public Works, Bureau of Sanitation. 2000. Hyperion Treatment Plant 1999 Annual Report. Los Angeles, CA.

Dalkey, A. and M. Leecaster. 2000. Comparison of Sediment Grain Size Analysis Among Two Methods and Three Instruments Using Environmental Samples. This annual report. pp. 289-295 *in:* This annual report. Southern California Coastal Water Research Project. Westminster, CA.

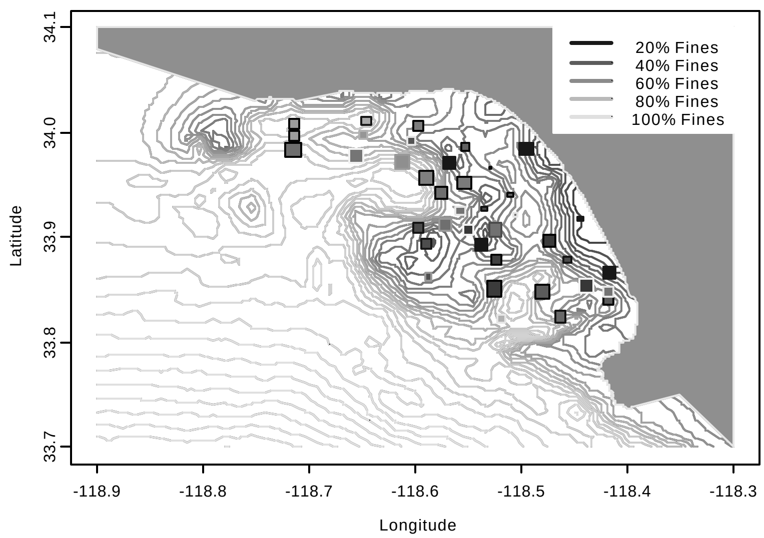
Dorsey, J.H., C.A. Phillips, A. Dalkey, J.D. Roney and G.B. Deets. 1995. Changes in assemblages of infaunal organisms around wastewater outfalls in Santa Monica Bay, California. *Bulletin of Southern California Academy of Sciences* 94:46-64.

Gotway, C.A., R.B. Ferguson, G.W. Hergert and T.A. Peterson. 1996. Comparison of kriging and inverse-distance methods for mapping soil parameters. *Soil Science Society of America Journal* 60:1237-1247.

Gotway Crawford, C.A. and G.W. Hergert. 1997. Incorporating spatial trends and anisotropy in geostatistical mapping of soil properties. *Soil Science Society of America Journal* 61:298-309.

Irvine, K.N., and G.W. Pettibone. 1993. Dynamics of indicator bacteria populations in sediment and river water near a combined sewer outfall. *Environmental Technology* 14:531-542.

FIGURE 6. Co-kriging prediction of percent fines for Santa Monica Bay. Squares represent validation data values and size signifies the deviation from prediction.



Isaaks, E.H. and R.M. Srivastava. 1989. Applied Geostatistics. Oxford University Press. New York, NY.

Kabrick, J.M., M.K. Clayton and K. McSweeny. 1997. Spatial patterns of carbon and texture on drumlins in northeastern Wisconsin. *Soil Science Society of America Journal* 61:541-548.

Laslett, G.M. and A.B. McBratney. 1990. Further comparison of spatial methods for predicting soil pH. *Soil Science Society of America Journal* 54:1553-1558.

Laslett, G.M., A.B. McBratney, P.J. Pahl and M.F. Huchinson. 1987. Comparison of several spatial prediction methods for soil pH. *Journal of Soil Science* 38:325-341.

Maurer, D., G. Robertson, T. Gerlinger and R. Gossett. 1996. Organic contaminants in sediments of the Newport Submarine Canyon, California, and the adjacent shelf. *Water Environment Research* 68:1024-1036.

McBratney, A.B. and R. Webster. 1981. The design of optimal sampling schemes for local estimation and mapping of regionalized variables: II. Program and examples. *Computers and Geosciences* 7:335-365.

McBratney, A.B. and R. Webster. 1983. Optimal interpolation and isarithmic mapping of soil properties: V. Co-regionalization and multiple sampling strategy. *Journal of Soil Science* 34:137-162.

McBratney, A.B., R. Webster and T.M. Burgess. 1981. The design of optimal sampling schemes for local estimation and mapping of regionalized variables: I. Theory and method. Computers and Geosciences 7:331-334.

Odeh, I.O.A., A.B. McBratney and D.J. Chittleborough. 1994. Spatial prediction of soil properties from landform attributes derived from digital elevation model. Geoderma 63:197-214.

Schiff, K. and R.W. Gossett. 1998. Southern California Bight 1994 Pilot Project: III. Sediment chemistry. Southern California Coastal Water Research Project. Westminster, CA.

Schiff, K. and S.B. Weisberg. 1997. Iron as a reference element for determining trace metal enrichment in California coastal shelf sediments. pp. 68-77 *in:* Southern California Coastal Water Research Project Annual Report 1996. Southern California Coastal Water Research Project. Westminster, CA.

Schiff, K.C. 2000. Sediment chemistry on the mainland shelf of the Southern California Bight. *Marine Pollution Bulletin* 40:268–276.

Streck, T. and J. Richter. 1997. Heavy metal displacement in a sandy soil at the field scale: I: Measurements and parameterization of sorptia. *Journal of Environmental Quality* 26:549-556.

Wu, R.S.S. and P K.S. Shin. 1997. Sediment characteristics and colonization of soft-bottom benthos: A field manipulation experiment. *Marine Biology* 128:475-487.

Zmarzly, D.L., T.D. Stebbins, D. Pasko, R.M. Duggan and K.L. Barwick. 1994. Spatial patterns and temporal succession in soft-bottom macroinvertebrate assemblages surrounding an ocean outfall on the southern San Diego shelf: Relation to anthropogenic and natural events. *Marine Biology* 118:293-307.

ACKNOWLEDGEMENTS

I wish to thank the United States Geological Survey for providing grain size data from their 1997 and 1998 cruises and bathymetry data from 1997. I also wish to thank the City of Los Angeles Environmental Monitoring Division for providing grain size data for the years 1987 to 1996.