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KRIGING AND AUTOMATED VARIOGRAM MODELING WITHIN A MOVING WINDOW

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Abstract—A spatial estimation procedure based on ordinary kriging is described and evaluated which consists of using only sampling sites contained within a moving window centered at the estimate location for modeling the covariance structure and constructing the kriging equations. The moving window, by depending on local data only to estimate the spatial covariance structure and calculate the estimate, is less affected by spatial trend in the data than conventional kriging approaches and implicitly models covariance nonstationarity. The window's covariance structure is estimated by automatically fitting a spherical variogram model to the unbiased estimates of semi-variance calculated at several lags. The automatic fit uses nonlinear least squares regression constrained by the nugget parameter being nonnegative.

This estimation method is compared to the more standard method of ordinary kriging over fixed subregions by using both procedures in the analysis of NADP/NTN sulfate deposition data in the conterminous U.S. For this analysis, we find that the moving window scheme provides local variogram models which are minimally affected by trend, and that also this use of an ensemble of variograms allows the accurate modeling of a spatially changing covariance structure.

Accurate spatial covariance modeling is needed by acid deposition effects researchers because it is a prerequisite for the calculation of defensible deposition confidence intervals from the error (kriging) variance.

Key word index: Kriging, spatial analysis, acid precipitation, nonlinear regression, variogram modeling, moving window estimation.

1. INTRODUCTION

Recently, there have been applications of kriging estimation procedures to environmental processes acting over large regions (Finkelstein, 1984; Lefohn *et al.*, 1987). For an introduction to the kriging technique of process estimation, see Venkatram (1988). Several researchers have noted the presence of mean nonstationarity in these processes (Seilkop, 1983; Cressie, 1986). In addition, given the variability of precipitation patterns and emissions sources at different localities in the conterminous U.S., covariance stationarity may also be present. Indeed, estimates of spatial covariance over subregions of the conterminous U.S. included in the discussion below suggest that there are marked differences. Several variations of the kriging procedure have been developed which allow for certain forms of mean nonstationarity, e.g. universal kriging and generalized covariance kriging, but there has been little effort toward accommodating covariance nonstationarity.

In this paper, we develop and test a method which minimizes the effect on the kriging point estimate and its associated estimate of estimation error variance (the so-called kriging variance) from both mean and covariance nonstationarity. We do this by taking advantage of the attenuation of trend, and covariance heterogeneity within subregions of the field the process is defined on. This is accomplished by performing the calculation of the semi-variance estimates, the modeling of the semi-variance function, and the calculation of a single, ordinary kriging estimate all inside a circular window centered at the estimate location. To generate an estimate surface, this window is moved to each desired estimate location (usually locations in a regular grid) and the above calculations repeated.

The rationale for why a moving window scheme is effective with nonstationary processes is derived from Journel and Huijbregts' (1978, pp. 33–34) definition and discussion of *quasi-stationarity*. Essentially, Journel and Huijbregts maintain that a nonstationary process defined over a large region will exhibit smaller absolute trend and a more homogeneous covariance structure over a subregion relative to the entire region, i.e. the process will be quasi-stationary within this subregion. This discussion suggests that covariance modeling should be performed over subregions. The window should be just large enough to contain enough sampling locations to estimate the semi-variance function with accuracy sufficient for the intended uses of the process estimates. Hence, a new subregion for every estimate location should be defined.

The implementation of this approach requires programmable heuristics for (a) window size determination, and (b) determination of initial nugget, sill, and range values for the iterative nonlinear least squares fitting of the variogram model.

As noted above, this approach requires for each window, a sampling site selection step, semi-variance estimate calculations, and an iterative nonlinear regression calculation in addition to the usual solution of the kriging equations. Hence, the computational load is greater for this approach than for standard kriging algorithms.

The paper is structured as follows. Section 2 describes the heuristics for window size determination. Section 3 gives the heuristics for automatic selection of starting values for the nonlinear least squares algorithm with a comparison of that algorithm's output to results from the NLIN procedure in SAS (1985). Section 4 reports an application of the moving window approach to estimating acid deposition in the conterminous U.S. with computing expense comparisons between this method and a more conventional kriging estimation approach. Section 5 gives our conclusions.

2. AUTOMATIC WINDOW SIZING

The size of a subregion is dependent on two conflicting criteria. The smaller the region, the better the approximation to stationarity; on the other hand, the larger the region, the more sites available for semi-variance estimates. The accuracy with which a semi-variance can be estimated is partly a function of the number of couples used in the estimate. Also, estimates at short lags are more important for later kriging estimation than those at longer lags.

For the NADP/NTN network (National Atmospheric Deposition Program, 1987), the above considerations were translated into a simple heuristic for window size determination, this was: recursively enlarge the window radius by 10% until at least 35 sites are included. Thereafter, increase the window radius in five site increments until: (a) at least one pair of sampling sites is found within the window for each separation distance bin, and (b) the automatic nonlinear regression fit of the spherical model (see section 3) to the semi-variance estimates converges. This heuristic was motivated by the observation that for the NADP/NTN network, about 35 sites in a circular window centered anywhere in the conterminous U.S. usually produces at least two couples for a 50 km lag isotropic semi-variance estimate. In our application, 50 km was the lag interval and hence the shortest lag for which a semi-variance was estimated. A 35 site circular window also produced couple counts between 7 and 60 for lags greater than 50 km and less than 140% of the window's radius. The distance of 140% of the window's radius also became the longest lag for which a semi-variance value was estimated. Although these heuristics were formulated specifically for the NADP/NTN network, the development of these rules is general: for any set of sampling sites, find a lag interval and window site count such that at least two couples are usually found at the shortest lag and at least two at the longest.

As we shall discuss in the following sections, even though the couple count was usually small for the two shortest lags, the iterative least squares algorithm was able to fit usable variogram models for every window in our application. This success is due to a characteristic of the semi-variance estimator employed in the analysis. We discuss this characteristic next.

Semi-variance ($\gamma(h)$) is defined to be $1/2E(Z(x)-Z(x+h))^2$. We used Matheron's unbiased semi-variance estimator

$$\hat{\gamma}(h)=1/2N_h\Sigma(Z(x)-Z(x+h))^2 \qquad (1)$$

(Matheron, 1963) where $Z(x)$ is an observation of the stochastic process at location x and N_h is the number of lag h couples. There are two sources of variation associated with this estimator. The first is due to using only a finite number of sample locations to estimate the semi-variance of a continuous process, called estimation variance by Journel and Huijbregts, and the second is due to the variation arising from using only one realization, called fluctuation variance by the same authors (Journel and Huijbregts, 1978, pp. 192–193). The contribution to the variance of the estimator at a particular lag from each of these sources is a function of the semi-variance at that lag. Since the semi-variance function is monotonically increasing, the estimate variance due to each of these sources increases when the lag of the estimated semi-variance increases. We note that if these two sources of error can be considered as independent then the total variance is the sum of the variance from each source. Journel and Huijbregts (1978, p. 193) give an example of the variance of Matheron's estimator. Let $Z(x)$ be a Gaussian random field defined on a one-dimensional space of length L and distributed $N(\mu,\sigma^2)$ at any point. Let the covariance structure be defined by $\gamma(h)=|h|$. Then, assuming the independence of the discrete sampling error and the single realization error sources, we have

$$E(\gamma(h)-\hat{\gamma}(h))^2=4\gamma(h)\sigma^2/N_h+4/3(h/L)\gamma(h)^2 \qquad (2)$$

for $h<L/3$. The first term is the variance due to using a finite number of couples (N_h), and the second is the variance due to using only one realization.

Hence, we suggest that since the semi-variance estimate at short lags has lower variance than an estimate at long lags, for the same number of couples, N_h, an estimate at a short lag can provide the same variance using fewer couples as an estimate of semi-variance at a long lag.

Even with the above argument, since precise estimates of the semi-variance at short lags is more important to the kriging step than precise estimates at long lags, we would prefer couple counts at short lags at least as large as those at longer lags.

As a final note on semi-variance estimation, even though the semi-variance functions are estimated in a moving window scheme with a minimum number of sampling sites, since an unbiased estimator is used, we can be confident that over a large region of similar covariance structure, the estimated semi-variance functions for each window will, on the average, represent the true covariance structure of that region.

3. AUTOMATIC VARIOGRAM MODEL FITTING

Once the window region has been determined and the semi-variance estimates calculated at the desired lags, a model is fitted to these estimates to determine the covariance structure needed in the kriging estimation step. The model used should explain the estimates well and also produce a positive definite covariance matrix for any set of lags. Models which guarantee a positive definite covariance matrix include the spherical, Gaussian, and exponential (Journel and Huijbregts, 1978). For our NADP/NTN data set of acid deposition, we choose the spherical model because of our prior success with fitting variogram models to deposition data with this function.

This model, like the other standard semi-variance models, is parameterized by the nugget, sill and range. These parameters are usually estimated from the semi-variance estimate data either by inspection or by nonlinear regression, the latter technique being possible to program as an automatic fitting procedure. All general purpose nonlinear regression algorithms are iterative, local optimization techniques and hence need starting estimates of the parameters which are already close (as measured in the parameter space) to the optimal estimates.

We chose the Levenberg–Marquardt algorithm with the least squares objective function and developed our automatic fitting procedure around the subroutine MRQMIN (Press *et al.*, 1986, pp. 521–527). This regression algorithm was chosen over two other candidate algorithms—the method of the steepest descent and the inverse Hessian method, because it essentially combines these two algorithms by varying a parameter controlling the step-size depending on whether the previous step produced a reduction in the sum of squares. For each window, the regression was begun as an unconstrained search, if a negative nuggest was returned, the nugget was fixed at zero and the subspace of the sill and range was searched again.

The heuristic for finding the starting nugget value for the iterative algorithm was to use 85% of the median of the semi-variance estimates at the three shortest lags. For the starting sill value, the heuristic was to use the median of the semi-variance estimates at the four longest lags. The median was chosen over the average due to the former's resistance to outliers. These starting nugget and sill values were then used in ten separate applications of the fitting algorithm wherein the starting value of the range was varied from one tenth of the maximum lag to the maximum lag in equal one tenth increments. The converged sum of squares was recorded from each of these fits and the parameter estimates from the regression with the smallest sum of squares were input to the kriging estimation step. If the algorithm failed to converge for any of these fits, the global search was repeated using just the median of the first three semi-variance estimates for the starting nugget, i.e. the 85% heuristic was dropped. If, after the global search, the nugget was larger than the sill, the nugget and sill were both set equal to the sample variance of the data within the window. This last was programmed because the nugget, being a measure of micro-scale spatial variability cannot be bigger than the variance of the process itself which is parameterized by the sill for a finite variance spatial stochastic process.

The fraction 85% was chosen to correct for the reduction of the semi-variance from the first lag to lag zero and was arrived at through experience with variograms estimated from the acid deposition process. The fitting procedure was not found to be highly sensitive to the particular value of this fraction, but generally, a slowly increasing semi-variance function should be fitted using a fraction near one.

The global search over the parameter space of the range was originally adopted because no reliable, simple heuristic could be devised for finding a starting range value. This simple global search of a one-dimensional space turned out, however, to be computationally inexpensive and to also provide more confidence that the true least squares parameter estimates had been found. Although these heuristics for finding starting parameter values were discovered through experience with a particular data set, we believe they may be applicable to data sets from other environmental process sampling networks.

To apply the algorithm to a set of data and starting parameter values, a convergence criterion had to be defined. Acting on recommendations in Press *et al.* (1986), we considered the algorithm to be converged when for 20 consecutive steps, the difference in the sum of squares of a latter and former step of any two

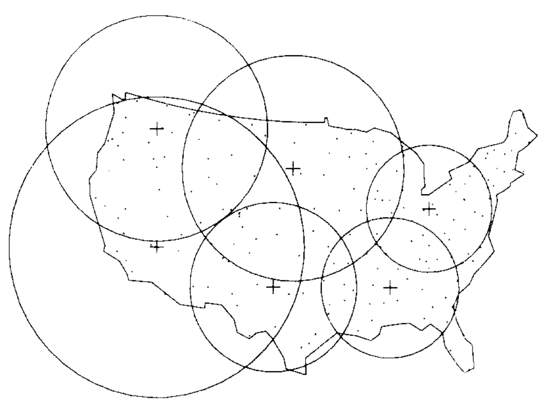

Fig. 1. Selected estimate locations (+s) and associated moving window subregions. The dots are the NADP/NTN sites operating during the winter of 1986 and for which the data met NADP/NTN quality assurance criteria. The number of sites within each window in the top row (from left to right) is 39, 55 and 42, respectively. For the bottom row, these are 65, 36 and 40.

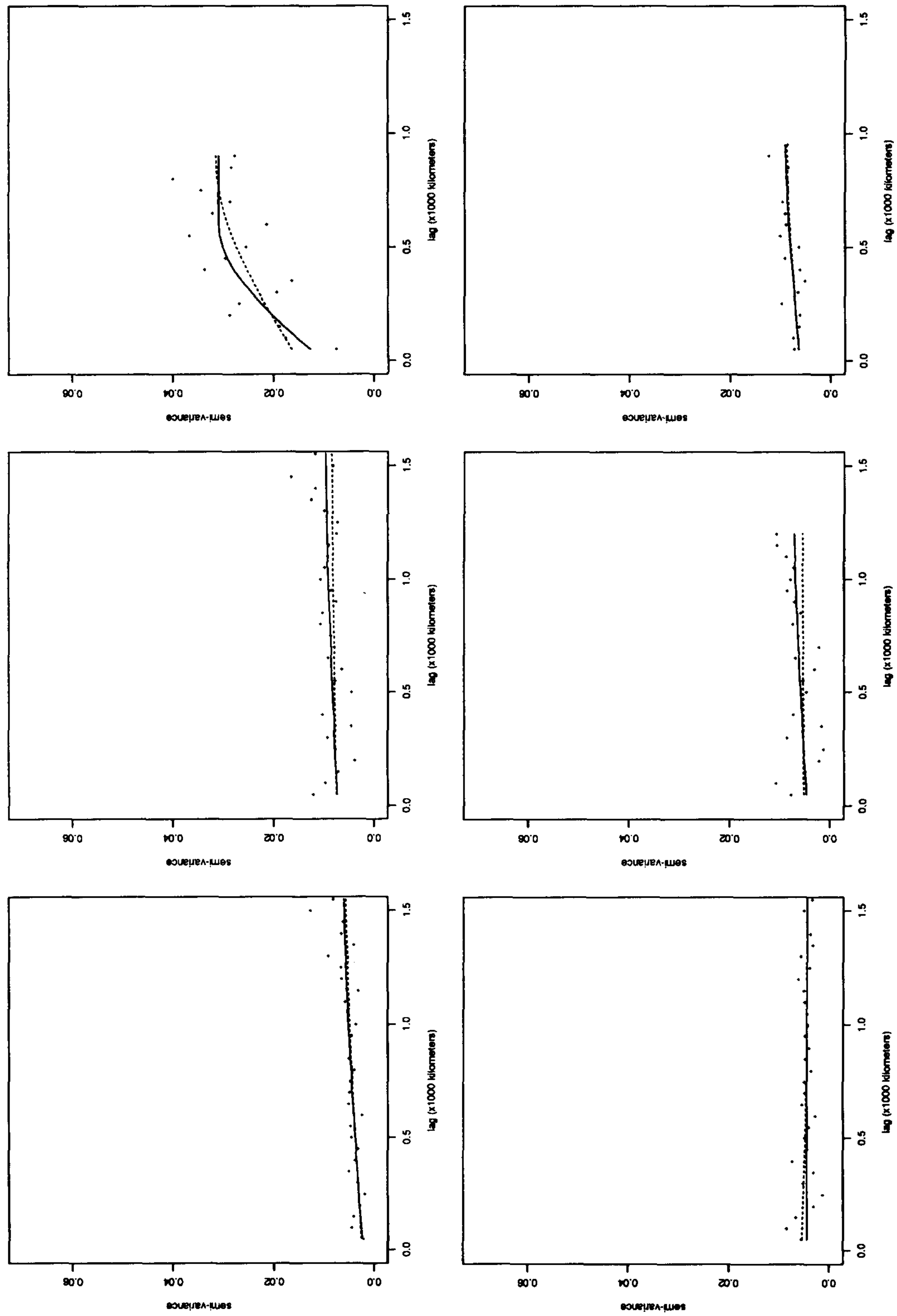

Fig. 2. Sample variogram values (asterisks) calculated within each of the windows given in Fig. 1. Relative plot layout is equivalent to the window layout in Fig. 1 (lower-left window is the lower-left plot, etc.). The solid line is the spherical model fit using the automatic, nonlinear regression routine in the moving window procedure. The dotted line is the spherical model fit using the NLIN procedure in SAS.

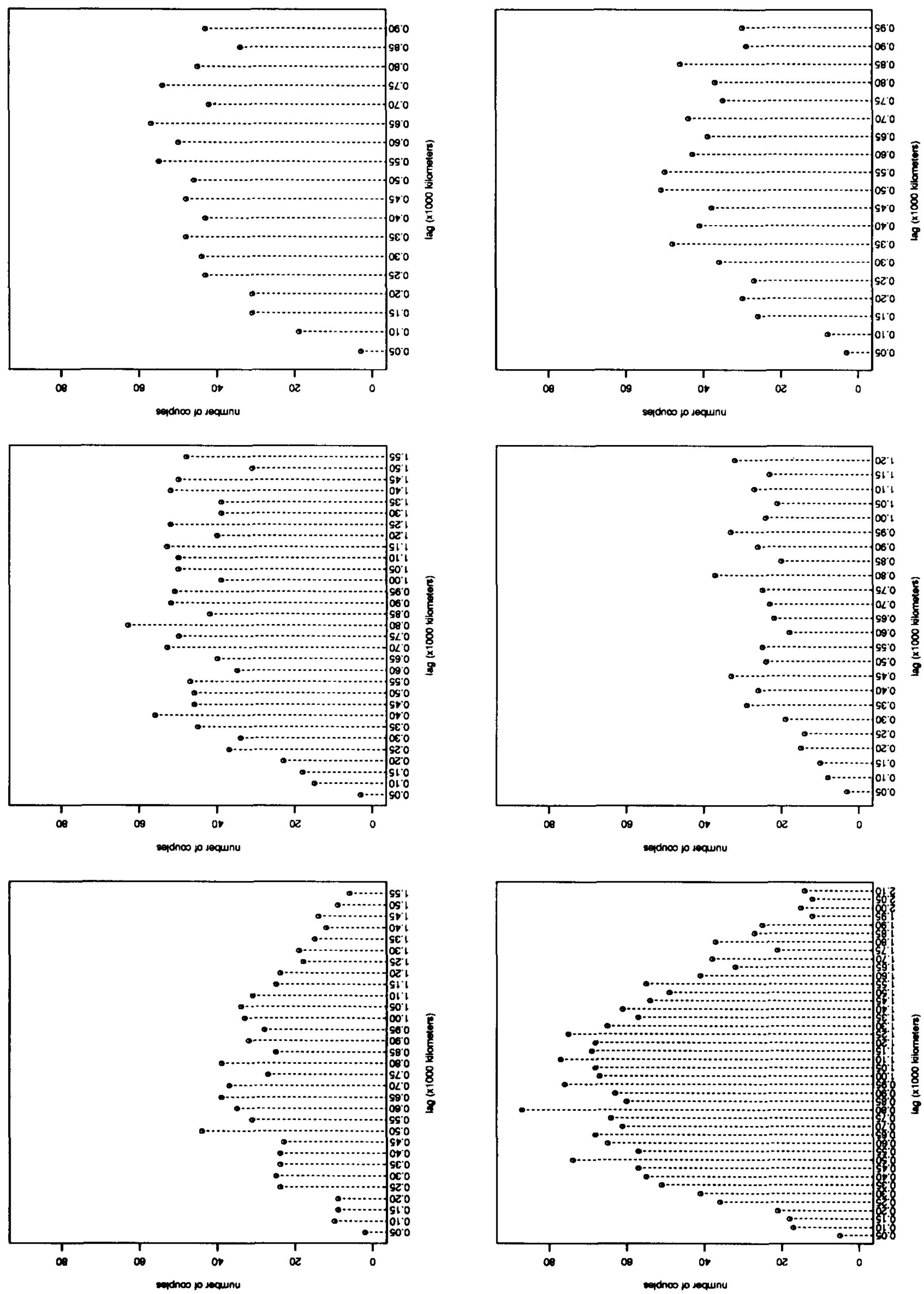

Fig. 3. Couple count distribution over the semi-variance estimate lags for each window in Fig. 1.

consecutive steps had either not changed at all or had decreased no more than 10^{-5} times the sum of squares at the former step. Note that this criterion allows the algorithm to tolerate a flat sum of squares surface.

To evaluate the automatic window sizing and subsequent variogram modeling procedures, we arbitrarily selected six estimate locations in the conterminous U.S. and used the above procedures to define subregions, calculate semi-variance estimates within these subregions, and fit the associated spherical variogram models. Figure 1 shows the NADP/NTN network and the windows found by the procedure at these selected estimate locations. Number the bottom row of windows 1, 2, 3 (left to right), and 4, 5, 6 for the top row.

The semi-variance estimates for these subregions along with the automatic regressions are in Fig. 2. The distributions of the number of site couples for these estimates are in Fig. 3. The couple distribution shows that our procedure does appear to provide at least two couples at the shortest lag but that the NADP/NTN network is not optimally designed for short lag semi-variance estimation.

To assess the correctness of the fitting algorithm, we compared the best converged parameter estimates from the automatic procedure to parameter estimate output from PROC NLIN of SAS using the "MARQUARDT" regression algorithm option (SAS, 1985). The search space was constrained to nonnegative nugget values and a range value between 0 and 3000 km. For a particular subregion, the NLIN fits used the same starting nugget, sill, and range values used in the best fit from the automatic procedure's 10 fit global search for that same subregion (see above).

The parameter estimates from these two regression algorithms were essentially identical for windows 3, 4 and 5. Window 1 resulted in an automatic regression fit with the nugget larger than the sill causing the automatic algorithm to set the nugget and sill equal to the within-window sample variance (see above). Only the fit in window 6 is distinctly different. Here, the automatic regression is superior (sum of squared residuals $= 5.5 \times 10^{-4}$) to that found by NLIN (sum of squared residuals $= 5.8 \times 10^{-4}$).

From the above comparisons then, we conclude that the window sizing and automated variogram model regression fitting procedures perform as desired.

4. COMPARISON OF THE MOVING WINDOW PROCEDURE TO FIXED SUBREGIONS

To assess the potential benefits and costs of process estimation using the moving window procedure, we estimated the winter, 1986 SO_4 deposition through rainfall over the conterminous U.S. using both the moving window procedure and a fixed subregion procedure. Both estimation methods used ordinary kriging to find the point estimate of deposition and its associated error variance. The ordinary kriging program was a modified version of the co-kriging program given by Carr *et al.* (1985). We calculated deposition at each NADP/NTN sampling site by multiplying the NADP winter 1986 precipitation total by the NADP/NTN precipitation volume weighted average of SO_4 concentration. The units on all plots of deposition are gm^{-2}.

The fixed subregion procedure divides the region for which an estimate surface is desired into a small number of fixed subregions and models variograms within these subregions. Ordinary kriging is then performed at each estimate point but the variogram model found for the subregion that the estimate point is located in is used to build the kriging equations no matter how close to an inter-subregion boundary that estimate point may be. This procedure then is very similar to standard, ordinary kriging except that several variograms are modeled before the kriging step as opposed to one in conventional kriging. Essentially, by kriging over fixed subregions, one is attempting to account for mean and covariance nonstationarity and still follow the maxim that the covariance structure should be modeled interactively and prior to the estimation calculation. The fixed subregions of the conterminous U.S. used in this study are shown in Fig. 4. The fitted variogram models for these subregions are in Fig. 5.

Figure 6 gives surface plots of the deposition estimate using both procedures and also surfaces of each procedure's 95% deposition confidence interval (C.I.) width based on the kriging variance and assumed normality of the errors. Both kriging procedures have been restricted to generating estimates only within the conterminous U.S.

The effect of variogram switching on the fixed subregion estimate can be seen at the boundaries of the fixed subregions. The discontinuities in the estimate surface suggests that an incorrect variogram model can introduce bias into the estimate. These subregion boundary effects of course are not present in the moving window procedure's estimate surface. Also, the window sizing and automatic regression

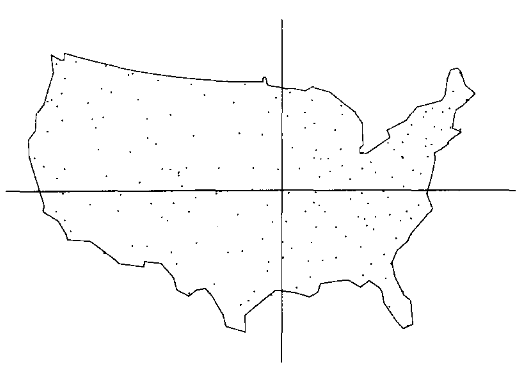

Fig. 4. Subregion definition for variogram modeling for the fixed subregions, ordinary kriging procedure.

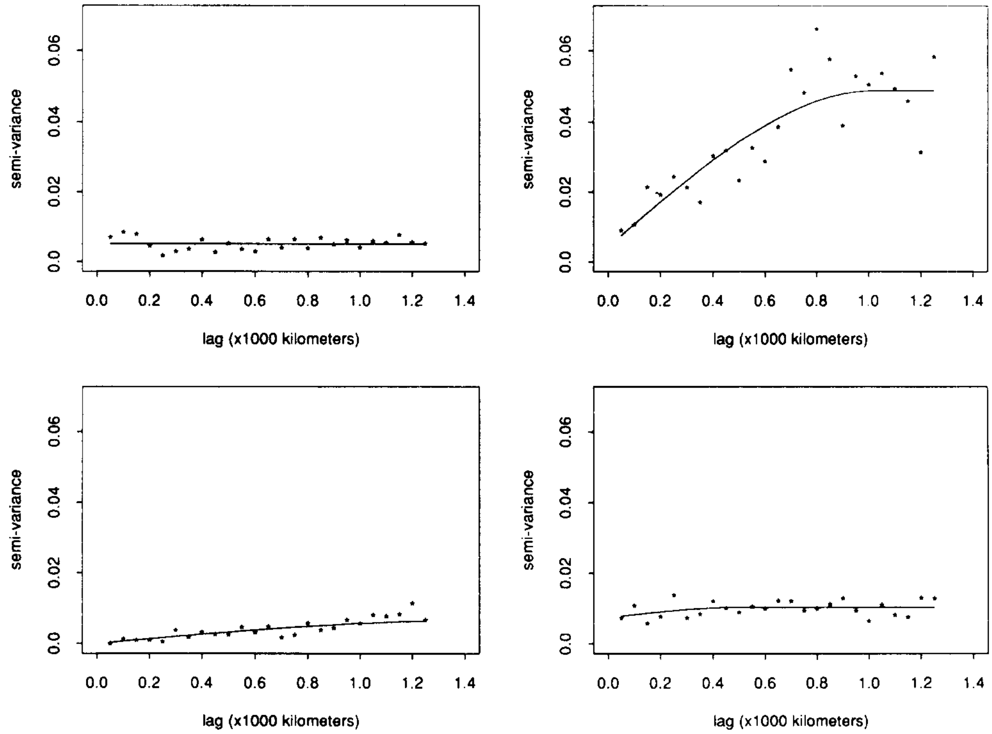

Fig. 5. Spherical variogram models fitted to semi-variance estimates over the subregions of Fig. 4 using the automatic regression routine.

algorithms appear to be robust for the following reasons. First, due to the recursive window enlargement procedures discussed above, automatic variogram model fits were found every estimate location. Second, Fig. 1 suggests that these converged regressions are not found by using excessively large window radii.

Figure 7a represents the surface generated by subtracting, at each estimate location, the fixed subregion's confidence interval width from that of the moving window's and reassigning this difference to zero if the result is negative. Hence, this is a surface of where the moving window procedure produces a larger C.I. width than the fixed subregion procedure. Figure 7b is the similar surface for where the fixed subregion procedure's C.I. width is larger than that of the moving window's. These two figures indicate that for the Northeast, the moving window procedure is

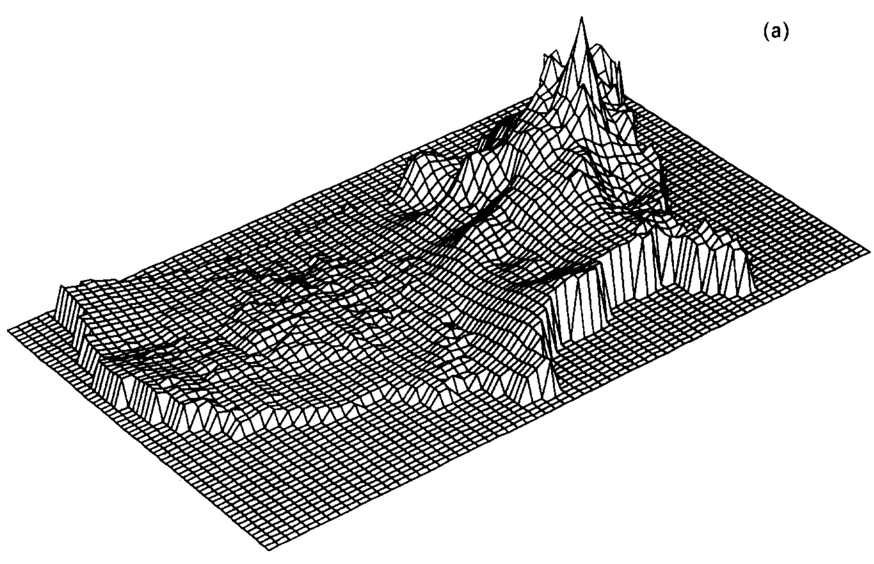

Fig. 6(a).

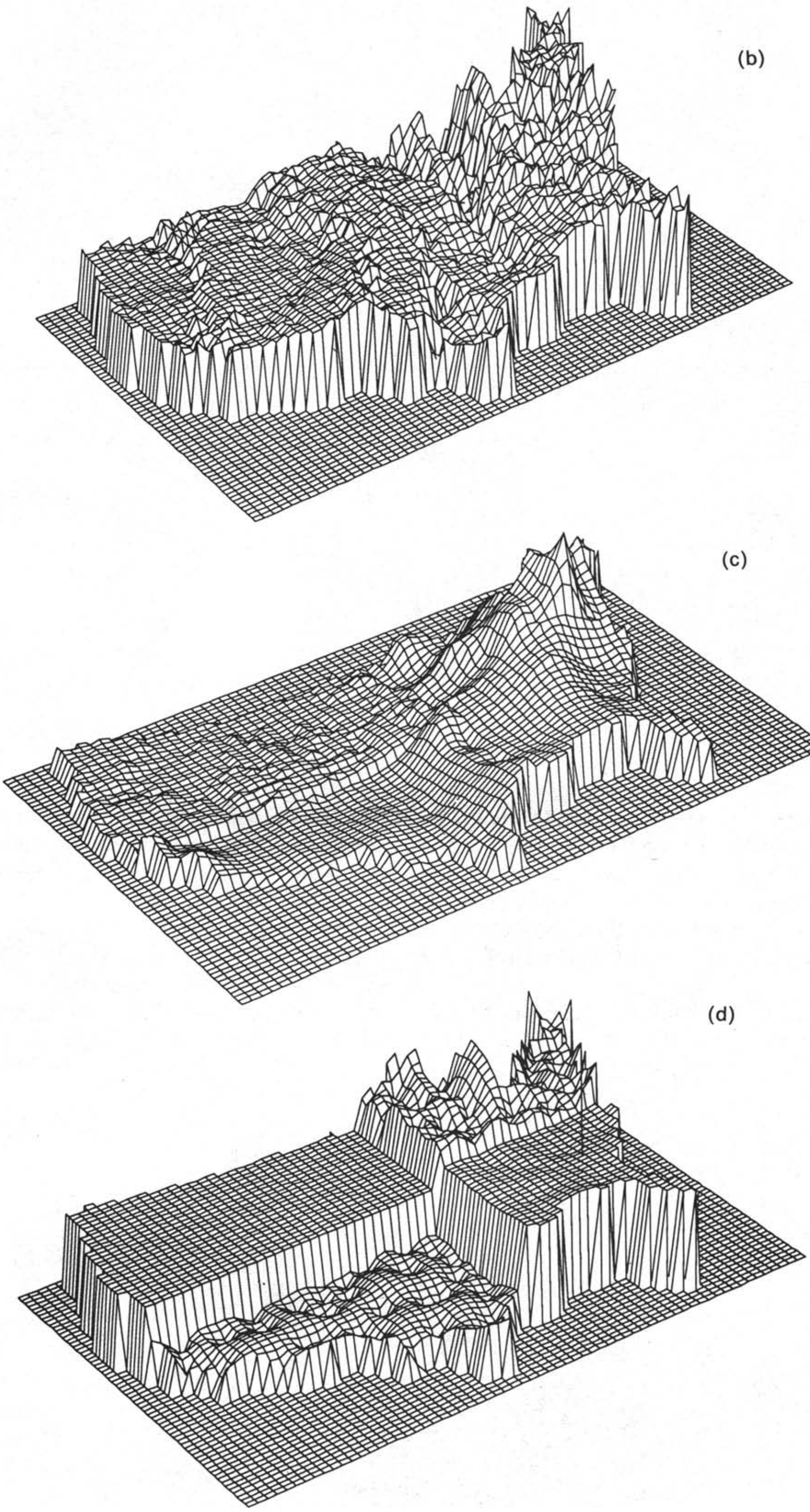

Fig. 6. Deposition estimate and 95% confidence interval width surfaces over a 65×65 regular grid using the moving window and fixed subregion procedures. Only locations within the conterminous U.S. are estimated, otherwise the surface value is set to zero. Figure 6a is the moving window estimate and Fig. 6b is the associated confidence interval width. Figures 6c and 6d are the corresponding surfaces using the fixed subregion procedure. The estimate surface and confidence interval width graphic scaling factors are different.

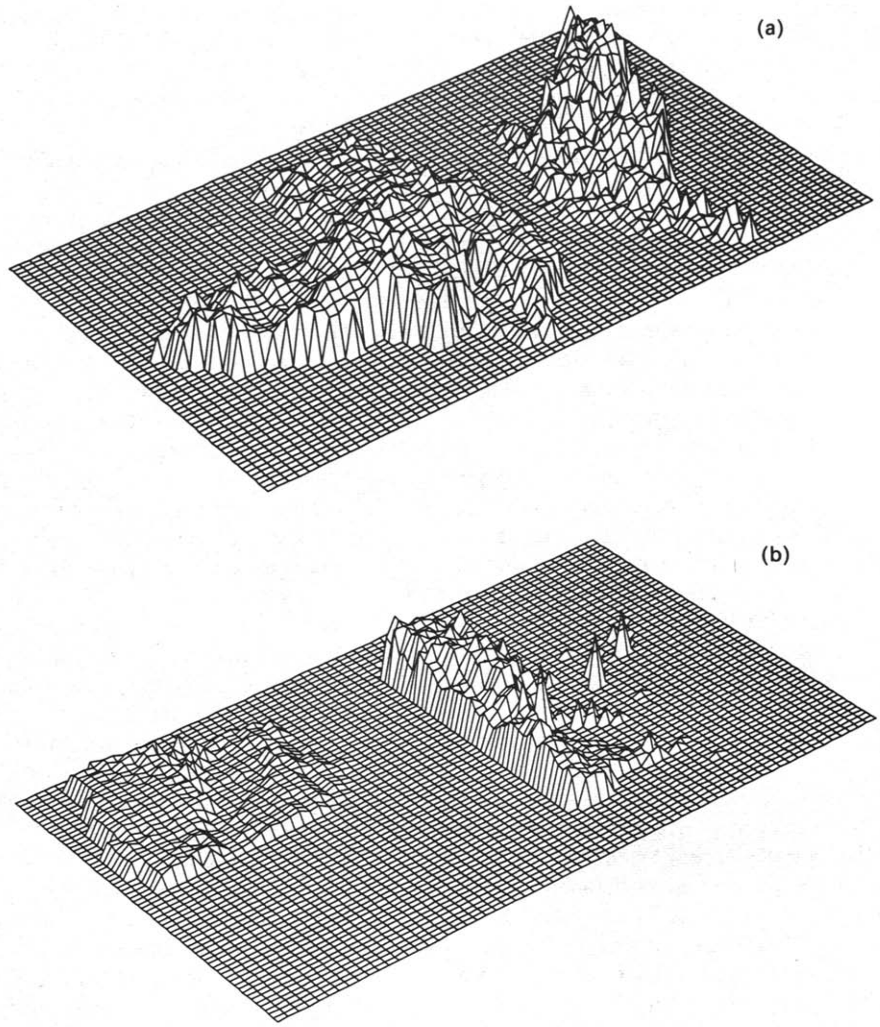

Fig. 7. Positive and negative surfaces of the moving window procedure's confidence interval width minus the fixed subregion's confidence interval width. Figure 7a is the surface of positive differences with negative differences reassigned to zero, i.e. the surface of where the moving window procedure gives a wider interval than the fixed subregion procedure. Figure 7b is the absolute value of the negative differences with positive differences assigned to zero, i.e. where the fixed subregion procedure's interval is wider than the moving window's.

usually producing kriging variances higher than the fixed subregion procedure. These higher kriging variances are because the moving window variogram models in the Northeast are of a process with low spatial covariance (sharply increasing variogram) and significant nugget effect, which in the kriging algorithm leads to higher kriging variances than the fixed Northeast subregion variogram model of a process with high spatial covariance. To see this difference in variogram models, compare the variogram of subregion 6 in Fig. 2 to that of the Northeast variogram in Fig. 5.

The reasons for these differing covariance structure models are explained as follows. The fixed Northeast subregion is large enough to include areas where the process is smoother (strong spatial covariance), e.g. the Great Lakes region, producing semi-variance estimates which do not increase rapidly over short lags. On the other hand, the variograms in the Northeast produced by the moving window procedure are over smaller subregions and hence form semi-variance estimates which increase rapidly over short lags (low spatial correlation), and then vacillate around a constant value for intermediate and long lags (negligible trend inflation). It should be noted that the fixed Northeast subregion is also large enough to allow trend effects to inflate the variogram. The presence of trend inflation in this subregion's variogram is detectable by noticing the continued increase of the semi-variance estimates over a large lag interval and the higher sill value of the Northeast variogram (Fig. 5) relative to window 6's sill value (Fig. 2).

Which procedure produces more accurate confidence intervals in the Northeast? Since the fixed subregion procedure is using a single Northeast variogram with trend inflation and higher spatial covariance than is likely to be true in (say) New England or the Ohio valley, we maintain that the moving window procedure's estimate and confidence interval width surface are closer to reality since the underlying variograms do not have substantial trend inflation and model the local spatial covariance more accurately.

The other distinct area of disagreement between the two procedures is in the Southwest. As can be noticed in Fig. 5, the fixed subregion procedure is using a variogram model with a zero nugget while the moving window procedure as suggested by subregion variograms 1 and 2 of Fig. 6 tends to model flat variograms having a nugget value nearly equal to the sill. This difference in covariance structure modeling explains the usually higher kriging variance produced by the moving window procedure. Again, the fixed Southwest subregion variogram exhibits trend inflation which, through the monotonicity of semivariance, results for this case in a regression estimate of a zero nugget.

Overall, the moving window procedure produced a deposition surface estimate free of subregion boundary effects and an variance at each estimate location more faithful to the process's stochastic characteristics in the immediate vicinity of that location.

The program for performing both analyses was written in standard FORTRAN 77 and run a SUN 3/50 utilizing the SUN's math coprocessor. The moving window estimate ran in 830 min of wall clock time while the fixed subregion procedure ran in 10 min, making the moving window procedure about 83 times more expensive to use than a more conventional kriging procedure. This ratio may appear to be prohibitive. We argue however that first, the timings are for a very large number of estimates (about 2000)—more than will usually be required for an effects model validation or a policy assessment study; second, the estimation can still be performed on workstation or fast PC hardware overnight; and third, this computation expense is trivial compared to the expense of acquiring the data or, more importantly, the potential cost of using inaccurate deposition estimates or their associated uncertainties when validating an effects model or evaluating the impact of a regulatory policy.

5. CONCLUSIONS

The development of a moving window kriging procedure and its application to the NADP/NTN data set has led us to the following conclusions.

(1) Subregions containing as few as 35 sampling sites can support the estimate of semivariances.

(2) Although Journel and Huijbregts caution against automatic fitting of variogram models (Journel and Huijbregts, 1978, pp. 232–233), we find that if regression heuristics are devised based on prior experience with the process to be estimated, a reliable and robust automatic fitting procedure can be developed.

(3) The moving window procedure, used in a region containing at least (say) 100 sampling locations with data from a process exhibiting trend, is capable of producing more accurate estimates of error variance than those found by using fixed subregions and ordinary kriging. This suggests that a moving window approach can be used successfully for estimating a process exhibiting trend. The advantage of the approach is that no assumption on the form of the trend is required.

(4) A moving window can also be effective with processes exhibiting covariance nonstationarity since a custom, local estimate of the covariance structure is made for each estimate location.

(5) The moving window procedure is more expensive to run than fixed subregion, ordinary kriging but is still a practical algorithm for use on work stations or fast PCs.

(6) Although not a focus of this article, the above moving window estimates leads us to suggest that acid deposition is not just a Northeastern phenomenon—sizable deposition occurs well into the South, Midwest and Northwest. Also, the ability to estimate deposition using NADP/NTN data is only moderately less certain in the Northeast than in the Southwest. This is surprising due to the high spatial variability of deposition in the Northeast but is accounted for by the correspondingly higher network density in that region.

The moving window kriging program is available from the author.

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