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ORIGINAL ARTICLE

Multi-lag cluster designs for estimating the semivariogram for sediments affected by effluent discharges offshore in San Diego

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Abstract Maps are useful tools for understanding, managing, and protecting the marine environment, yet few useful and statistically defensible maps of environmental quality and aquatic resources have been developed in near-coastal regions. Current environmental management efforts, such as ocean monitoring by sewage dischargers, routinely sample areas of potential impact using sparse sampling grids. Heterogeneous oceanic conditions often make extrapolation from these grids to non-sampled locations questionable. Although rarely applied in coastal monitoring, kriging offers a more rigorous statistical approach to mapping and allows confidence intervals to be calculated for predictions. Its usefulness relies on accurate models of the spatial variability through estimating the semivariogram. Many optimal designs for estimating the semivariogram have been proposed, but these designs are often difficult to implement in practice. In this paper, we present simple design strategies for augmenting existing monitoring designs with the goal of estimating the semivariogram. In particular, we investigate a multi-lag cluster design strategy, where clusters of sites, spaced at various lag distances, are placed around fixed stations on an existing sampling grid. We find that these multi-lag cluster designs provide improved accuracy in estimating the parameters of the semivariogram. Based on simulation study findings, we apply a multi-lag cluster enhancement to the monitoring grid for the City of San Diego's Point Loma Wastewater Treatment Plant as part of a special study to map chemical contaminants in sediments around its sewage outfall.

Keywords Environmental surveys · Kriging · Mapping · Spatial variability

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1 Introduction

Maps are useful tools for understanding and managing the marine environment. Because spatial patterns are recognized more easily with visual displays, maps provide scientists with valuable summaries of changing ecological conditions. Using maps, resource managers can quickly locate disturbance, assess its relative magnitude and spatial extent, and weigh risks to neighboring areas. In addition, cumulative effects resulting from multiple sources and types of disturbance can be determined. Perhaps most importantly, maps are effective and efficient media for communicating information to the public.

Despite the benefits, few useful and statistically defensible maps of environmental quality and aquatic resources have been developed in the near-coastal regions. Current environmental management efforts, such as ocean monitoring by sewage dischargers, routinely sample areas of potential impact using fixed grids of relatively few sample sites (e.g., <30). Simple interpolation methods, such as linear interpolation or triangulation, typically are applied to data collected from these sparse grids. However, these few samples cannot adequately capture the heterogeneous oceanic conditions and lack the spatial intensity to predict reliably at unsampled locations. Further, these simple interpolation methods do not provide estimates of precision. Kriging offers a more sophisticated statistical alternative for creating maps that provide predictions, as well as estimates of prediction errors, and kriging is available in many statistical or mapping software packages. The usefulness of kriging, however, requires an adequate understanding of the spatial variability of the data. In many cases this information is unavailable.

With kriging, spatial variability is estimated through modeling the semivariogram. The semivariogram is equal to one-half the variance of paired sample differences taken at some fixed or "lag" distance apart. By measuring the variability of sample differences as a function of distance, the semivariogram provides a measure of the strength of the spatial autocorrelation that determines the weights associated with kriging predictions. In addition, the semivariogram can be used to assess the errors associated with those predictions, so that, in conjunction with a cost or objective function, one can estimate the optimal grid spacing for future designs (Burgess et al. 1981, McBratney et al. 1981).

Our ability to model the semivariogram accurately depends on the sample design. Many optimal sampling schemes have been proposed in the literature for estimating the semivariogram. These methods rely on optimization with respect to some complex objective function. For example, Muller and Zimmerman (1999) suggest maximizing the determinant of the information matrix using method of moments. Lark (2002) uses spatial simulated annealing and maximum likelihood to maximize the precision of the kriging variance. Other suggested approaches include minimization of the dispersion of distances between sites (Russo 1984), fitting of lags to a distribution (Warrick and Myers 1987), and maximization of the equivalent uncorrelated pairs (Morris 1991). Although these designs are optimal with regard to their particular objective function, their sophistication and difficulty of implementation often make them prohibitive for use by coastal monitoring agencies.

In this study, we investigate simple design strategies that can be implemented easily by coastal monitoring agencies to build off their existing monitoring grid for the purpose of estimating the semivariogram. In particular, we introduce multi-lag cluster designs, where clusters of sites, spaced at various lag distances, are placed around fixed locations on an existing grid. We examine different strategies for allocating sampling resources within the mult-lag clusters, including replication at particular lag distances, spatial coverage, and sample configuration (i.e., how samples are placed around grid sites). We use our findings to develop a special mapping study for the City of San Diego's Point Loma Wastewater Treatment Plant (PLWTP) to estimate the semivariogram for a host of chemical contaminants found in sediments around its sewage outfall. The estimated semivariogram will then be used to determine appropriate grid spacing for more cost-efficient surveys.

2 Methods

In this section, we present the multi-lag cluster design as a simple strategy for augmenting fixed grids for modeling the semivariogram. We focus on estimating three parameters (nugget, range, and sill), typically used to describe semivariogram models. The nugget measures the variability between paired sample differences taken at very close proximities. The nugget represents laboratory measurement error plus small-scale spatial variability. The sill measures the variability achieved between sample differences that are spaced far enough apart so that there is no spatial autocorrelation. The range is the lag distance at which the sill is achieved and provides the extent of the spatial autocorrelation between sample locations. For a more technical description of kriging and the semivariogram (see Cressie 1993 or Webster and Oliver 2001).

We perform two simulation studies that assess the usefulness of multi-lag cluster designs for estimating semivariogram parameters. The first study examines four different resource allocations within the class of multi-lag cluster designs. The results of the study are used to design a survey for the PLWTP for estimating the semivariogram of chemical contaminants in sediment around its sewage outfall. The second simulation study assesses the ability of this particular design to estimate the semivariogram parameters under varying degrees of spatial dependence. In both simulation studies, we assume the mean is constant and the variability of paired sample differences does not depend on their particular sample locations, but only on the distance between them (i.e., first-order stationarity). Further, we assume that the variability does not depend on direction (i.e., isotropy).

2.1 Multi-lag cluster designs

Multi-lag cluster designs are enhancements to fixed grid designs where clusters of sample sites are placed around existing grid stations. The multi-lag component to the design allows for replication of sample pairs at multiple spatial distances by placing sites within each cluster at various lag distances from the existing grid stations. Clusters can be placed around all or a subset of existing grid stations. Thus, multiple lag distances and spatial coverage can be addressed in the design.

The class of multi-lag cluster designs allows for great flexibility in terms of the number of clusters, the number of lags within a cluster, the number of replicates within each lag class, and the size of each lag class. We present four multi-cluster alternatives in our simulation studies that represent some of the possibilities for these designs.

Two simulation studies were conducted to investigate the utility of multi-lag cluster designs for estimating the semivariogram. The first simulation study compared semivariogram parameter estimation among four multi-lag cluster designs and two fixed grids. The designs were chosen to explore different strategies for allocating sampling resources within the class of multi-lag cluster designs for fixed cost (e.g., sample size). The results of the first simulation study were used to develop a multi-lag cluster design to estimate semivariograms of chemical contaminants for the PLWTP outfall area. Our second simulation study then examined how accurately this particular multi-lag cluster design estimated the semivariogram parameters under different degrees of spatial autocorrelation.

2.2 Simulation study 1: four multi-lag cluster enhancements to the 5 × 5 fixed grid

In this first simulation study, we compared the accuracy of semivariogram parameter estimation based on data simulated across four multi-lag cluster designs (STAR, S, Short Lag Star, and Long Lag Star) and two fixed grid designs (FixGrid5 and FixGrid10). Our first two designs, STAR and S, explored the difference between the number of clusters (sample coverage) and the number of sites within a cluster (cluster size). Our second two designs, Short Lag Star and Long Lag Star, had fewer lags represented in each cluster and examined the difference between shorter and longer lag distances.

The four multi-lag cluster designs were based on enhancements to a fixed 5 × 5 sampling grid, FixGrid5 (Fig. 1a). The first multi-lag cluster design, STAR, consisted of clusters of 16 sites arranged in a star-shaped pattern around four fixed grid stations (Fig. 1b). Within each cluster, four samples were placed at each of four different lag distances from the grid station. The four lags were 1, 3, 7, and 13 km (units to correspond to our PLWTP application). The S multi-lag cluster design consisted of clusters of eight sites arranged in a S-shaped pattern around eight fixed grid stations (Fig. 1c). The S-clusters, in the S design, were formed by splitting each star-cluster in half, in the STAR design. Within each of the S-clusters, two samples were placed at each of four different lag distances from the grid station. The Short Lag Star multi-lag cluster design consisted of clusters of eight sites arranged in a STAR-shaped pattern around eight fixed grid stations. Within each cluster, four samples were placed at each of the two shorter lag distances, 1 and 3 km, from the grid station (Fig. 1d). The Long Lag Star multi-lag cluster design also consisted of clusters of eight sites arranged in a STAR-shaped pattern around eight fixed grid stations, only samples were placed at each of the longer two lag distances, 7 and 13 km (Fig. 1e). Finally, a 10 × 10 grid (FixGrid10) design was included for comparison (Fig. 1f). All multi-lag cluster designs had 89 sample locations. The FixGrid5 had 25 sample locations and was included simply as a reference for improvement with increased sampling density. The FixGrid10, with 100 sample locations, was used to compare the multi-lag cluster designs with a fixed grid of similar sample size. A summary of sample allocations for each of the multi-lag cluster designs is given in Table 1.

The differences among designs can be seen in their distribution of the lag distances representing the replication of pairwise distances between sample sites (Fig. 2a). Lag distributions for the fixed grid designs are characterized by replication at only a few lag distances, revealing "holes" where lag distances were not represented. The multi-lag cluster designs resulted in a much greater representation across lag distances.

Simulations proceeded by fitting a semivariogram model to sample data generated from the various sample designs. With each run of the simulation, spatially correlated

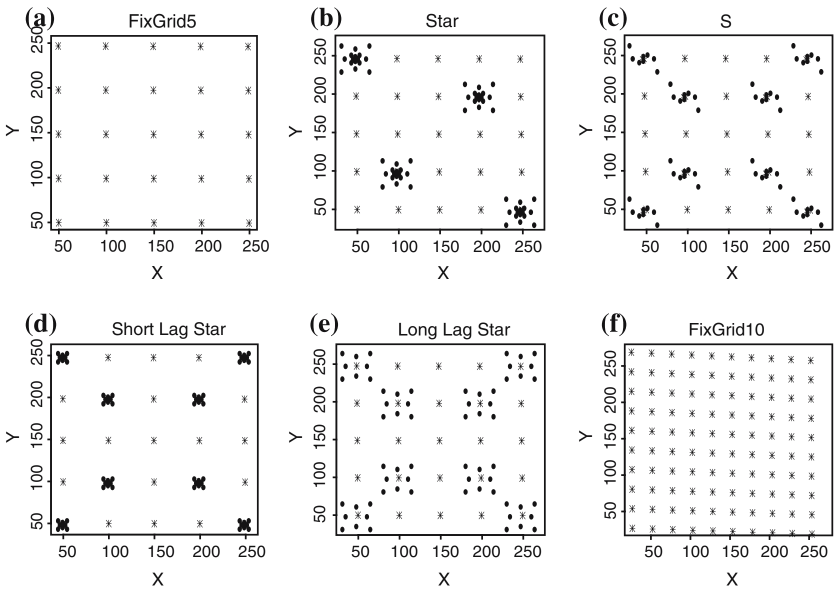

Fig. 1 (**a–f**) Schematic sampling locations for fixed grids and multi-lag cluster designs. FixGrid5 (**a**) has 25 samples arranged in an equally spaced grid pattern. The multi-lag cluster designs [Star (**b**), S (**c**), Short Lag Star (**d**), and Long Lag Star (**e**)] consist of 64 additional sites placed around various grid points of FixGrid5 for a total of 89 sampling locations. The Star design adds four clusters of 16 sites, arranged in a STAR-shape in which four distinct lag classes are represented. The S design is formed by dividing each STAR-shaped cluster into two s-shaped clusters, so that there are eight S-shaped clusters of eight sites where each of the four lag classes is represented in each cluster. Short Lag Star adds eight STAR-shaped clusters of eight sites, where only the two shorter lag clusters are represented in each cluster. Long Lag Star adds eight STAR-shaped clusters of eight sites where only the two longer lag classes are represented. The F. FixGrid10 is a fixed grid design of 100 samples

Table 1 Summary of sampling allocations for multi-lag cluster designs (Simulation 1)

Design	Number of Lags (Lag Distances)	Number of Clusters (Number of Sites in Each Cluster)	Total Sample Size
STAR	4 (1, 3, 7, 13)	4 (16)	89
S	4 (1, 3, 7, 13)	8 (8)	89
Short Lag Star	2 (1, 3)	8 (8)	89
Long Lag Star	2 (7, 13)	8 (8)	89

data were generated across all six designs using *rfsim* in the Splus S+Spatial Statistics module (Kaluzny et al. 1998). The spherical model was chosen to represent the underlying variability of the data with three different range values (10, 30, and 60 km), two different nuggets (0 and 0.2), and one sill value (1).

The fitting algorithm for estimating the semivariogram model parameters was done with *variogram.fit* in Splus S+Spatial Statistics module (Kaluzny et al. 1998). This automated procedure is based on minimizing the weighted least squares objective function given by Cressie (1985). Prior specifications to the *variogram.fit* procedure were the same for each design (semivariogram model = spherical, number of lag

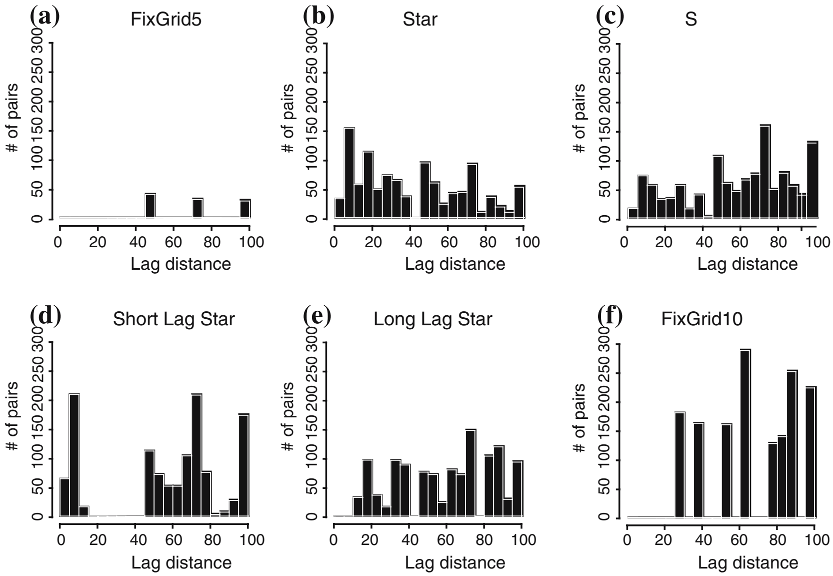

Fig. 2 **(a–f)** Distribution lag distances between sampling points represented in each of the five sample designs (FixGrid5 (**a**), Star (**b**), S (**c**), Short Lag Star (**d**), Long Lag Star (**e**), and FixGrid10 (**f**)) used in the first simulation study

classes = 50, maximum lag distance = 100). These specifications were determined by manually fitting the semivariogram to data simulated for each of the sampling designs and selecting those specifications that generally gave the most reliable results with the automated semivariogram fitting procedure.

Performances among the six designs for estimating the semivariogram parameters were assessed using two measures. First, we calculated the median deviation from the true parameter value for each design. Second, we computed the percentage of times (simulated runs) that each design yielded estimates closest to the true parameter value, across all other designs. In the case where more than one design gave an estimate that was closest to the true value (i.e., ties), each of the "winners" received credit for being closest. Consequently, percentages may sum to greater than 100%. Percentages were also computed for all design pairs in order to verify that a particular resource allocation was preferred (e.g., shorter lags versus longer lags, more clusters versus more sites within a cluster). Results were based on 1,000 simulations.

2.3 Application of the multi-lag cluster enhancement to the City of San Diego's PLWTP montoring grid

As part of its regulatory requirements governing sewage effluent discharge offshore, the City of San Diego agreed to participate in a special study to improve the estimation of sediment contaminants surrounding the Point Loma Ocean Outfall (NPDES Permit No. CA0107409, Order No. R9-2002-0025, Addendum No. 1). Because regular monitoring of ocean sediments off Point Loma relies mostly on a fixed grid of only 22 sites, there was little information available that could be used to reliably estimate the semivariogram. Therefore, efforts were directed toward building off the existing monitoring grid to estimate the semivariogram parameters for a host of chemical contaminants around the outfall. These estimates are intended to aid in determining cost-efficient sample spacing for subsequent monitoring surveys, where kriging could be applied to produce a map of chemical contaminants surrounding the outfall.

Using data collected previously from the existing PLWTP monitoring grid across 2 years, we roughly estimated semivariograms for a host of chemical contaminants. Chemicals included chromium, copper, lead, mercury, and total organic carbon. We found that the estimated range of the spatial autocorrelation was between approximately 2 and 8 km, depending on sampling event and chemical constituent (Fig. 3). This information was used to choose appropriate lag spacing for the multi-lag cluster enhancements.

Based on results from the first simulation study, we chose a modification of the STAR multi-lag cluster enhancement to a subset of stations from the existing PLWTP monitoring grid (Fig. 4). The subset consisted of 12 sites, spaced 1–12 km from each other. The study design allowed for 100 additional samples to be taken. The chosen design consisted of clusters of 16 sites placed around three existing monitoring stations and two new stations of special concern. The two additional sites of interest were located near the US. EPA's LA5 dredge-dumping site, at a depth between 60 and 90 m. The four lag distances in the STAR design were 0.05, 0.25, 1.00, and 3.00 km. Eight additional samples were placed at old monitoring stations located along the shallower depth contour of the original Point Loma outfall discharge site (~60 m). Nine field

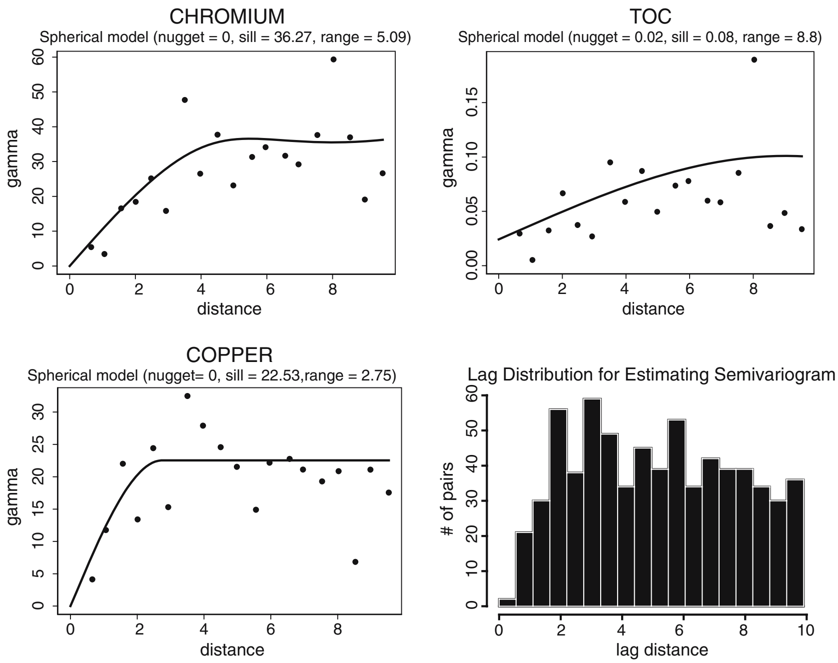

Fig. 3 Empirical semivariograms ("gamma") and fitted models for three chemical constituents from PLWTP existing monitoring grid and the distribution of lags from PLWTP fixed monitoring grid. Fitted model and estimated parameters provided in subtitle

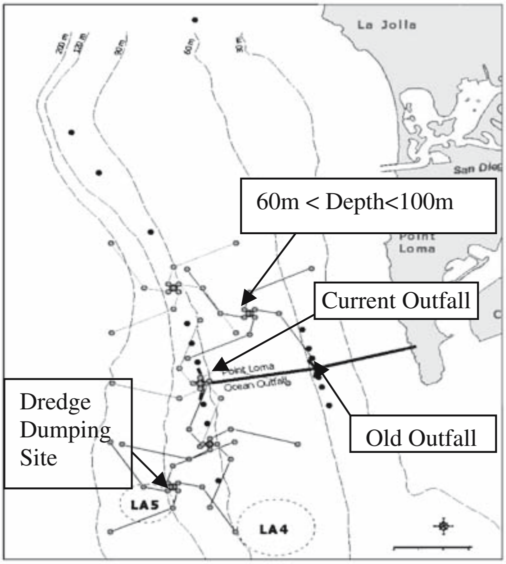

Fig. 4 Multi-lag cluster design for PLWTP. *Note*: Connected points represent sites within the same "star"-shaped cluster; Black dots represents sites on existing and previously monitored fixed sampling grid

duplicates were also allocated; five to the star centers and four at core grid stations. A total of 112 samples were allocated for sampling in this mapping study.

2.4 Simulation study 2: assessment of multi-lag cluster enhancement to PLWTP monitoring grid

A second simulation study was performed to assess the accuracy of multi-lag cluster enhancement to the PLWTP monitoring grid for estimating the nugget, sill, and range. As with the first simulation study, spatially correlated sample data were generated using *rfsim* in the Splus S+Spatial Statistics module. The spherical model was chosen to represent the "true" spatial variability and semivariogram model fits were performed automatically by means of *variogram.fit*. We simulated semivariogram estimation under several semivariogram parameter values in order to investigate the usefulness of the design under varying degrees of spatial autocorrelation. These included six values for the range ($R = 1, 2, \ldots, 6$), three values for the nugget ($N = 0, 0.1$, and 0.2), and one value for the sill ($S = 1$). The spherical model and the parameter values were chosen based on rough approximations to empirical semivariograms provided by previous surveys across multiple chemical constituents. Performance was based on median estimates for each of the three parameters, across 1,000 simulations.

3 Results

3.1 Simulation study 1

The multi-lag cluster designs provided substantial improvement over the fixed grid designs for estimating the semivariogram parameters (Table 2a–c). The multi-lag cluster designs were particularly effective when the range parameter value was less than the minimum distance between fixed grid stations. Designs with more replication

Table 2 **A**–**C** Median deviation and percentage of times ("runs") design yielded estimate closest to the target value for various combinations of parameter values (Nugget = 0.2, Range = 10, 30, 60, Sill=1)

Nugget = 0.2				Nugget = 0.0			
Design	Range = 10	Range =30	Range = 60	Design	Range = 10	Range =30	Range = 60
A. Estimating target nugget (Nugget = 0.2, 0.0)							
FixGrid5	−0.17 (15)	0.16 (1)	−0.17 (0)	FixGrid5	0.02 (13)	0.02 (8)	0.02 (8)
STAR	−0.01 (24)	0.07 (29)	−0.02 (26)	STAR	0.00 (53)	0.00 (57)	0.00 (58)
S	−0.01 (21)	0.08 (23)	−0.00 (23)	S	0.00 (54)	0.00 (57)	0.00 (61)
Short Lag Star	0.00 (39)	0.06 (38)	−0.02 (31)	Short Lag Star	0.00 (53)	0.00 (50)	0.00 (59)
Long Lag Star	0.81 (1)	0.20 (9)	−0.02 (12)	Long Lag Star	0.82 (20)	0.00 (53)	0.00 (59)
FixGrid10	0.83 (3)	0.79 (1)	−0.02 (7)	FixGrid10	0.86 (3)	0.83 (3)	0.00 (52)
B. Estimating target range (Range =10, 30, 60)							
FixGrid5	40.00 (0)	20.00 (2)	−10.00 (23)	FixGrid5	40.00 (0)	20.00 (2)	−10.00 (17)
STAR	2.19 (30)	1.38 (21)	−0.98 (15)	STAR	2.08 (29)	1.12 (25)	3.09 (14)
S	2.01 (30)	1.37 (21)	−3.01 (9)	S	1.93 (31)	2.48 (18)	1.35 (11)
Short Lag Star	0.58 (31)	1.17 (17)	−8.79 (6)	Short Lag Star	1.05 (31)	3.42 (18)	3.52 (7)
Long Lag Star	16.84 (8)	1.91 (24)	0.80 (9)	Long Lag Star	8.71 (8)	3.29 (25)	2.89 (12)
FixGrid10	28.15 (2)	8.17 (15)	0.61 (39)	FixGrid10	28.11 (2)	8.18 (12)	1.65 (41)
C. Estimating target sill (Sill =1)							
FixGrid5	0.14 (23)	0.15 (21)	0.13 (22)	FixGrid5	−0.05 (20)	−0.05 (22)	−0.06 (22)
STAR	0.09 (22)	0.07 (18)	0.05 (15)	STAR	0.00 (25)	0.02 (19)	0.01 (15)
S	0.06 (19)	0.04 (17)	0.06 (12)	S	−0.01 (27)	0.02 (18)	0.00 (9)
Short Lag Star	0.01 (24)	0.02 (16)	0.05 (9)	Short Lag Star	−0.03 (18)	−0.02 (12)	0.00 (8)
Long Lag Star	−0.69 (6)	0.08 (23)	0.12 (12)	Long Lag Star	−0.72 (8)	−0.01 (25)	−0.01 (13)
FixGrid10	−0.86 (5)	−0.82 (6)	0.02 (31)	FixGrid10	−0.91 (2)	−0.85 (4)	−0.07 (33)

Note that due to ties, percentages may sum to greater than 100%; Percentages are given in parentheses

at shorter lag distances (Short Lag Star, STAR, and S) tended to provide nugget estimates closer to the true value than those with less replication at longer lag distances (FixGrid5, FixGrid10, and Long Lag Star). Designs with greater replication at lag distances shorter than the target range provided better estimates of the range than those whose shortest distance exceeded the range. Relative performances among the designs with regard to estimating the sill generally mirrored performance with regard to estimating the range. There was little difference in performance between the STAR and S designs, due to the difference in spatial coverage. Differences between shorter and longer lag distances depended on the parameter value being estimated, but neither performed as well, overall, as designs with both shorter and longer lag distances. Pairwise comparisons among the designs confirmed these findings.

When examining the distribution of parameter estimates across all designs, we found many extreme values. These can be explained, in part, by the poor semivariogram fits that often resulted from the automated semivariogram fitting procedure. Upon closer inspection, the automated fit produced a curve that was very different from the curve that probably would have resulted if the fit had been done manually. In addition, the automated procedure tended to yield a zero nugget estimate when no information was obtained at short lag distances. Excluding these extreme estimates

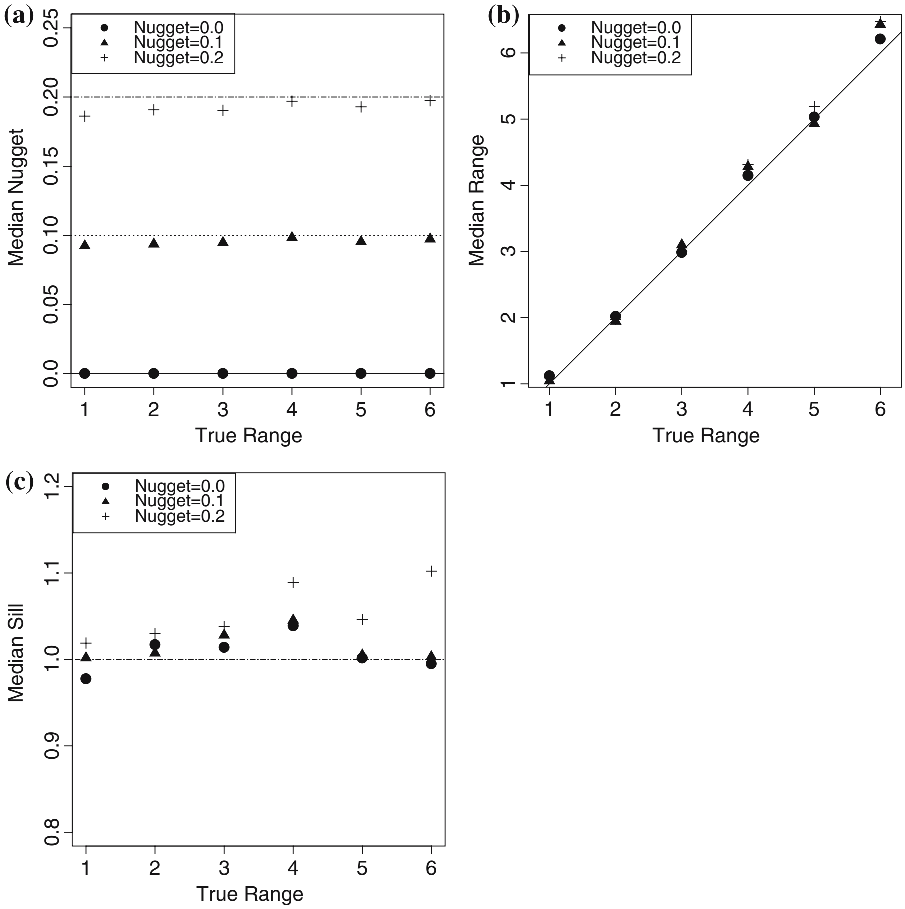

Fig. 5 **(a)** Median of nugget estimates, **(b)** median of range estimates, **(c)** Median of sill estimates

resulted in only slightly better median estimates than those reported and did not change the relative performance standing among the designs.

3.2 Simulation study 2

The modified STAR enhancement to the PLWTP monitoring grid provided median estimates of semivariogram parameters close to target values across all the nugget, sill, and range parameter values selected for data simulation (Fig. 5a–c). Nugget accuracy tended to increase as the range parameter increased. Median range estimates were closer to the target value for smaller range and nugget parameter values. The design tended to overestimate the range as the target range increased. Sill estimates tended to be higher than the true value, especially for larger target nugget values. As with the first simulation study, we saw that parameter estimation gave many extreme values. We believe that deficiencies of the automated semivariogram fitting procedure accounted for a substantial number of these poor estimates.

4 Discussion

Critical to constructing statistically defensible maps and developing cost-efficient surveys is our ability to accurately model the spatial variability or the semivariogram. Reliable estimates of the semivariogram require a sample design to have adequate spatial coverage and sufficient replication at multiple spatial distances. Sample locations that are spaced too far apart can result in model misspecification because there is not sufficient replication at moderate and smaller spatial distances to characterize the shape of the semivariogram or to estimate the nugget. Sample locations that are spaced too close together waste resources and can fail to capture the range and/or estimate the sill. Ideally, we would like to have a dense sampling grid that covers the entire study area. Unfortunately, economic considerations limit the total number of sites that can be visited and samples that can be collected. How we allocate our samples, then, requires us to be selective and strategic.

This study demonstrates that multi-lag cluster designs offer a simple approach for augmenting existing grids that can greatly improve semivariogram parameter estimation. The first simulation study demonstrated that the semivariogram cannot be estimated dependably from sampling grids that have few sampling points or that lack sites spaced at multiple distances (particularly sites very close together). Even with increased sample size, as with FixGrid10, the fixed grid outperformed the multi-lag cluster designs only under limited conditions. However, due to the truncation of pairwise distances to model the semivariogram, the number of pairs of points used to estimate the semivariogram was smaller for the FixGrid10 than for the multi-lag design. This might relate, in part, to the poor semivariogram fit with this design. Regardless, the FixGrid10 did lack adequate information at smaller spatial scales to model the semivariogram at shorter distances or to estimate the nugget effectively. In addition, our study showed that the ability of the multi-lag cluster designs to estimate semivariogram parameters accurately depends on how samples are allocated to the clusters and the strength of spatial autocorrelation.

Since there are many ways to allocate sampling resources in multi-lag cluster designs, we offer a number of important recommendations. First, lag distances selected for clusters should be shorter than the true range, as shown by Range 10 simulations and FixGrid10 designs in Table 2. If possible, use information from previous surveys to get an idea of the extent of the spatial autocorrelation of the data. Such information will help in selecting maximum lag distances for use in each multi-lag cluster. Second, multiple lag distances are preferred over increased replication at one or two lag distances, when little is known about the true spatial range, as replication at both moderate and long lag distances is necessary to cover all potential range values. This finding is demonstrated in Table 2, in comparison of the STAR and S design rows with the Short Lag Star and Long Lag Star rows. Third, multi-lag clusters with replication at short lag distances ensure more accurate estimation of the nugget, as demonstrated by Short Lag Star compared to Long Lag Star and FixGrid (Table 2). If possible, collect field duplicates at some stations. Stein (1990) remarks that the critical issue to constructing defensible maps is accurately estimating the semivariogram near the origin. Fourth, the choice between greater spatial coverage (e.g., more clusters, as in the S design) and more samples in a cluster (e.g., as in the STAR design) depends on the goals of the study and the physical properties of the study area. Substrata, such as grain size and different depth zones within the study area, might lead to different models of spatial variability or varying strengths of spatial autocorrelation. If spatial variability changes are expected with different substrata, then target particular substrata. If the area of interest is uniform, then increase the number of clusters and hence the spatial coverage. Fifth, if variability is expected to change with direction, use either STAR designs or S designs, with clusters rotated to cover various directions. Finally, and probably most importantly, examine the distribution of lag distances associated with candidate designs. Such inspection will allow checking for "holes" where lag distances are not represented in the design, as seen in the FixGrids and the Short Lag Star designs (Fig. 2a–f).

Many considerations influenced the choice of the STAR multi-lag cluster design for the PLWTP mapping study. The multi-lag cluster enhancement enabled PLWTP to sample new sites for estimation of the semivariogram while simultaneously sampling the existing grid as required under its sewage discharge permit. Also, PLWTP had five primary areas of interest. These areas were thought to represent different strata in terms of depth, grain size, and relative levels of chemical contamination. Thus, these areas were important for examining potential differences in mean concentrations and spatial variability (i.e., non-stationarity). Further, the STAR-shaped pattern allowed for spatial variability to be estimated in multiple directions. Due to the steeper depth gradient perpendicular to the shoreline and oceanic currents, the strength of spatial autocorrelation was likely to change, depending not only on distance, but also on direction (i.e., anisotropy). Although, we did not explore the effects of anisotropy in this study because of time constraints, we did consider the potential for anisotropy when constructing the clusters, so that the spatial variability across multiple directions could be explored. The clusters of size 16 had two lag distances represented in eight different directions. Finally, from the first set of simulations, the clusters of size 16 were useful for estimating multiple parameters under varying degrees of spatial autocorrelation.

The multi-lag cluster design has several advantages for monitoring agencies, including ease of implementation, flexibility, and the ability to provide more accurate estimates of the semivariogram. Because semivariogram estimation is based on statistical models, randomness is not a requirement for these designs. Therefore, monitors can target specific areas of interest. Also, because the enhancement is to the existing monitoring grid, sampling can be done in conjunction with current monitoring efforts, so that resources are conserved and time-series information is not lost.

Although this study showed that the multi-lag cluster design offers an effective strategy for estimating semivariogram parameters, further research is needed to examine more carefully the relationship between semivariogram parameter values and the estimation accuracy with regard to choosing the number and size of clusters and lag classes. In addition, we should consider alternative semivariogram fitting algorithms, such as ML and REML, non-stationarity and anisotropy, and compare them with other design alternatives, including random nested designs.

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