

A comparison of design-based and model-based approaches for finite population spatial data.

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Abstract

1. The design-based and model-based approaches to frequentist statistical inference lie on fundamentally different foundations. In the design-based approach, inference depends on random sampling. In the model-based approach, inference depends on distributional assumptions. We compare the approaches for finite population spatial data.
2. We provide relevant background for the design-based and model-based approaches and then study their performance using simulations and an analysis of real mercury concentration data. In the simulations, a variety of sample sizes, location layouts, dependence structures, and response types are considered. In the simulations and real data analysis, the population mean is the parameter of interest and performance is measured using statistics like bias, squared error, and interval coverage.
3. When studying the simulations and mercury concentration data, we found that regardless of the strength of spatial dependence in the data, sampling plans that incorporate spatial locations (spatially balanced samples) generally outperform sampling plans that ignore spatial locations (non-spatially balanced samples). We also found that model-based analyses tend to

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outperform design-based analyses, even when the data are skewed (and by consequence, the model-based distributional assumptions violated). The performance gap between the analysis approaches is small when spatially balanced samples are used but large when non-spatially balanced samples are used. This suggests that the sampling choice (spatially balanced samples versus non-spatially balanced samples) is most important when using a design-based analysis.

4. There are many benefits and drawbacks practitioners must consider when choosing between design-based and model-based approaches for finite population spatial data. We provide relevant background contextualizing each approach and study their properties in a variety of scenarios, making recommendations for use based on the practitioner's goals.

Keywords

Design-based inference; Finite Population Block Kriging (FPBK); Generalized Random Tessellation Stratified (GRTS) algorithm; Model-based inference; Spatially balanced sampling; Spatial covariance;

1. Introduction

There are two general approaches for using data to make frequentist statistical inferences about a population: design-based and model-based. When data cannot be collected for all units in a population (i.e., population units), data are collected on a subset of the population units. This subset is called a sample. In the design-based approach, inferences about the underlying population are informed via a probabilistic process assigning some population units to be part of the sample. Alternatively, in the model-based approach, inferences are made from specific assumptions about the underlying process generating the data. Each

55 paradigm has a deep historical context (Sterba, 2009) and its own set of benefits
56 and drawbacks (Hansen et al., 1983).

57 Though the design-based and model-based approaches apply to statistical
58 inference in a broad sense, we focus on comparing these approaches for spatial
59 data. We define spatial data as data that incorporates the specific locations of
60 the population units into either the design or estimation process. De Gruijter
61 and Ter Braak (1990) give an early comparison of design-based and model-based
62 approaches for spatial data, quashing the belief that design-based approaches
63 could not be used for spatially correlated data. Since then, there have been
64 several general comparisons between design-based and model-based approaches
65 for spatial data (Brus and De Gruijter, 1997; Brus, 2021; Ver Hoef, 2002, 2008;
66 Wang et al., 2012). Cooper (2006) reviews the two approaches in an ecological
67 context before introducing a “model-assisted” variance estimator that combines
68 aspects from each approach. In addition to Cooper (2006), there has been
69 substantial research and development into estimators that use both design and
70 model-based principles (see e.g., Sterba (2009), Cicchitelli and Montanari (2012),
71 Chan-Golston et al. (2020) for a Bayesian approach).

72 Certainly comparisons between design-based and model-based approaches to
73 spatial data have been studied. But no numerical comparison has been made
74 between design-based approaches incorporating spatial information and design-
75 based approaches. In this manuscript, we compare design-based approaches
76 incorporating spatial information to model-based approaches for spatial data.
77 We focus on finite populations, but these comparisons generalize to infinite
78 populations as well. A finite population contains a finite number of population
79 units; an example is lakes (treated as a whole with the lake centroid representing
80 location) in the contiguous United States. An infinite population contains an
81 infinite number of population units; an example is locations within a single lake.

82 The rest of the manuscript is organized as follows. In Section 1.1, we
83 introduce and provide relevant background for the design-based and model-based
84 approaches to finite population spatial data. In Section 2, we describe how we
85 compare performance of the approaches with a simulation study and an analysis
86 of real data that contains mercury concentration in lakes from the contiguous
87 United States. In Section 3, we present results from the simulation study and the
88 analysis of mercury concentrations. And in Section 4, we end with a discussion
89 and provide directions for future research.

90 *1.1. Background*

91 The design-based and model-based approaches incorporate randomness in
92 fundamentally different ways. In this section, we describe the role of randomness
93 for each approach and the subsequent effects on statistical inferences for spatial
94 data.

95 *1.1.1. Comparing Design-Based and Model-Based Approaches*

96 The design-based approach assumes the population is fixed. Randomness is
97 incorporated via the selection of units in a sampling frame. A sampling frame
98 is the set of all units available to be sampled. Units from the sampling frame
99 are selected as part of the sample according to a sampling design, which assigns
100 a positive probability of inclusion (inclusion probability) to each unit from the
101 sampling frame. Some examples of commonly used sampling designs include
102 simple random sampling, stratified random sampling, and cluster sampling.
103 When sampling designs incorporate spatial locations into sampling, we call
104 the resulting samples “spatially balanced.” One approach to selecting spatially
105 balanced samples is the Generalized Random Tessellation Stratified (GRTS)
106 algorithm (Stevens and Olsen, 2004), which we discuss in more detail in Section
107 1.1.2. When sampling designs do not incorporate spatial locations into sampling,
108 we call the resulting samples “non-spatially balanced.”

109 Fundamentally, the design-based approach combines the randomness of the
 110 sampling design with the data collected via the sample to justify the estimation
 111 and uncertainty quantification of fixed, unknown parameters of a population (e.g.,
 112 a population mean). Treating the data as fixed and incorporating randomness
 113 through the sampling design yields estimators having very few other assumptions.
 114 Confidence intervals for these types of estimators are typically derived using
 115 limiting arguments that incorporate all possible samples. Sample means, for
 116 example, are asymptotically normal (Gaussian) by the Central Limit Theorem
 117 (under some assumptions). If we repeatedly select samples from the population,
 118 then 95% of all 95% confidence intervals constructed from a procedure with
 119 appropriate coverage will contain the true, fixed mean. Särndal et al. (2003)
 120 and Lohr (2009) provide thorough reviews of the design-based approach.

121 The model-based approach assumes the data are a random realization of
 122 a data-generating stochastic process. Randomness is incorporated through
 123 distributional assumptions on this process. Strictly speaking, randomness need
 124 not be incorporated through random sampling, though Diggle et al. (2010) warn
 125 against preferential sampling. Preferential sampling occurs when the process
 126 generating the data locations and the process being modeled are not independent
 127 of one another. To guard against preferential sampling, model-based approaches
 128 often still implement some form of random sampling.

129 Instead of estimating fixed, unknown population parameters, as in the design-
 130 based approach, often the goal of model-based inference is to predict a realized
 131 variable, or value. For example, suppose the realized mean of all population
 132 units is the value of interest. Instead of *estimating* a fixed, unknown mean, we
 133 are *predicting* the value of the mean, a random variable. Prediction intervals are
 134 then derived using assumptions of the data-generating stochastic process. If we
 135 repeatedly generate response values from the same data-generating stochastic

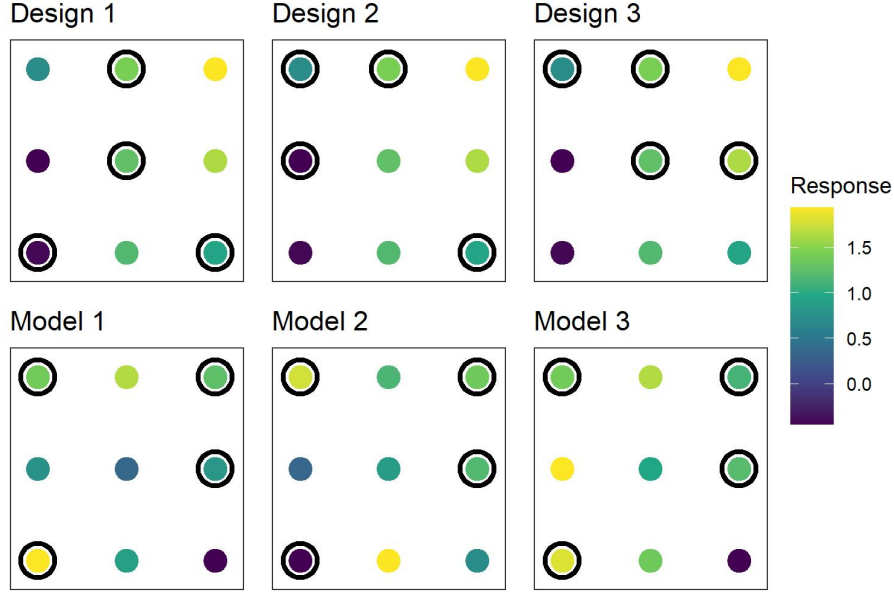


Figure 1: A visual comparison of the design-based and model-based approaches. In the top row, there is one fixed population with nine population units and three random samples of size four (points circled are those sampled). The response values at each site are fixed, but we obtain different estimates for the mean response in each random sample. In the bottom row, there are three realizations of the same data-generating stochastic process that are all sampled at the same four locations. The data-generating stochastic process has a single mean, but the mean of the nine population units is different in each of the three realizations

process and select samples, then 95% of all 95% prediction intervals constructed from a procedure with appropriate coverage will contain their respective realized means. Cressie (1993) and Schabenberger and Gotway (2017) provide thorough reviews of model-based approaches for spatial data. In Fig. 1, we provide a visual comparison of the design-based and model-based approaches (Ver Hoef (2002) and Brus (2021) provide similar figures).

1.1.2. Spatially Balanced Design and Analysis

We previously mentioned that the design-based approach can be used to select spatially balanced samples (samples that incorporate spatial locations of the population units and are “well-spread” in space). Spatially balanced samples are useful because parameter estimates from these samples tend to

147 vary less than parameter estimates from samples that are not spatially balanced
 148 (Barabesi and Franceschi, 2011; Benedetti et al., 2017; Grafström and Lundström,
 149 2013; Robertson et al., 2013; Stevens and Olsen, 2004; Wang et al., 2013).
 150 The first spatially balanced sampling algorithm seeing widespread use is the
 151 Generalized Random Tessellation Stratified (GRTS) algorithm (Stevens and
 152 Olsen, 2004). To quantify the spatial balance of a sample, Stevens and Olsen
 153 (2004) proposed loss metrics based on Voronoi polygons (Dirichlet Tessellations).
 154 After the GRTS algorithm was developed, several other spatially balanced
 155 sampling algorithms emerged, such as the Local Pivotal Method (Grafström et
 156 al., 2012; Grafström and Matei, 2018), Spatially Correlated Poisson Sampling
 157 (Grafström, 2012), Balanced Acceptance Sampling (Robertson et al., 2013),
 158 Within-Sample-Distance Sampling (Benedetti and Piersimoni, 2017), and Halton
 159 Iterative Partitioning Sampling (Robertson et al., 2018). In this manuscript, we
 160 select spatially balanced samples using the Generalized Random Tessellation
 161 Stratified (GRTS) algorithm because it has several attractive properties. More
 162 specifically, the GRTS algorithm accommodates finite and infinite sampling
 163 frames, equal, unequal, and proportional (to size) inclusion probabilities, legacy
 164 (historical) sampling (Foster et al., 2017), a minimum distance between units in
 165 a sample, and replacement units (replacement units are population units that
 166 can be sampled when a population unit originally selected can no longer be
 167 sampled). The GRTS algorithm selects samples by utilizing a particular mapping
 168 between two-dimensional and one-dimensional space that preserves proximity
 169 relationships. Via this mapping, units in two-dimensional space are partitioned
 170 using a hierarchical address. This hierarchical address is used to map population
 171 units to a one-dimensional line. On the one dimensional line, each population
 172 unit's line length equals its inclusion probability. Then, a systematic sample of
 173 population units is selected on the line, yielding desired sample. Stevens and

174 Olsen (2004) provides more technical details.

After selecting a sample and collecting data, unbiased estimates of population means and totals can be obtained using the Horvitz-Thompson estimator (Horvitz and Thompson, 1952). If τ is a population total, the Horvitz-Thompson estimate of τ , denoted by $\hat{\tau}_{ht}$, is given by

$$\hat{\tau}_{ht} = \sum_{i=1}^n Z_i \pi_i^{-1}, \quad (1)$$

175 where Z_i is the value of the i th population unit in the sample and π_i is the
176 inclusion probability of the i th population unit in the sample. An estimate of
177 the population mean is obtained by dividing $\hat{\tau}_{ht}$ by N , the number of population
178 units.

179 It is also important to quantify uncertainty $\hat{\tau}_{ht}$. Horvitz and Thompson
180 (1952) and Sen (1953) provide variance estimators for $\hat{\tau}_{ht}$, but these estimators
181 have two drawbacks. First, they rely on calculating π_{ij} , the probability that
182 population unit i and population unit j are both in the sample – this quantity
183 can be challenging if not impossible to calculate analytically. Second, these
184 estimators ignore the spatial locations of the population units. To address these
185 two drawbacks simultaneously, Stevens and Olsen (2003) proposed the local
186 neighborhood variance estimator. The local neighborhood variance estimator
187 does not rely on π_{ij} and incorporates spatial locations – for technical details see
188 Stevens and Olsen (2003). Stevens and Olsen (2003) show the local neighborhood
189 variance estimator tends to reduce the estimated variance of $\hat{\tau}$ and yield narrower
190 confidence intervals compared to variance estimators that ignore spatial locations.

191 1.1.3. Finite Population Block Kriging

192 Finite Population Block Kriging (FPBK) is a model-based approach that
193 expands the geostatistical Kriging framework to the finite population setting

194 (Ver Hoef, 2008). Instead of developing inference based on a specific sampling
 195 design, we assume the data are generated by a spatial stochastic process. We
 196 summarize some of the basic principles of FBPK next (for more technical details,
 197 see Ver Hoef (2008)) Let $\mathbf{z} \equiv \{z(s_1), z(s_2), \dots, z(s_N)\}$ be an $N \times 1$ response vector
 198 at locations s_1, s_2, \dots, s_N that can be measured at the N population units.
 199 Suppose we want to use a sample to predict some linear function of the response
 200 variable, $f(\mathbf{z}) = \mathbf{b}'\mathbf{z}$, where \mathbf{b}' is a $1 \times N$ vector of weights (e.g, the population
 201 mean is represented by a weights vector whose elements all equal one). Denoting
 202 quantities that are part of the sampled population units with a subscript s and
 203 quantities that are part of the unsampled population units with subscript u , let

$$\begin{pmatrix} \mathbf{z}_s \\ \mathbf{z}_u \end{pmatrix} = \begin{pmatrix} \mathbf{X}_s \\ \mathbf{X}_u \end{pmatrix} \boldsymbol{\beta} + \begin{pmatrix} \boldsymbol{\delta}_s \\ \boldsymbol{\delta}_u \end{pmatrix}, \quad (2)$$

204 where \mathbf{X}_s and \mathbf{X}_u are the design matrices for the sampled and unsampled
 205 population units, respectively, $\boldsymbol{\beta}$ is the parameter vector of fixed effects, and
 206 $\boldsymbol{\delta} \equiv [\boldsymbol{\delta}_s \ \boldsymbol{\delta}_u]'$, where $\boldsymbol{\delta}_s$ and $\boldsymbol{\delta}_u$ are random errors for the sampled and unsampled
 207 population units, respectively.

FBPK assumes $\boldsymbol{\delta}$ in Equation 2 has mean-zero and a spatial correlation
 structure that can be modeled using a covariance function. This covariance
 function is commonly assumed to be non-negative (between zero and one), second-
 order stationary (depending only on the distance between population units),
 isotropic (independent of direction), and decay with distance between population
 units (Cressie, 1993). Henceforth, it is implied that we have made these same
 assumptions regarding $\boldsymbol{\delta}$, though Chiles and Delfiner (1999), pp. 80-93 discuss
 covariance functions that are not second-order stationary, not isotropic, or both.
 A variety of flexible covariance functions can be used to model $\boldsymbol{\delta}$ (Cressie, 1993);
 one example is the exponential covariance function (for a thorough list of spatial

covariance functions, see Cressie (1993). The i, j th element of the exponential covariance matrix, $\text{cov}(\boldsymbol{\delta})$, is

$$\text{cov}(\delta_i, \delta_j) = \begin{cases} \sigma_1^2 \exp(-h_{i,j}/\phi) & h_{i,j} > 0 \\ \sigma_1^2 + \sigma_2^2 & h_{i,j} = 0 \end{cases}, \quad (3)$$

where σ_1^2 is the variance parameter quantifying the variability that is dependent (coarse-scale), σ_2^2 is the variance parameter quantifying the variability that is independent (fine-scale), ϕ is the range parameter measuring the distance-decay rate of the covariance, and $h_{i,j}$ is the Euclidean distance between population units i and j . The proportion of variability attributable to dependent random error is $\sigma_1^2/(\sigma_1^2 + \sigma_2^2)$. Similarly, the proportion of variability attributable to independent random error is $\sigma_2^2/(\sigma_1^2 + \sigma_2^2)$. Finally we note that σ_1^2 and σ_2^2 are often called the partial sill and nugget, respectively.

With the above model formulation, the Best Linear Unbiased Predictor (BLUP) for $f(\mathbf{b}'\mathbf{z})$ and its prediction variance can be computed. While details of the derivation are in Ver Hoef (2008), we note here that the predictor and its variance are both moment-based, meaning that they do not rely on any distributional assumptions.

Other approaches, such as k-nearest-neighbors (Fix and Hodges, 1989; Ver Hoef and Temesgen, 2013), random forests (Breiman, 2001), Bayesian models (Chan-Golston et al., 2020), among others, could also be used to obtain predictions for a mean or total from spatially correlated responses of a finite population. Compared to the k-nearest-neighbors and random forest approach, we prefer FBPK because it is model-based and relies on theoretically-based variance estimators leveraging the model's spatial covariance structure, whereas k-nearest-neighbors and random forests use ad-hoc variance estimators (Ver Hoef and Temesgen, 2013). Additionally, Ver Hoef and Temesgen (2013) studied

230 compared FBPK, k-nearest-neighbors, and random forests in a variety of spatial
 231 data contexts, and FBPK tended to perform best. Compared to the Bayesian
 232 approach, we prefer FBPK mostly because it is much more computationally
 233 efficient.

234 2. Materials and Methods

235 2.1. Simulation Study

236 We used a simulation study to investigate performance of four sampling-
 237 analysis combinations: IRS with a design-based analysis, called “IRS-Design”;
 238 IRS with a model-based analysis, called “IRS-Model”; GRTS sampling with a
 239 design-based analysis, called “GRTS-Design”; GRTS sampling with a model-
 240 based analysis, called “GRTS-Model”. These combinations are also provided in
 241 Table 1.

	Design	Model
IRS	IRS-Design	IRS-Model
GRTS	GRTS-Design	GRTS-Model

Table 1: Sampling-analysis combinations in the simulation study. The rows give the two types of sampling designs and the columns give the two types of analyses.

242 Performance for the four sampling-analysis combinations was evaluated in 36
 243 different simulation scenarios. The 36 scenarios resulted from the crossing of three
 244 sample sizes, two location layouts, two response types, and three proportions of
 245 dependent random error. The three sample sizes (n) were $n = 50$, $n = 100$, and
 246 $n = 200$. Samples were always selected from a population size (N) of $N = 900$.
 247 The two location layouts (of the population units) were random and gridded.
 248 Locations in the random layout were randomly generated inside the unit square
 249 $([0, 1] \times [0, 1])$. Locations in the gridded layout were placed on a fixed, equally
 250 spaced grid inside the unit square. The two response types were normal and

lognormal. For the normal response type, the response was simulated using mean-zero random errors with the exponential covariance (Equation 3) for varying proportions of dependent random error. The proportion of dependent random error is represented by $\sigma_1^2/(\sigma_1^2 + \sigma_2^2)$, where σ_1^2 and σ_2^2 are the dependent random error variance (partial sill) and independent random error variance (nugget), respectively, from Equation 3. The total variance, $\sigma_1^2 + \sigma_2^2$, was always 2. The range was always $\sqrt{2}/3$, which means that the correlation in the dependent random error decayed to nearly zero at the largest possible distance between two units in the domain. For the lognormal response type, the response was first simulated using the same approach as for the normal response type, except that the total variance was 0.6931 instead of 2. The response was then exponentiated, yielding a random variable whose total variance is 2. The lognormal responses were used to evaluate performance of the sampling-analysis approaches for data that were skewed (i.e., not normal).

Sample Size (n)	50	100	200
Location Layout	Random	Gridded	-
Proportion of Dependent Error	0	0.5	0.9
Response Type	Normal	Lognormal	-

Table 2: Simulation scenario options. All combinations of sample size, location layout, response type, and proportion of dependent random error composed the 36 simulation scenarios. In each simulation scenario, the total variance was two.

In each of the 36 simulation scenarios, there were 2000 independent simulation trials. In each trial, IRS and GRTS samples were selected and then design-based and model-based analyses were used to estimate (design-based) or predict (model-based) the mean and construct confidence (design-based) or prediction (model-based) intervals. Then we recorded the bias, squared error, and interval coverage for all sampling-analysis combinations. After all 2000 trials, we summarized the long-run performance of the combinations by calculating average bias, RMS(P)E (root-mean-squared error for the design-based approaches and root-mean-squared-

prediction error for the model-based approaches), and the proportion of times the true mean is contained in its 95% interval. The GRTS algorithm and the local neighborhood variance estimator are available in the **R** package **spsurvey** (Dumelle et al., 2021). FPBK is available in the **sptotal** **R** package (Higham et al., 2021) and covariance parameters were estimated using Restricted Maximum Likelihood (Harville, 1977; Patterson and Thompson, 1971; Wolfinger et al., 1994).

2.2. Application

The Environmental Protection Agency (EPA), states, and tribes periodically conduct National Aquatic Research Surveys (NARS) in the United States to assess the water quality of various bodies of water. We will use data from the 2012 National Lakes Assessment (NLA), which measures various aspects of lake health and water quality for lakes in the contiguous United States (USEPA, 2012). Specifically, we will analyze mercury concentration in lakes. Although we know the true mean mercury concentration values for the 986 lakes from the 2012 NLA, we will explore whether or not we obtain an adequately precise estimate for the realized mean mercury concentration if we sample only 100 of the 986 lakes. For each of the four familiar sampling-analysis combinations (IRS-Design, IRS-Model, GRTS-Design, and GRTS-Model), we estimate

3. Results

3.1. Simulation Study

The average bias was nearly zero for all four combinations in all 36 scenarios, so we omit a more detailed summary of those results here. Tables for average bias in all 36 simulation scenarios are provided in the supporting information.

Fig. 2 shows the relative rMS(P)E of the four approaches from Table 1 using the random location layout with “IRS-Design” as the baseline.

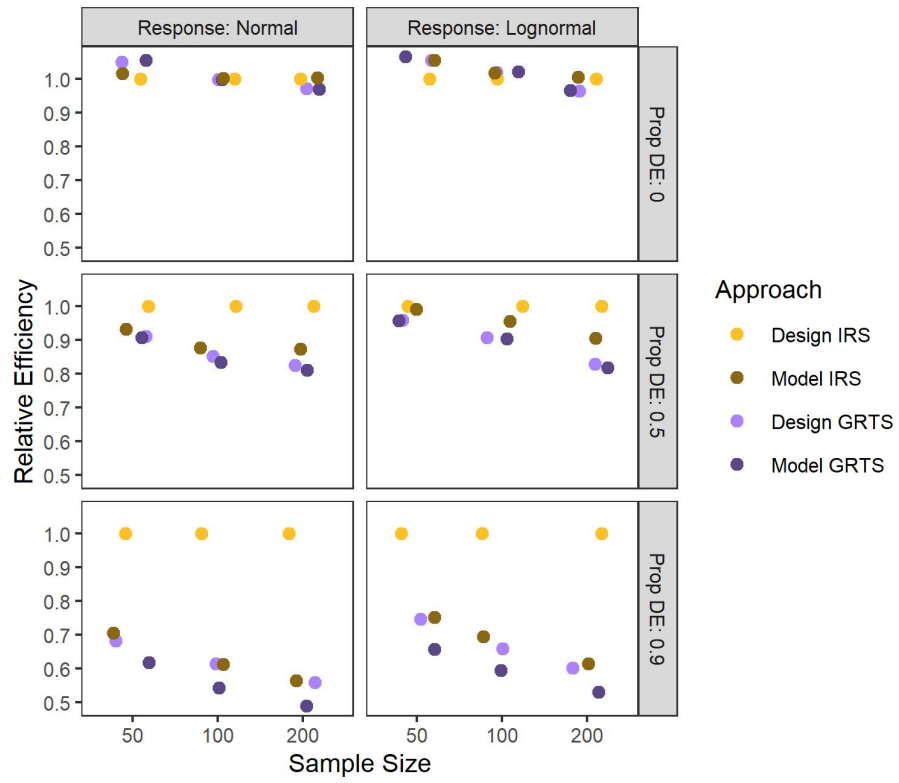


Figure 2: Relative rms(P)E for the four sampling-analysis combinations. The rows indicate the proportion of dependent error and the columns indicate the response type.

The relative rMS(P)E is defined as

$$\frac{\text{rMS(P)E of sampling-analysis combination}}{\text{rMS(P)E of IRS-Design}},$$

When there is no spatial correlation (Fig. 2, “Prop DE: 0” row), the four sampling-analysis combinations have approximately equal rMS(P)E. So using the GRTS sampling plan or a model-based analysis does not result in much, if any, loss in efficiency compared to IRS-Design when there is no spatial correlation. When there is spatial correlation (Fig. 2, “Prop DE: 0.5” and “Prop DE: 0.9” rows), GRTS-Model tends to perform best, followed by GRTS-Design, IRS-Model, and finally IRS-Design, though the difference in relative rMS(P)E among GRTS-Model, GRTS-Design, and IRS-Model is relatively small. As the strength of spatial correlation increases, the gap in rMS(P)E between IRS-Design and the other sampling-analysis combinations widens. Finally we note that when there is spatial correlation, IRS-Model outperforms IRS-Design by a large margin, suggesting that the poor design properties of IRS are largely mitigated by the model-based analysis. These conclusions are similar to those observed in the grid location layout, so we omit a grid location layout figure here. Tables for rMS(P)E in all 36 simulation scenarios are provided in the supporting information.

We also studied 95% interval coverage among the sampling-analysis combinations. The design-based confidence intervals and model-based prediction intervals were constructed using the normal distribution. Justification for this comes from the asymptotic normality of means via the Central Limit Theorem.

Fig. 3 shows the 95% interval coverage for each of the four sampling-analysis combinations in the random location layout.

Within each scenario, the sampling-analysis combinations tend to have fairly similar interval coverage. Coverage in the normal response scenarios was usually near 95%, while coverage in the lognormal response scenarios varied

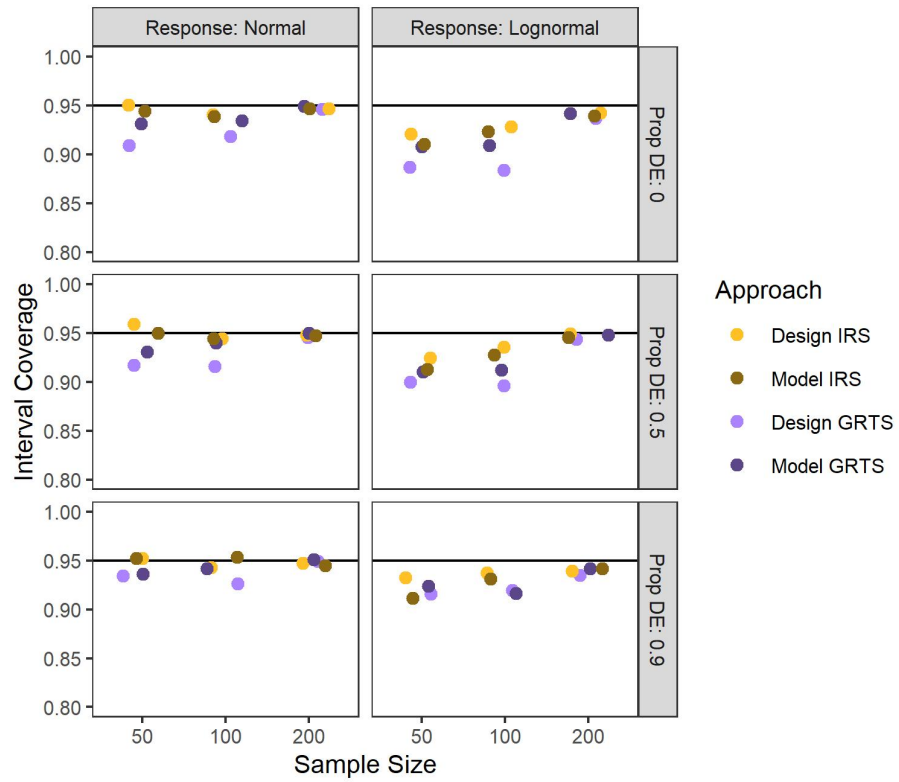


Figure 3: Interval coverage for the four sampling-analysis combinations. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid, black line in each plot represents 95% coverage.

323 from from 90% to 95%. Coverage tended to always increase with the sample
324 size. At a sample size of 200, all four sampling-analysis combinations had
325 approximately 95% interval coverage in both response scenarios for all dependent
326 error proportions. These conclusions are similar to those observed in the grid
327 location layout, so we omit a grid location layout figure here. Tables for interval
328 coverage in all 36 simulation scenarios are provided in the supporting information.

329 *3.2. Application*

330 Fig. 4 shows that mercury concentration is right-skewed, with most lakes
331 having a low value of mercury concentration but a few having a much higher
332 concentration. Mercury concentration exhibits some spatial patterning, with
333 high mercury concentrations in lakes in the northeast and north central United
334 States. Fig. 4 also shows the spatial dependence in mercury concentration via
335 the empirical semivariogram. The empirical semivariogram can be used as a
336 tool to visualize spatial dependence. It quantifies the halved squared differences
337 (semivariance) among mercury concentration at different distances apart. When
338 a process is spatially correlated, the semivariance tends to be smaller at small
339 distances and larger at large distances. Together, the map, histogram, and
340 semivariogram in Fig. 4 suggest that mercury concentration is skewed and
341 exhibits spatial dependence. Lastly we note that the realized mean mercury
342 concentration in the 986 lakes is 103.2 ng / g.

343 We selected a single IRS sample and a single GRTS sample and estimated
344 (design-based) or predicted (model-based) the mean mercury concentration and
345 its standard error using using design-based and model-based approaches. For the
346 model-based analyses, the exponential covariance was used. Table 3 shows the
347 results from these analyses. For all four sampling-analysis combinations, the true
348 realized mean mercury concentration is within the bounds of the 95% confidence
349 (design-based) or prediction (model-based) intervals. Though we should not

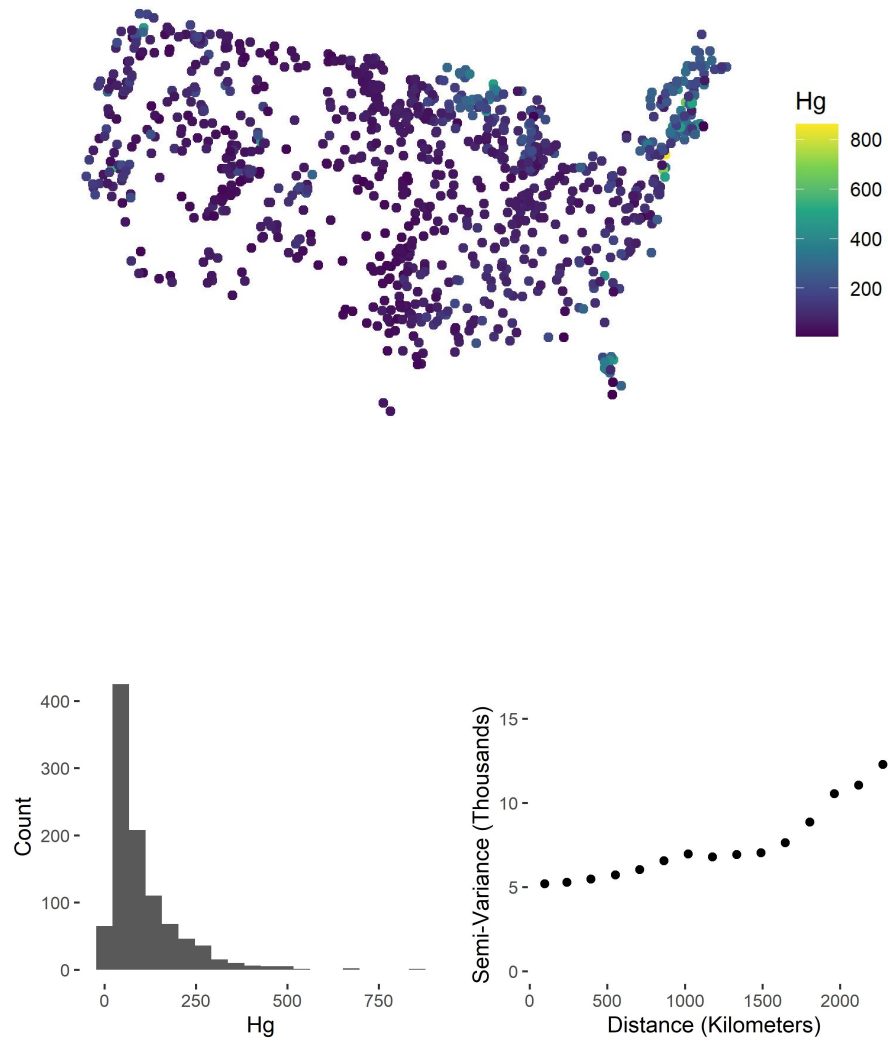


Figure 4: Mercury concentration visualizations for the population (Hg) for 986 lakes in the contiguous United States. A spatial layout is in the top row, a histogram is in the bottom row and left column, and an empirical semivariogram is in the bottom row and right column.

350 generalize these results to other samples from these data, we do note a couple
 351 of patterns. The design-based IRS analysis shows the largest standard error:
 352 a likely reason is that this is the only approach that does not incorporate any
 353 spatial information regarding mercury concentration. Both analyses using GRTS
 354 sampling have lower standard errors than both analyses using IRS sampling.
 355 We expect that these patterns are consistent with other samples from these
 356 data because mercury concentration exhibits spatial patterning, so a spatially
 357 balanced sample should usually yield a lower standard error.

Approach	Estimate	SE	95% LB	95% UB
IRS-Design	112.7	8.8	95.4	129.9
IRS-Model	110.5	7.9	95.0	125.9
GRTS-Design	101.8	6.1	89.8	113.7
GRTS-Model	102.3	5.9	90.8	113.9

Table 3: Application of design-based and model-based approaches to the NLA data set on mercury concentration. The true mean concentration is 103.2 ng / g.

358 **4. Discussion**

359 The design-based and model-based approaches to statistical inference are
 360 fundamentally different paradigms by which samples are selected and data are
 361 analyzed. The design-based approach incorporates randomness through sampling
 362 to estimate population parameters. The model-based approach incorporates
 363 randomness through distributional assumptions to predict realized values of a
 364 random process. Though these approaches have often been compared in the
 365 literature both from theoretical and analytical perspectives, our contribution
 366 lies in studying them in a spatial context while implementing spatially balanced
 367 sampling. Aside from the theoretical differences described, a few analytical
 368 findings from the simulation study are particularly notable. First, the sampling
 369 decision (GRTS vs IRS) is most important when using a design-based analysis.
 370 Though GRTS-Model still outperformed IRS-Model, the model-based analysis

371 mitigated much of the inefficiency of the IRS sample. Second, independent of
 372 the analysis approach, we found no reason to prefer IRS over GRTS for sampling
 373 spatial data – GRTS-Design and GRTS-Model generally performed at least
 374 as well as their IRS counterparts when there was no spatial correlation and
 375 noticeably better than their IRS counterparts when there was spatial correlation.
 376 Third, as the strength of spatial correlation increases, the gap in rMS(P)E
 377 between IRS-Design and the other sampling-analysis combinations also increases.
 378 Fourth and finally, when the response was normal, interval coverage for all
 379 sampling-analysis combinations was very close to 95% for all sample sizes; when
 380 the response was lognormal, interval coverage for all sampling and analysis was
 381 between 90% and 95% and closest to 95% when $n = 200$.

382 There are several benefits and drawbacks of the design-based and model-
 383 based approaches for finite population spatial data. Some we have discuss, but
 384 others we have not and they are worthy of consideration in future research.
 385 Design-based approaches are often computationally efficient, while model-based
 386 estimation can be computationally burdensome, especially for likelihood-based
 387 methods such as REML that rely on inverting a covariance matrix. The design-
 388 based approach also more naturally handles binary data, free from the more
 389 complicated logistic regression framework commonly used to analyze binary
 390 data in a model-based approach. The model-based approach, however, can
 391 more naturally quantify the relationship between covariates (predictor variables)
 392 and response variable. The model-based approach also yields estimated spatial
 393 covariance parameters, which help better understand the dependence structure
 394 in the process of study. Model selection is also possible using model-based
 395 approaches and criteria such as cross validation, likelihood ratio tests, or AIC
 396 (Akaike, 1974). Model-based approaches are capable of more efficient small-area
 397 estimation than design-based approaches by leveraging distributional assumptions

398 in areas with few observed sites. Model-based approaches can also compute site-
399 by-site predictions at unobserved locations and use them to construct informative
400 visualizations. The benefits and drawbacks of both approaches, alongside our
401 theoretical and analytical comparisons, can motivate the process of choosing among
402 them. This is especially true from an analysis perspective, as we found that
403 using a spatially balanced sampling algorithm benefits both design-based and
404 model-based analyses.

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414 **Conflict of Interest Statement**

415 There are no conflicts of interest for any of the authors.

416 **Data and Code Availability**

417 This manuscript has a supplementary R package that contains all of the
418 data and code used in its creation. The supplementary R package is hosted on
419 GitHub. Instructions for download are available at

420 <https://github.com/michaeldumelle/DvMsp>.

421 **Supporting Information**

422 In the supporting information, we provide tables presenting summary statis-
423 tics for all 36 simulation scenarios.

424 **Author Contributions**

425 All authors conceived the ideas; All authors designed methodology; MD and
426 MH performed the simulations and analyzed the data; MD and MH led the
427 writing of the manuscript; All authors contributed critically to the drafts and
428 gave final approval for publication.

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