

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 rest on fundamentally different foundations. In the design-based approach, inference relies on random sampling. In the model-based approach, inference relies 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 approaches tend to

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outperform design-based approaches, even when the data are skewed (and by consequence, the model-based distributional assumptions violated). The performance gap between these approaches is small when spatially balanced samples are used but large when non-spatially balanced samples are used. This suggests that the sampling choice (whether to select a sample that is spatially balanced) is most important when performing design-based inference.

4. There are many benefits and drawbacks to the design-based and model-based approaches for finite population spatial data that practitioners must consider when choosing between them. 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; Local neighborhood variance estimator; Model-based inference; Restricted Maximum Likelihood (REML) estimation; Spatially balanced sampling; Spatial covariance

1. Introduction

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. There are two general approaches for using samples to make frequentist statistical inferences about a population: design-based and model-based. In the design-based approach, inference relies on randomly assigning some population units to be in the sample (e.g., random sampling). Alternatively, in

the model-based approach, inference relies on distributional assumptions about the underlying stochastic process that generated the sample. Each paradigm has a deep historical context (Sterba, 2009) and its own set of benefits and drawbacks (Hansen et al., 1983).

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

Certainly comparisons between design-based and model-based approaches have been studied in spatial contexts. But no numerical comparison has been made between design-based approaches that incorporate spatial locations into sampling and analysis and model-based approaches. In this manuscript, we compare design-based approaches that incorporate spatial locations into sampling and analysis to model-based approaches for finite population spatial data. A finite population contains a finite number of population units (we assume the finite number is known); an example is lakes (treated as a whole with the

lake centroid representing location) in the contiguous United States. Though here we focus on finite populations, the comparisons we discuss generalize to infinite populations as well. An infinite population contains an infinite number of population units; an example is locations within a single lake.

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

1.1. Background

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

1.1.1. Comparing Design-Based and Model-Based Approaches

The design-based approach assumes the population is fixed. Randomness is incorporated via the selection of population units according to a sampling design. A sampling design assigns a positive probability of inclusion (inclusion probability) in the sample to each population unit. These inclusion probabilities are later used to estimate population parameters. Some examples of commonly used sampling designs include simple random sampling, stratified random sampling, and cluster sampling.

When sampling designs incorporate spatial locations into sampling, we call the resulting samples “spatially balanced.” One approach to selecting spatially

109 balanced samples is the Generalized Random Tessellation Stratified (GRTS)
 110 algorithm (Stevens and Olsen, 2004), which we discuss in more detail in Section
 111 1.1.2. When sampling designs do not incorporate spatial locations into sampling,
 112 we call the resulting samples “non-spatially balanced.”

113 Fundamentally, the design-based approach combines the randomness of the
 114 sampling design with the data collected via the sample to justify the estimation
 115 and uncertainty quantification of fixed, unknown parameters of a population (e.g.,
 116 a population mean). Treating the data as fixed and incorporating randomness
 117 through the sampling design yields estimators having very few other assumptions.
 118 Confidence intervals for these types of estimators are typically derived using
 119 limiting arguments that incorporate all possible samples. Sample means, for
 120 example, are asymptotically normal (Gaussian) by the Central Limit Theorem
 121 (under some assumptions). If we repeatedly select samples from the population,
 122 then 95% of all 95% confidence intervals constructed from a procedure with
 123 appropriate coverage will contain the true fixed population mean. Särndal et al.
 124 (2003) and Lohr (2009) provide thorough reviews of the design-based approach.

125 The model-based approach assumes the sample is a random realization of a
 126 data-generating stochastic process. Randomness is formally incorporated through
 127 distributional assumptions on this process. Strictly speaking, randomness need
 128 not be incorporated through random sampling, though Diggle et al. (2010)
 129 warn against preferential sampling. Preferential sampling occurs when the
 130 process generating the data locations and the process being modeled are not
 131 independent of one another. To guard against preferential sampling, model-
 132 based approaches often still implement some form of random sampling. When
 133 model-based approaches implement random sampling, the inclusion probabilities
 134 are ignored when analyzing the sample (in contrast to the design-based approach,
 135 which relies on these inclusion probabilities to analyze the sample).

136 Instead of estimating fixed, unknown population parameters, as in the design-
 137 based approach, often the goal of model-based inference is to predict a realized
 138 variable, or value. For example, suppose the realized mean of all population
 139 units is the value of interest. Instead of a fixed, unknown mean, we are the value
 140 of the mean, a random variable. Prediction intervals are then derived using
 141 assumptions of the data-generating stochastic process. If we repeatedly generate
 142 response values from the same process and select samples, then 95% of all 95%
 143 prediction intervals constructed from a procedure with appropriate coverage
 144 will contain their respective realized means. Cressie (1993) and Schabenberger
 145 and Gotway (2017) provide thorough reviews of model-based approaches for
 146 spatial data. In Fig. 1, we provide a visual comparison of the design-based
 147 and model-based approaches (Ver Hoef (2002) and Brus (2021) provide similar
 148 figures).

149 1.1.2. *Spatially Balanced Design and Analysis*

150 We previously mentioned that the design-based approach can be used to
 151 select spatially balanced samples (samples that incorporate spatial locations of
 152 the population units). Spatially balanced samples are useful because parameter
 153 estimates from these samples tend to vary less than parameter estimates from
 154 samples that are not spatially balanced (Barabesi and Franceschi, 2011; Benedetti
 155 et al., 2017; Grafström and Lundström, 2013; Robertson et al., 2013; Stevens and
 156 Olsen, 2004; Wang et al., 2013). The first spatially balanced sampling algorithm
 157 to see widespread use was the Generalized Random Tessellation Stratified (GRTS)
 158 algorithm (Stevens and Olsen, 2004). To quantify the spatial balance of a
 159 sample, Stevens and Olsen (2004) proposed loss metrics based on Voronoi
 160 polygons (Dirichlet Tessellations). After the GRTS algorithm was developed,
 161 several other spatially balanced sampling algorithms emerged, including the
 162 Local Pivotal Method (Grafström et al., 2012; Grafström and Matei, 2018),

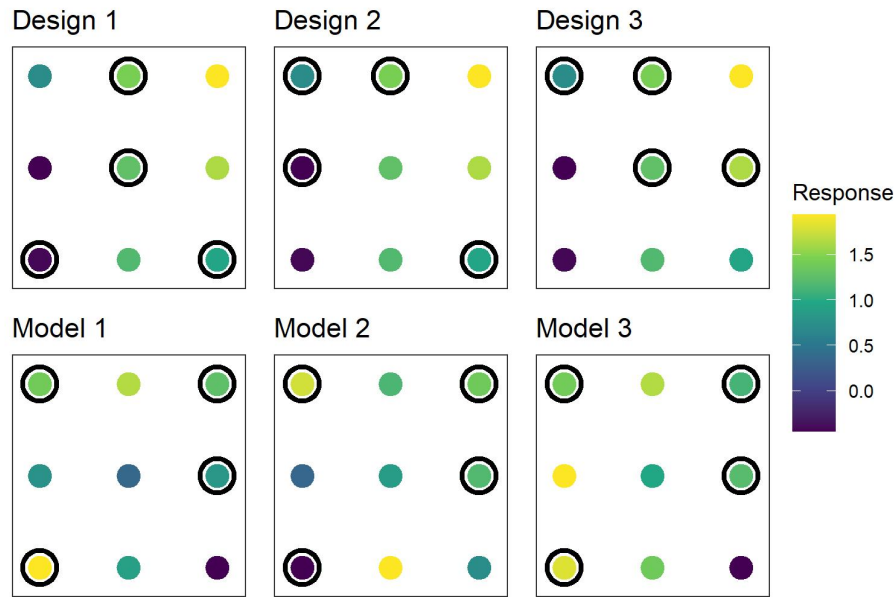


Figure 1: A visual comparison of the design-based and model-based approaches. In the top row, the design-based approach is highlighted. There is one fixed population with nine population units and three random samples of size four (points circled are those sampled). The response values at each site are fixed, but we obtain different estimates for the mean response in each random sample. In the bottom row, the model-based approach is highlighted. 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.

163 Spatially Correlated Poisson Sampling (Grafström, 2012), Balanced Acceptance
 164 Sampling (Robertson et al., 2013), Within-Sample-Distance Sampling (Benedetti
 165 and Piersimoni, 2017), and Halton Iterative Partitioning Sampling (Robertson
 166 et al., 2018). In this manuscript, we select spatially balanced samples using
 167 the Generalized Random Tessellation Stratified (GRTS) algorithm because it
 168 has several attractive properties: the GRTS algorithm accommodates finite and
 169 infinite sampling frames, equal, unequal, and proportional (to size) inclusion
 170 probabilities, legacy (historical) sampling (Foster et al., 2017), a minimum
 171 distance between units in a sample, and replacement units (replacement units are
 172 population units that can be sampled when a population unit originally selected
 173 can no longer be sampled). The GRTS algorithm selects samples by utilizing a
 174 particular mapping between two-dimensional and one-dimensional space that
 175 preserves proximity relationships. Via this mapping, units in two-dimensional
 176 space are partitioned using a hierarchical address. This hierarchical address is
 177 used to map population units to a one-dimensional line. On the one dimensional
 178 line, each population unit's line length equals its inclusion probability. Then, a
 179 systematic sample of population units is selected on the line and mapped back
 180 to two-dimensional space, yielding the desired sample. Stevens and Olsen (2004)
 181 provide 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 estimator for τ , denoted by $\hat{\tau}_{ht}$, is given by

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

182 where Z_i is the value of the i th population unit in the sample, π_i is the inclusion
 183 probability of the i th population unit in the sample, and n is the sample size. An

184 estimate of the population mean is obtained by dividing $\hat{\tau}_{ht}$ by N , the number
 185 of population units.

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

199 1.1.3. Finite Population Block Kriging

200 Finite Population Block Kriging (FPBK) is a model-based approach that
 201 expands the geostatistical Kriging framework to the finite population setting
 202 (Ver Hoef, 2008). Instead of developing inference based on a specific sampling
 203 design, we assume the data are generated by a spatial stochastic process. We
 204 summarize some of the basic principles of FBPK next – for technical details, see
 205 Ver Hoef (2008). Let $\mathbf{z} \equiv \{z(s_1), z(s_2), \dots, z(s_N)\}$ be an $N \times 1$ response vector
 206 at locations s_1, s_2, \dots, s_N that can be measured at the N population units.
 207 Suppose we want to use a sample to predict some linear function of the response
 208 variable, $f(\mathbf{z}) = \mathbf{b}'\mathbf{z}$, where \mathbf{b}' is a $1 \times N$ vector of weights (e.g, the population
 209 mean is represented by a weights vector whose elements all equal $1/N$). Denoting
 210 quantities that are part of the sampled population units with a subscript s and

quantities that are part of the unsampled population units with a subscript u ,
let

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

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

FBPK assumes $\boldsymbol{\delta}$ in Equation 2 has mean-zero and a spatial dependence structure that can be modeled using a covariance function. This covariance function is commonly assumed to be non-negative, 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 not either. A variety of flexible covariance functions can be used to model $\boldsymbol{\delta}$ (Cressie, 1993); one example is the exponential covariance function (Cressie (1993) provides a thorough list of spatial covariance functions). 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. Distributional assumptions are used, however, when constructing prediction intervals.

Other approaches, such as k-nearest-neighbors (Fix and Hodges, 1989; Ver Hoef and Temesgen, 2013) and random forest (Breiman, 2001), among others, could also be used to obtain predictions for a mean or total from finite population spatial data. 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 compared FBPK, k-nearest-neighbors, and random forest in a variety of spatial data contexts, and FBPK tended to perform best.

2. Materials and Methods

2.1. Simulation Study

We used a simulation study to investigate performance of four sampling-analysis combinations. The first sampling-analysis combination was IRS-Design. In IRS-Design, samples were selected with the Independent Random Sampling

(IRS) algorithm. The IRS algorithm ignores the spatial locations of the population units, thus the IRS samples were not spatially balanced. In IRS-Design, samples were analyzed using the design-based approach via the Horvitz-Thompson mean estimator and an IRS variance estimator that ignored the spatial locations of the units in the sample. The second sampling-analysis combination was IRS-Model, where samples were selected with the IRS algorithm and analyzed using the model-based approach via Restricted Maximum Likelihood (REML) estimation (Harville, 1977; Patterson and Thompson, 1971; Wolfinger et al., 1994). The third sampling-analysis combination was GRTS-Design, where samples were selected with the GRTS algorithm and analyzed using the design-based approach via the Horvitz-Thompson mean estimator and the local neighborhood variance estimator (which does incorporate the spatial locations of the units in the sample). The fourth and final sampling-analysis combination was GRTS-Model, where samples were selected with the GRTS algorithm and analyzed using the model-based approach via REML estimation. These sampling-analysis combinations are also provided in Table 1. Lastly we note that for both the IRS and GRTS samples, equal inclusion probabilities were assumed for all population units. When IRS assumes equal inclusion probabilities for all population units, the algorithm is equivalent to simple random sampling (SRS).

	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.

Performance for the four sampling-analysis combinations was evaluated in 36 different simulation scenarios. The 36 scenarios resulted from the crossing of three sample sizes, two location layouts (of the population units), two response types, and three proportions of dependent random error. The three sample sizes

(n) were $n = 50, n = 100$, and $n = 200$. Samples were always selected from a population size (N) of $N = 900$. The two location layouts were random and gridded. Locations in the random layout were randomly generated inside the unit square ($[0, 1] \times [0, 1]$). Locations in the gridded layout were placed on a fixed, equally 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) from Equation 3, respectively. The total variance, $\sigma_1^2 + \sigma_2^2$, was always 2. The range was always $\sqrt{2}/3$, chosen so that the correlation in the dependent random error decayed to nearly zero at $\sqrt{2}$, the largest possible distance between two population 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 lognormal random variable whose total variance was 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 2.

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 95% confidence (design-based) or 95% prediction (model-based) intervals. Then we recorded the bias, squared error, standard error, and interval coverage for all sampling-analysis combinations. After all 2000 trials, we summarized the long-run performance of the combinations by calculating mean bias, rMS(P)E (root-mean-squared error for the design-based approaches and root-mean-squared-prediction error for the model-based approaches), MStdE (mean standard error), and the proportion of times the true mean is contained in its 95% confidence (design-based) or 95% prediction (model-based) interval. The 95% intervals were constructed using the normal distribution. Justification for this comes from the asymptotic normality of means via the Central Limit Theorem (under some assumptions). Quantifying mean bias and rMS(P)E is important because they help us understand how far (under different loss metrics) the estimates (design-based) or predictions (model-based) tend to be from the true mean. Quantifying MStdE is important because it helps us understand how precise intervals tend to be. Quantifying interval coverage is important because it helps us understand how often our 95% intervals actually contain the true mean.

The IRS algorithm, IRS variance estimator, GRTS algorithm, and local neighborhood variance estimator are available in the **spsurvey R** package (Dumelle et al., 2021). FPBK is available in the **sptotal R** package (Higham et al., 2021).

2.2. Application

The United States Environmental Protection Agency (USEPA), states, and tribes periodically conduct National Aquatic Research Surveys (NARS) to assess the water quality of various bodies of water in the contiguous United States. One component of NARS is the National Lakes Assessment (NLA), which measures various aspects of lake health and water quality (USEPA, 2012). We will analyze mercury concentration data collected at 986 lakes from the 2012

NLA. Although we can calculate the true mean mercury concentration values for these 986 lakes, here we will explore whether or not we can obtain an adequately precise estimate (design-based) or prediction (model-based) 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 (design-based) or predict (model-based) the mean mercury concentration and construct 95% intervals from this sample of 100 lakes and compare to the true mean mercury concentration from all 986 lakes.

3. Results

3.1. Simulation Study

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

Fig. 7 shows the relative rMS(P)E of the four sampling analysis combinations using the random location layout with “IRS-Design” as the baseline. 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 covariance (Fig. 7, “Prop DE: 0” row), the four sampling-analysis combinations have approximately equal rMS(P)E and using the GRTS algorithm or a model-based analysis does not result in much, if any, loss in efficiency compared to IRS-Design. When there is spatial covariance (Fig. 7, “Prop DE: 0.5” and “Prop DE: 0.9” rows), GRTS-Model tends to have the lowest rMS(P)E, followed by GRTS-Design, IRS-Model, and finally IRS-Design, though the difference in relative rMS(P)E among GRTS-Model,

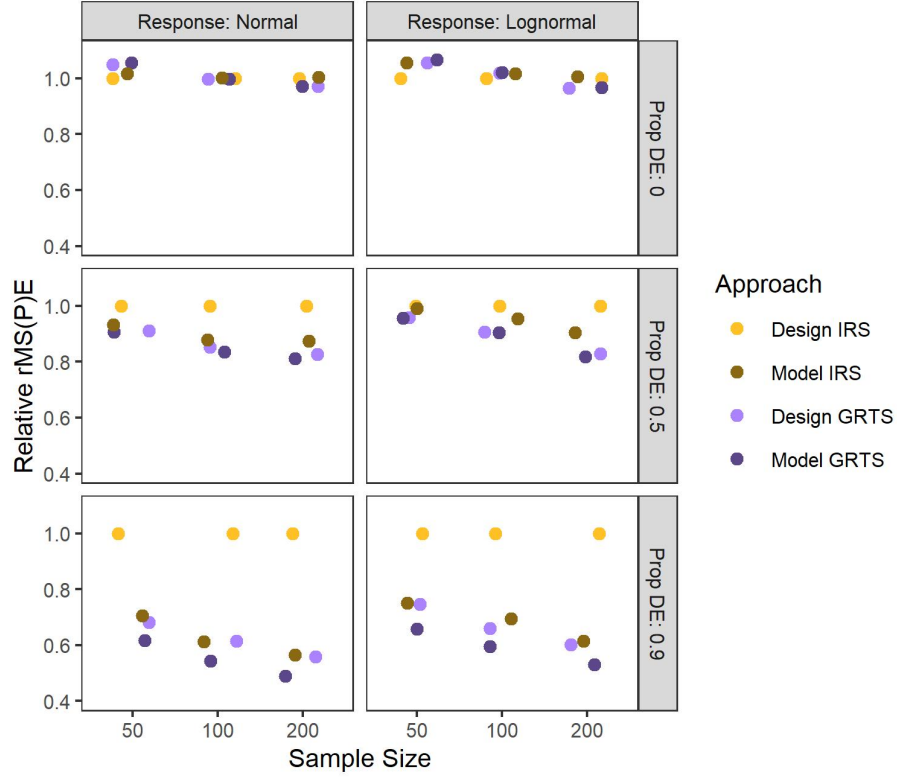


Figure 2: Relative rMS(P)E in the simulation study for the four sampling-analysis combinations. The rows indicate the proportion of dependent error and the columns indicate the response type.

339 GRTS-Design, and IRS-Model is relatively small. As the strength of spatial
 340 covariance increases, the gap in rMS(P)E between IRS-Design and the other
 341 sampling-analysis combinations widens. Finally we note that when there is spatial
 342 covariance, IRS-Model has a much lower rMS(P)E than IRS-Design, suggesting
 343 that the poor design properties of IRS are largely mitigated by the model-based
 344 analysis. These rMS(P)E conclusions are similar to those observed in the grid
 345 location layout, so we omit a grid location layout figure here. Tables for rMS(P)E
 346 in all 36 simulation scenarios are provided in the supporting information.

Fig. 8 shows the relative MStdE of the four sampling-analysis combinations using the random location layout with “IRS-Design” as the baseline. The relative

MStdE is defined as

$$\frac{\text{MStdE of sampling-analysis combination}}{\text{MStdE of IRS-Design}},$$

Many general takeaways regarding MStdE are similar to general takeaways regarding rMS(P)E: there seems to be no benefit to using IRS, even when there is no spatial covariance; as the strength of spatial covariance increases, the gap in MStdE between IRS-Design and the other sampling-analysis combinations widens; and IRS-Model outperforms IRS-Design by a noticeable margin. These fact that the rMS(P)E and MStdE findings are similar is not particularly surprising because the mean bias for all sampling-analysis combinations was nearly zero, thus rMS(P)E is driven by the standard error of the estimators (design-based) or predictors (model-based). We do note that between GRTS-Design and GRTS-Model, GRTS-Design had lower MStdE when there was no spatial covariance or a medium amount of spatial covariance (Fig. 8, “Prop DE: 0” and “Prop DE: 0.5” rows), and GRTS-Model had lower MStdE when there was a high amount of spatial covariance (Fig. 8, “Prop DE: 0.9” row). These MStdE conclusions are similar to those observed in the grid location layout, so we omit a grid location layout figure here. Tables for MStdE in all 36 simulation scenarios are provided in the supporting information.

Fig. 9 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, though when $n = 50$ or $n = 100$, GRTS-Design coverage is usually a few percentage points lower than the other combinations. Coverage in the normal response scenarios was usually near 95%, while coverage in the lognormal response scenarios usually varied from 90% to 95% but increased with the sample size. At a sample size of 200, all four sampling-analysis combinations had approximately 95% interval

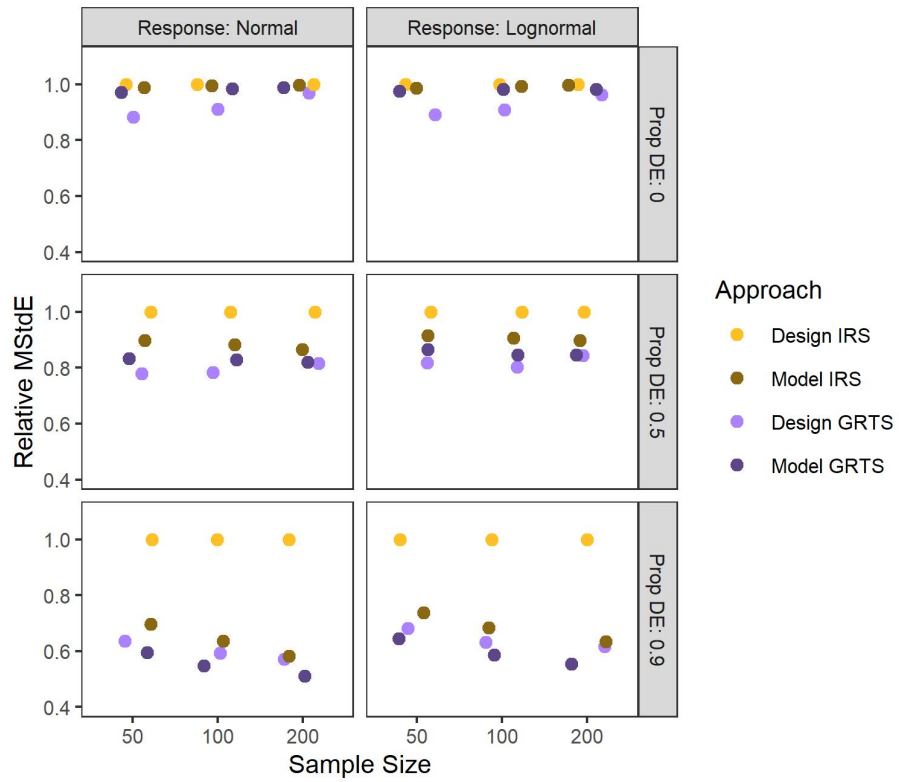


Figure 3: Relative MStdE in the simulation study for the four sampling-analysis combinations. The rows indicate the proportion of dependent error and the columns indicate the response type.

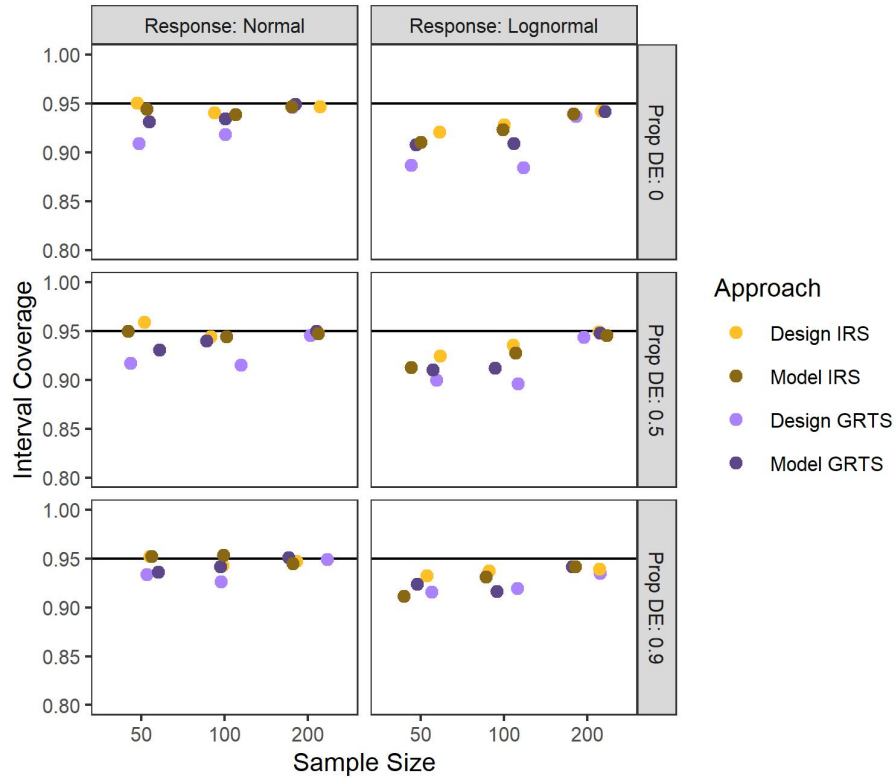


Figure 4: Interval coverage in the simulation study for the four sampling-analysis combinations. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid, black line represents 95% coverage.

coverage in both response scenarios for all dependent error proportions. These interval coverage conclusions are similar to those observed in the grid location layout, so we omit a grid location layout figure here. Tables for interval coverage in all 36 simulation scenarios are provided in the supporting information.

3.2. Application

Fig. 6 shows a map and histogram of mercury concentration in all 986 NLA lakes. The map shows mercury concentration exhibits some spatial patterning, with high mercury concentrations in the northeast and north central United States. The histogram shows that mercury concentration is right-skewed, with

most lakes having a low value of mercury concentration but a few having a much higher concentration. Fig. 6 also shows mercury concentration's empirical semivariogram. The empirical semivariogram can be used as a tool to visualize spatial dependence. It quantifies the mean of the halved squared differences (semivariance) among all pairs of mercury concentrations at different distances apart. When a process has spatial covariance (exhibits spatial dependence), the mean semivariance tends to be smaller at small distances and larger at large distances. The empirical semivariogram in Fig. 6 suggests that mercury concentration exhibits spatial dependence. Lastly we note that the true mean mercury concentration in the 986 NLA lakes is 103.2 ng / g.

We selected a single IRS sample and a single GRTS sample and estimated (design-based) or predicted (model-based) the mean mercury concentration and constructed 95% confidence (design-based) and 95% (model-based) prediction intervals. For the model-based analyses, the exponential covariance was used. Table 3 shows the results from these analyses. Though we should not generalize these results to other samples from this population, we do mention a few findings. First, IRS-Design has the largest standard error. Second, compared to IRS-Design and IRS-Model, GRTS-Design and GRTS-Model are much closer to the true mean mercury concentration (have bias closer to zero) and have much lower standard errors (more precise intervals). Third, GRTS-Model has the least amount of bias and the lowest standard error (most precise interval). Finally, we note that for all sampling-analysis combinations, the true mean mercury concentration (103.2 ng / g) is within the bounds of the combination's 95% interval.

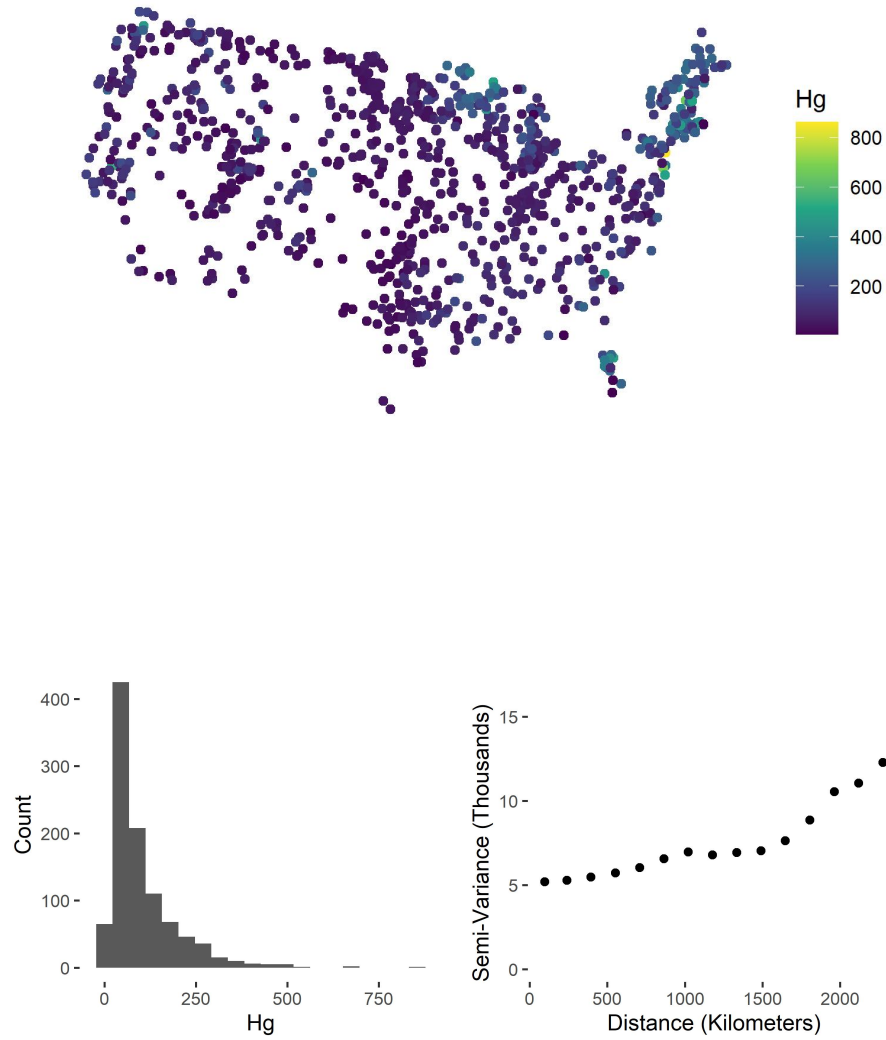


Figure 5: Mercury concentration (Hg) visualizations for all 986 lakes in the NLA data. A spatial layout is in the top row, a histogram is in the bottom row and left column, and an empirical semivariogram is in the bottom row and right column.

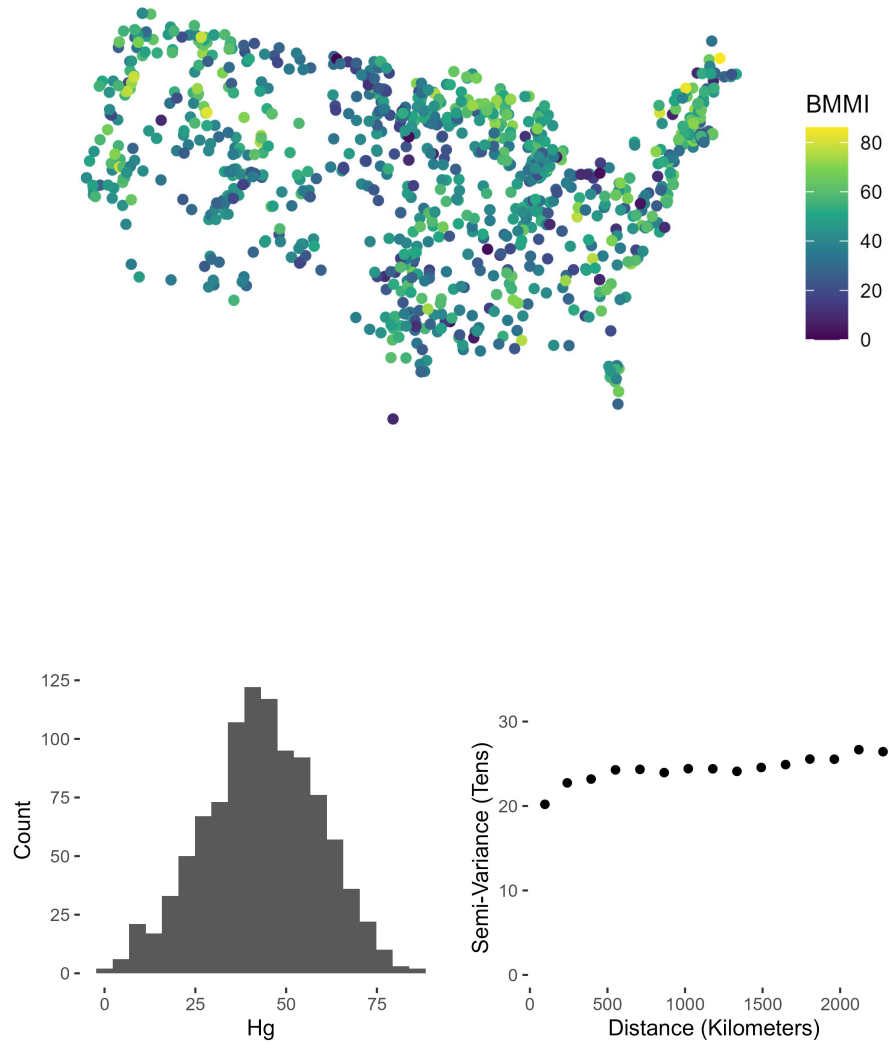


Figure 6: BMMI visualizations for all 986 lakes in the NLA data. A spatial layout is in the top row, a histogram is in the bottom row and left column, and an empirical semivariogram is in the bottom row and right column.

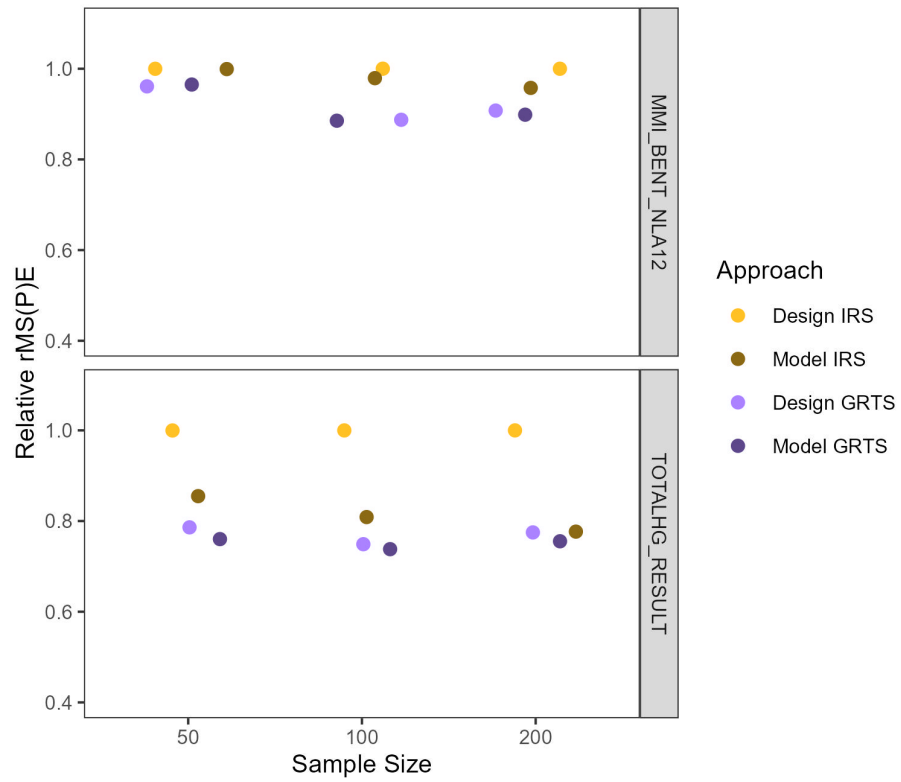


Figure 7: Relative RMS(P)E in the data study for the four sampling-analysis combinations. The rows indicate the proportion of dependent error and the columns indicate the response type.

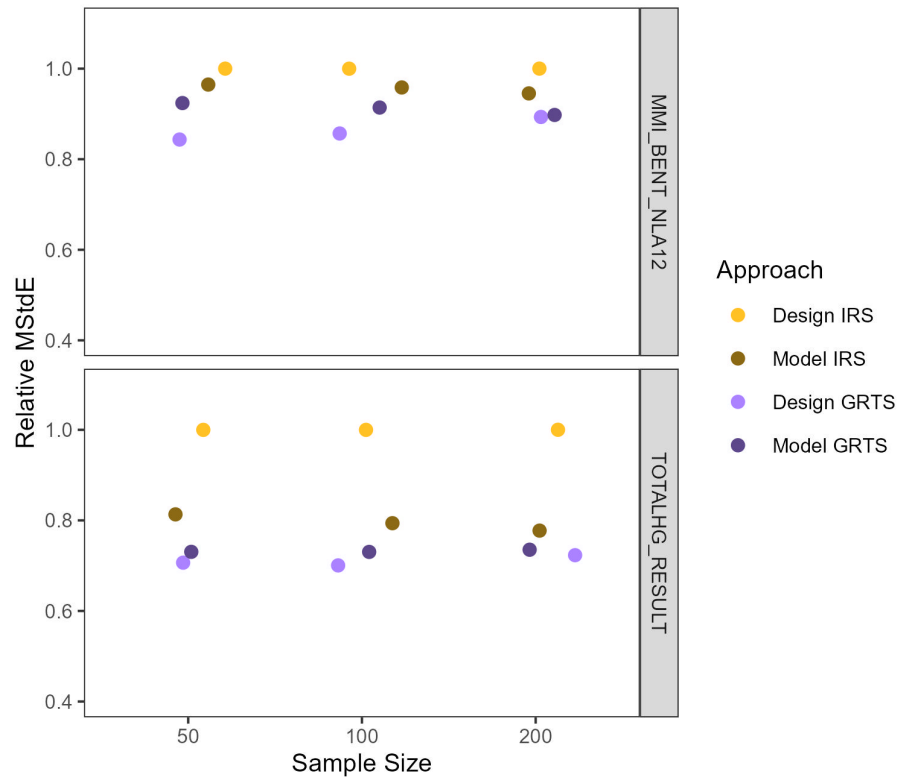


Figure 8: Relative MStdE in the data study for the four sampling-analysis combinations. The rows indicate the proportion of dependent error and the columns indicate the response type.

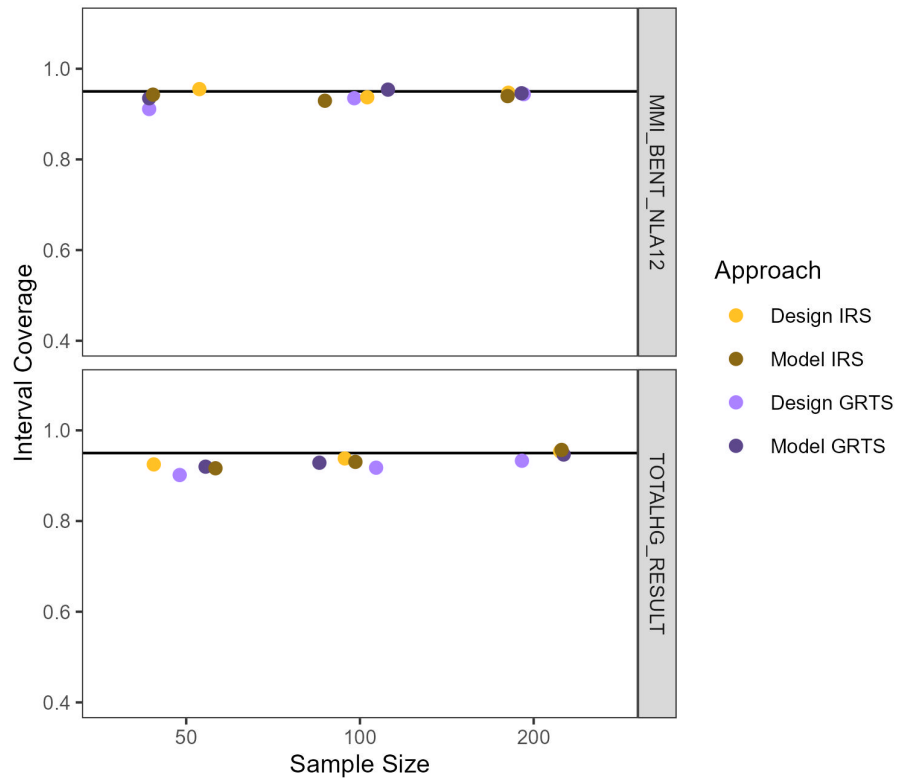


Figure 9: Interval coverage in the data study for the four sampling-analysis combinations. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid, black line represents 95% coverage.

Approach	True Mean	Est/Pred	SE	95% LB	95% UB
IRS-Design	103.2	112.7	8.8	95.4	129.9
IRS-Model	103.2	110.5	7.9	95.0	125.9
GRTS-Design	103.2	101.8	6.1	89.8	113.7
GRTS-Model	103.2	102.3	5.9	90.8	113.9

Table 3: For each sampling-analysis combination (Approach), the true mean mercury concentration (True Mean), estimates/predictions (Est/Pred), standard errors (SE), lower 95% interval bounds (95% LB), and upper 95% interval bounds (95% UB) for mean mercury concentration computed using a sample of 100 lakes in the NLA data.

3.3. New Application

4. Discussion

The design-based and model-based approaches to statistical inference are fundamentally different paradigms. The design-based approach relies on random sampling to estimate population parameters. The model-based approach relies on distributional assumptions to predict realized values of a stochastic process. Though the model-based approach does not rely on random sampling, it can still be beneficial as a way to guard against preferential sampling. While the design-based and model-based approaches have often been compared in the literature from theoretical and analytical perspectives, our contribution lies in studying them in a spatial context while implementing spatially balanced sampling and the design-based, local neighborhood variance estimator. Aside from the theoretical differences described, a few analytical findings from the simulation study are particularly notable. First, independent of the analysis approach, we found no reason to prefer IRS over GRTS when sampling spatial data – GRTS-Design and GRTS-Model generally had similar rMS(P)E as their IRS counterparts when there was no spatial covariance and lower rMS(P)E than their IRS counterparts when there was spatial covariance. Second, the sampling decision (IRS vs GRTS) is most important when using a design-based analysis. Though GRTS-Model still had lower rMS(P)E than IRS-Model, the model-based analysis mitigated most of the rMS(P)E inefficiencies that result from the IRS samples lacking

spatial balance. Third, as the strength of spatial covariance increases, the gap in rMS(P)E and MStdE between IRS-Design and the other sampling-analysis combinations also increases, likely because IRS-Design is the only combination that ignores spatial locations in sampling and analysis. Fourth and finally, when the response was normal, interval coverage for all sampling-analysis combinations was usually close to 95% for all sample sizes; when the response was lognormal, interval coverage for all sampling-analysis combinations was usually between 90% and 95% and closest to 95% when $n = 200$.

There are several benefits and drawbacks of the design-based and model-based approaches for finite population spatial data. Some we have discussed, but others we have not, and they are worthy of consideration in future research. Design-based approaches are often computationally efficient, while model-based approaches can be computationally burdensome, especially for likelihood-based estimation methods like REML that rely on inverting a covariance matrix. The design-based approach also more naturally handles binary data, free from the more complicated logistic regression framework commonly used to analyze binary data in a model-based approach. The model-based approach, however, can more naturally quantify the relationship between covariates (predictor variables) and the response variable. The model-based approach also yields estimated spatial covariance parameters, which help better understand the dependence structure in the stochastic process of study. Model selection is also possible using model-based approaches and criteria such as cross validation, likelihood ratio tests, or AIC (Akaike, 1974). Model-based approaches are capable of more efficient small-area estimation than design-based approaches by leveraging distributional assumptions in areas with few observed units. Model-based approaches can also compute unit-by-unit predictions at unobserved locations and use them to construct informative visualizations like smoothed maps. In short, when

452 deciding whether the design-based or model-based approach is more appropriate
453 to implement, the benefits and drawbacks of each approach should be considered
454 alongside the particular goals of the study.

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464 **Conflict of Interest Statement**

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

466 **Author Contribution Statement**

467 All authors conceived the ideas; All authors designed the methodology; MD
468 and MH performed the simulations and analyzed the data; MD and MH led the
469 writing of the manuscript; All authors contributed critically to the drafts and
470 gave final approval for publication.

471 **Data and Code Availability**

472 This manuscript has a supplementary **R** package that contains all of the
473 data and code used in its creation. The supplementary **R** package is hosted on
474 GitHub. Instructions for download at available at

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

If the manuscript is accepted, this repository will be archived in Zenodo.

Supporting Information

In the supporting information, we provide tables of summary statistics for all 36 simulation scenarios.

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