

sampling (SRS) algorithm, which does not explicitly incorporate spatial locations into sampling. We also found that model-based inference tends to outperform design-based inference, even for skewed data where the model-based distributional assumptions are violated. The performance gap between design-based inference and model-based inference is small when GRTS samples are used but large when SRS samples are used, suggesting that the sampling choice (whether to use GRTS or SRS) 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 sampling and inference 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 (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

55 units to be in the sample (random sampling). Alternatively, in the model-based
 56 approach, inference relies on distributional assumptions about the underlying
 57 data-generating stochastic process (superpopulation). Each paradigm has a deep
 58 historical context (Sterba, 2009) and its own set of benefits and drawbacks (Brus
 59 and De Gruijter, 1997; Hansen et al., 1983). In this manuscript, we compare
 60 design-based and model-based approaches for finite population spatial sampling
 61 and inference.

62 Spatial data are data that have some sort of spatial index (usually specified
 63 via coordinates). De Gruijter and Ter Braak (1990) and Brus and DeGruijter
 64 (1993) give early comparisons of design-based and model-based approaches for
 65 spatial data, quashing the belief that design-based approaches could not be
 66 used for spatially correlated data. Since then, there have been several general
 67 comparisons between design-based and model-based approaches for spatial data
 68 (Brus and De Gruijter, 1997; Brus, 2021; Ver Hoef, 2002, 2008). Cooper (2006)
 69 reviews the two approaches in an ecological context before introducing a “model-
 70 assisted” variance estimator that combines aspects from each approach. In
 71 addition to Cooper (2006), there has been substantial research and development
 72 into estimators that use both design-based and model-based principles (see e.g.,
 73 Sterba (2009) and Cicchitelli and Montanari (2012), and for Bayesian approaches,
 74 see Chan-Golston et al. (2020) and Hofman and Brus (2021)).

75 While comparisons between design-based and model-based approaches have
 76 been studied in spatial contexts, our contribution is comparing design-based
 77 approaches specifically built for spatial data to model-based approaches. Though
 78 the broad comparisons we draw between design-based and model-based ap-
 79 proaches generalize to finite and infinite populations, we focus on finite popu-
 80 lations. A finite population contains a finite number of population units (we
 81 assume the finite number is known) – an example is lakes (treated as a whole

82 with the lake centroid representing location) in the conterminous United States.
83 An infinite population contains an infinite number of population units – an
84 example is locations within a single lake.

85 The rest of the manuscript is organized as follows. In Section 1.1, we introduce
86 and provide relevant background for design-based and model-based approaches
87 to finite population spatial sampling and inference. In Section 2, we describe
88 how we intend to compare performance of the approaches using simulated and
89 real data. The real data is from the United States Environmental Protection
90 Agency’s 2012 National Lakes Assessment (NLA) (USEPA, 2012). In Section 3,
91 we present analysis results for the simulated data and NLA data. And in Section
92 4, we end with a discussion and provide directions for future research.

93 *1.1. Background*

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

98 *1.1.1. Comparing Design-Based and Model-Based Approaches*

99 The design-based approach assumes the population is fixed. Randomness is
100 incorporated via the selection of population units according to a sampling design.
101 A sampling design assigns a probability of selection to each sample (subset of
102 population units). Some examples of commonly used sampling designs include
103 simple random sampling, stratified random sampling, and cluster sampling.
104 The inclusion probability of a population unit is calculated by summing each
105 sample’s probability of selection over all samples that contain the population unit.
106 Inclusion probabilities are often used when selecting samples and estimating
107 population parameters.

108 When samples are chosen in a manner such that the layout of sampled units
 109 reflects the layout of the population units, we call the resulting sample spatially
 110 balanced. By “reflecting the layout of the population units”, we mean that if
 111 population units are concentrated in specific areas, the units in the sample should
 112 be concentrated in the same areas. Because spatially balanced samples reflect
 113 the layout of the population units, they are not necessarily spread out in space
 114 in some equidistant manner. One method of selecting spatially balanced samples
 115 is the generalized random tessellation stratified (GRTS) algorithm (Stevens and
 116 Olsen, 2004), which we discuss in more detail in Section 1.1.2. To quantify the
 117 spatial balance of a sample, Stevens and Olsen (2004) proposed loss metrics
 118 based on Voronoi polygons (i.e., Dirichlet Tessellations).

119 Fundamentally, the design-based approach combines the randomness of the
 120 sampling design with the data collected via the sample to justify the estimation
 121 and uncertainty quantification of fixed, unknown parameters of a population (e.g.,
 122 a population mean). Treating the data as fixed and incorporating randomness
 123 through the sampling design yields estimators having very few other assumptions.
 124 Confidence intervals for these types of estimators are typically derived using
 125 limiting arguments that incorporate all possible samples. Sample means, for
 126 example, are asymptotically normal (Gaussian) by the central limit theorem
 127 (under some assumptions). If we repeatedly select samples from the population,
 128 then 95% of all 95% confidence intervals constructed from a procedure with
 129 appropriate coverage will contain the true fixed population mean. Särndal et al.
 130 (2003) and Lohr (2009) provide thorough reviews of the design-based approach.

131 The model-based approach assumes the population is a random realization of a
 132 data-generating stochastic process. Randomness is formally incorporated through
 133 distributional assumptions on this process. Strictly speaking, randomness need
 134 not be incorporated through random sampling, though Diggle et al. (2010)

135 warn against preferential sampling. Preferential sampling occurs when the
 136 process generating the data locations and the process being modeled are not
 137 independent of one another. To guard against preferential sampling, model-
 138 based approaches can implement some form of random sampling. It is common,
 139 however, for model-based approaches to sample non-randomly. When model-
 140 based approaches do implement random sampling, the inclusion probabilities are
 141 ignored when analyzing the sample (in contrast to the design-based approach,
 142 which relies on these inclusion probabilities to analyze the sample).

143 Instead of estimating fixed, unknown population parameters, as in the design-
 144 based approach, often the goal of model-based inference is to predict the value
 145 of a realized variable. For example, suppose the realized mean of all population
 146 units (the realized population mean) is the variable of interest. Instead of a fixed,
 147 unknown mean, we are predicting the value of the mean, a random variable.
 148 Prediction intervals are then derived using assumptions of the data-generating
 149 stochastic process. If we repeatedly generate realizations from the same process
 150 and select samples, then 95% of all 95% prediction intervals constructed from a
 151 procedure with appropriate coverage will contain their respective realized means.
 152 Cressie (1993) and Schabenberger and Gotway (2017) provide thorough reviews
 153 of model-based approaches for spatial data. In Fig. 1, we provide a visual
 154 comparison of the design-based and model-based approaches (Ver Hoef (2002)
 155 and Brus (2021) provide similar figures). Fig. 1 contrasts the design-based
 156 approach with a fixed population and random sampling to the model-based
 157 approach with random populations and non-random sampling.

158 *1.1.2. Spatially Balanced Design and Analysis*

159 We previously mentioned that the design-based approach can be used to select
 160 spatially balanced samples. Spatially balanced samples are useful because pa-
 161 rameter estimates from these samples tend to vary less than parameter estimates

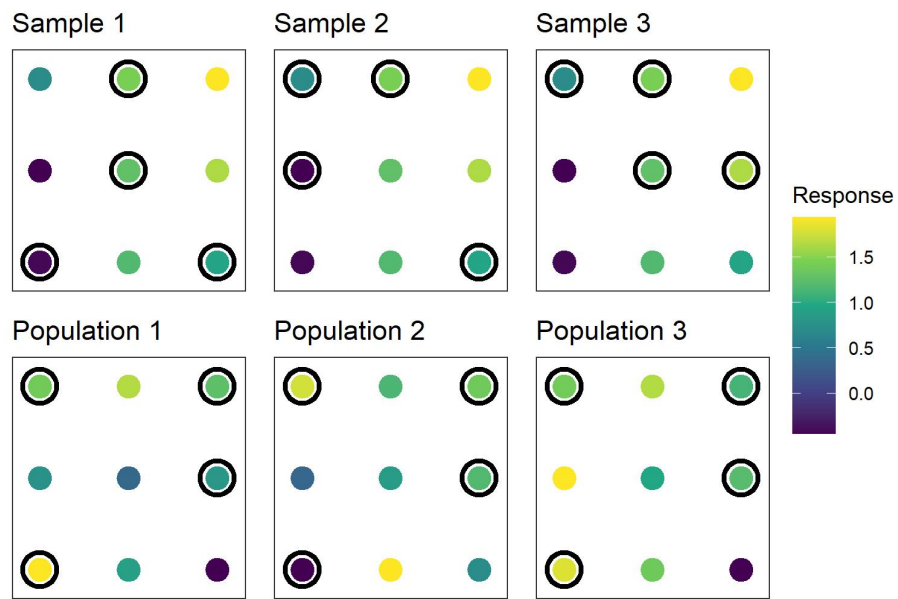
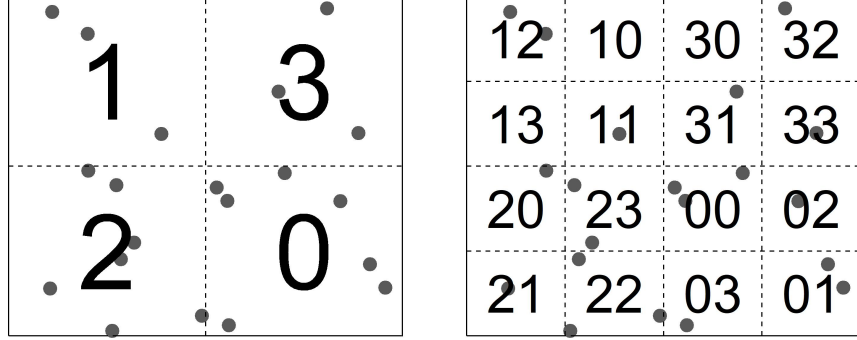


Figure 1: A visual comparison of the design-based and model-based approaches. In the top row, the design-based approach is highlighted. There is one fixed population with nine population units and three random samples of size four (points circled are those sampled). The response values at each site are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

from samples lacking spatial balance (Barabesi and Franceschi, 2011; Benedetti et al., 2017; Grafström and Lundström, 2013; Robertson et al., 2013; Stevens and Olsen, 2004; Wang et al., 2013). The first spatially balanced sampling algorithm to see widespread use was the generalized random tessellation stratified (GRTS) algorithm (Stevens and Olsen, 2004). After the GRTS algorithm was developed, several other spatially balanced sampling algorithms emerged, including stratified sampling with compact geographical strata (Walvoort et al., 2010), the local pivotal method (Grafström et al., 2012; Grafström and Matei, 2018), spatially correlated Poisson sampling (Grafström, 2012), balanced acceptance sampling (Robertson et al., 2013), within-sample-distance sampling (Benedetti and Piersimoni, 2017), and Halton iterative partitioning sampling (Robertson et al., 2018). In this manuscript, we select spatially balanced samples using the GRTS algorithm because it is readily available in the **spsurvey** **R** package (Dumelle et al., 2022) and naturally accommodates finite and infinite sampling frames, unequal inclusion probabilities, and replacement units. Replacement units are additional population units that can be sampled when a population unit originally selected can no longer be sampled. A couple of reasons why an originally selected site can no longer be sampled include its location being physically inaccessible or it is on private land that the researcher does not have permission to access.

The GRTS algorithm selects samples by utilizing a particular mapping between two-dimensional and one-dimensional space that preserves proximity relationships. First, the bounding box of the domain is split up into four distinct, equally sized squares called level-one cells. Each level-one cell is randomly assigned a level-one address of 0, 1, 2, or 3. The set of level-one cells is denoted by \mathcal{A}_1 and defined as $\mathcal{A}_1 \equiv \{a_1 : a_1 = 0, 1, 2, 3\}$. Within each level-one cell, the inclusion probability for each population unit (which is



(a) Assignment of level-one cells to the spatial domain. Grey circles indicate population units. (b) Assignment of level-two cells to the spatial domain. Grey circles indicate population units.

Figure 2: Assignment of level-one and level-two cells to the spatial domain. In (a), each level-one cell is randomly given a level-one address of 0, 1, 2, or 3. In (b), each level-two cell within each level-one cell is randomly given a level-two address of 0, 1, 2, or 3.

pre-specified) is summed, and if any of these sums exceed one, a second level of cells is added. Then each level-one cell is split into four distinct, equally sized squares called level-two cells. Each level-two cell is randomly assigned a level-two address of 0, 1, 2, or 3. The set of level-two cells is denoted by \mathcal{A}_2 and defined as $\mathcal{A}_2 \equiv \{a_1 a_2 : a_1 = 0, 1, 2, 3; a_2 = 0, 1, 2, 3\}$. The inclusion probabilities within each level-two cell are summed, and if any of these sums exceed one, a third level of cells is added. This process continues for k steps, until all level- k cells have inclusion probability sums no larger than one. Then $\mathcal{A}_k \equiv \{a_1 \dots a_k : a_1 = 0, 1, 2, 3; \dots; a_k = 0, 1, 2, 3\}$. Figure 2 provides some intuition regarding the assignment of level-one and level-two cells.

After determining \mathcal{A}_k , the set is placed into hierarchical order. Hierarchical order is a numeric order that first sorts \mathcal{A}_k by the level-one addresses from smallest to largest, then sorts \mathcal{A}_k by the level-two addresses from smallest to largest, and so on. For example, \mathcal{A}_2 in hierarchical order is the set $\{00, 01, 02, 03, 10, \dots, 13, 20, \dots, 23, 30, \dots, 33\}$. Because hierarchical ordering sorts by level-one cells, then level-two cells, and so on, population units that have

similar hierarchical addresses tend to be nearby one another in space. Next, each population unit is mapped to a one-dimensional line in hierarchical order where each population unit's inclusion probability equals its line-length. If a level- k cell has multiple population units in it, they are randomly placed within the cell's respective line segment. A uniform random variable is then simulated in $[0, 1]$ and a systematic sample is selected on the line, yielding n sample points for a sample size n . Each of these sample points falls on some population unit's line segment, and thus that population unit is selected in the sample. For further details regarding the GRTS algorithm, see Stevens and Olsen (2004).

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

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

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

It is also important to quantify the uncertainty in $\hat{\tau}_{ht}$. The Horvitz-Thompson (Horvitz and Thompson, 1952) and Sen-Yates-Grundy (Sen, 1953; Yates and Grundy, 1953) variance estimators are often used to estimate $\text{Var}(\hat{\tau}_{ht})$, but these estimators have two drawbacks. First, they rely on calculating π_{ij} , the probability that population unit i and population unit j are both in the sample – this quantity can be challenging if not impossible to calculate analytically for GRTS samples. Second, these estimators tend to ignore the spatial locations of the population units. To address these two drawbacks simultaneously, Stevens

and Olsen (2003) proposed the local neighborhood variance estimator. The local neighborhood variance estimator does not rely on π_{ij} and estimates the variance of $\hat{\tau}$ conditional on the random properties of the GRTS sample – the idea being that this conditioning should yield a more precise estimate of $\hat{\tau}$. They show that the contribution from each sampled population unit to the overall variance is dominated by local variation. Thus the local neighborhood variance estimator is a weighted sum of variance estimates from each sampled population unit’s local neighborhood. These local neighborhoods contain the sampled population unit itself and its three nearest neighbors (among all other sampled population units). For more details, see Stevens and Olsen (2003).

1.1.3. Finite Population Block Kriging

Finite population block kriging (FPBK) is a model-based approach that expands the geostatistical Kriging framework to the finite population setting (Ver Hoef, 2008). Instead of developing inference based on a specific sampling design, we assume the data are generated by a spatial stochastic process. We summarize some of the basic principles of FPBK next – see Ver Hoef (2008) for technical details and see Higham, Ver Hoef, Madsen, et al. (2021) for an extension to cases of imperfect detection among population units. Let $\mathbf{z} \equiv \{z(s_1), z(s_2), \dots, z(s_N)\}$ be an $N \times 1$ response vector at locations s_1, s_2, \dots, s_N that can be measured at the N population units. Suppose we want to use a sample to predict some linear function of the response variable, $f(\mathbf{z}) = \mathbf{b}'\mathbf{z}$, where \mathbf{b}' is a $1 \times N$ vector of weights (e.g, the population mean is represented by a weights vector whose elements all equal $1/N$). Denoting 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

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

251 where \mathbf{X}_s and \mathbf{X}_u are the design matrices for the sampled and unsampled
 252 population units, respectively, $\boldsymbol{\beta}$ is the parameter vector of fixed effects, and
 253 $\boldsymbol{\delta} \equiv [\boldsymbol{\delta}_s \ \boldsymbol{\delta}_u]'$, where $\boldsymbol{\delta}_s$ and $\boldsymbol{\delta}_u$ are random errors for the sampled and unsampled
 254 population units, respectively.

FPBK 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 separation vector (e.g., distance) between population units), and isotropic (independent of direction) (Cressie, 1993). Henceforth, it is implied that we have made these same assumptions regarding $\boldsymbol{\delta}$. 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

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

255 where σ_1^2 is the variance parameter that quantifies the spatially dependent (cor-
 256 related) variability, σ_2^2 is the variance parameter the quantifies that spatially
 257 independent (not correlated) variability, ϕ is the distance parameter that mea-
 258 sures the distance-decay rate of the covariance, and $h_{i,j}$ is the Euclidean distance
 259 between population units i and j . In geostatistical literature, σ_1^2 is called the
 260 partial sill, σ_2^2 is called the nugget, and ϕ is called the range. We denote $\boldsymbol{\theta}$ as the

261 vector of covariance parameters that composes $\boldsymbol{\delta}$. In Equation 3, $\boldsymbol{\theta} = \{\sigma_1^2, \sigma_2^2, \phi\}$.

The parameters in Equation 2 can be estimated using a variety of techniques, but we focus on restricted maximum likelihood (REML) (Harville, 1977; Patterson and Thompson, 1971; Wolfinger et al., 1994). REML is preferred over maximum likelihood (ML) because ML estimates can be badly biased for small sample sizes, due to the fact that ML makes no adjustment for the simultaneous estimation of $\boldsymbol{\beta}$ and $\boldsymbol{\theta}$ (Patterson and Thompson, 1971). Minus twice the REML log-likelihood of the sampled sites is given by

$$\ln |\boldsymbol{\Sigma}| + (\mathbf{z}_s - \mathbf{X}_s \tilde{\boldsymbol{\beta}})^T \boldsymbol{\Sigma}_{ss}^{-1} (\mathbf{z}_s - \mathbf{X}_s \tilde{\boldsymbol{\beta}}) + \ln |\mathbf{X}_s^T \boldsymbol{\Sigma}_{ss}^{-1} \mathbf{X}_s| + (n - p) \ln(2\pi), \quad (4)$$

262 where $\tilde{\boldsymbol{\beta}} = (\mathbf{X}_s^T \boldsymbol{\Sigma}_{ss}^{-1} \mathbf{X}_s)^{-1} \mathbf{X}_s^T \boldsymbol{\Sigma}_{ss}^{-1} \mathbf{z}_s$ and $\boldsymbol{\Sigma}_{ss}$ is the covariance matrix of the
 263 sampled sites. Minimizing Equation 4 yields $\hat{\boldsymbol{\theta}}_{reml}$, the REML estimates of
 264 $\boldsymbol{\theta}$. Then $\hat{\boldsymbol{\beta}}_{reml}$, the REML estimate of $\boldsymbol{\beta}$, is given by $(\mathbf{X}_s^T \hat{\boldsymbol{\Sigma}}_{ss}^{-1} \mathbf{X}_s)^{-1} \mathbf{X}_s^T \hat{\boldsymbol{\Sigma}}_{ss}^{-1} \mathbf{z}_s$,
 265 where $\hat{\boldsymbol{\Sigma}}_{ss}$ is $\boldsymbol{\Sigma}_{ss}$ evaluated at $\hat{\boldsymbol{\theta}}_{reml}$.

266 With the model formulation in Equation 2, the best linear unbiased predictor
 267 (BLUP) of $f(\mathbf{b}'\mathbf{z})$ and its prediction variance can be computed. While details
 268 of the derivation are in Ver Hoef (2008), we note here that the predictor and
 269 its variance are both moment-based, meaning that they do not rely on any
 270 distributional assumptions. Distributional assumptions are used, however, when
 271 constructing prediction intervals.

272 Other approaches, such as k-nearest-neighbors (Fix and Hodges, 1989; Ver
 273 Hoef and Temesgen, 2013) and random forest (Breiman, 2001), among others,
 274 could also be used to obtain predictions for a mean or total from finite population
 275 spatial data. Compared to the k-nearest-neighbors and random forest approach,
 276 we prefer FPBK because it is model-based and relies on theoretically-based
 277 variance estimators leveraging the model's spatial covariance structure, whereas
 278 k-nearest-neighbors and random forests use ad-hoc variance estimators (Ver Hoef

279 and Temesgen, 2013). Additionally, Ver Hoef and Temesgen (2013) compared
 280 FPBK, k-nearest-neighbors, and random forest in a variety of spatial data
 281 contexts, and FPBK tended to perform best.

282 2. Materials and Methods

In this section we describe how we used simulated and real data to investigate performance between simple random sampling (SRS) and GRTS sampling as well as performance between design-based (DB) and model-based (MB) inference. In SRS and GRTS sampling, all population units had equal inclusion probabilities and were selected without replacement. The important distinction between SRS and GRTS is that SRS ignores spatial locations while sampling but GRTS explicitly incorporates them. Together, the two sampling plans (SRS and GRTS) combined with the two inference approaches (DB and MB) yielded four sampling-inference combinations: SRS-DB, SRS-MB, GRTS-DB, and GRTS-MB. For SRS-DB, the Horvitz-Thompson estimator (1) was used to estimate means and the commonly-used SRS variance formula (Lohr, 2009; Särndal et al., 2003) was used to estimate variances. This variance formula is given by

$$\frac{f[\sum_{i=1}^n (z_i - \bar{z})^2]}{n(n-1)}, \quad (5)$$

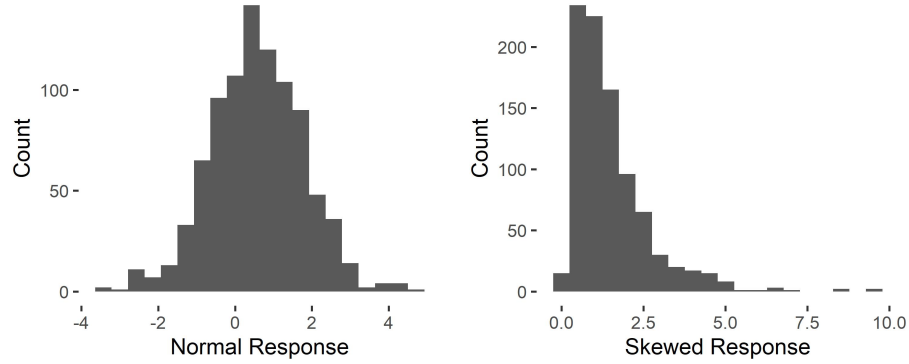
283 where z_i is the response value of the i th sampled population unit, \bar{z} is the mean
 284 of all z_i , n is the sample size, N is the population size, and $f = (1 - n/N)$ (f is
 285 often called the finite population correction factor). For GRTS-DB, the Horvitz-
 286 Thompson estimator was used to estimate means and the local neighborhood
 287 variance was used to estimate variances. For SRS-MB and GRTS-MB, FPBK
 288 was used to estimate means and variances using restricted maximum likelihood.
 289 SRS, GRTS sampling, and design-based inference were implemented using the
 290 `spsurvey` **R** package (Dumelle et al., 2022). FPBK was implemented using the

291 **sptotal** R package (Higham, Ver Hoef, Frank, et al., 2021).

292 The simulated and real data were used for distinct objectives. The simulated
 293 data was used to compare the sampling-inference combinations across many
 294 realized populations (from the same data-generating stochastic process) and
 295 random samples. The real data was used to compare the sampling-inference
 296 combinations within a single realized population but across random samples.
 297 With the simulated data, we were in control of the data-generating stochastic
 298 process and the random sampling process. With the real data, we were only in
 299 control of the random sampling process (which is typically the case in practice).

300 2.1. Simulated Data

301 We evaluated performance of the four sampling-inference combinations in
 302 36 different simulation scenarios. The 36 scenarios resulted from the crossing of
 303 three sample sizes, two location layouts (of the population units), two response
 304 types, and three proportions of dependent random error (DRE). The three sample
 305 sizes (n) were $n = 50$, $n = 100$, and $n = 200$. Samples were always selected from
 306 a population size (N) of $N = 900$. The two location layouts were random and
 307 gridded. Locations in the random layout were randomly generated inside the
 308 unit square $([0, 1] \times [0, 1])$. Locations in the gridded layout were placed on a fixed,
 309 equally spaced grid inside the unit square. The two response types were normal
 310 and skewed. For the normal response type, the response was simulated using
 311 mean-zero random errors with the exponential covariance (Equation 3) for three
 312 proportions of dependent random error (DRE): 0% DRE, 50% DRE, and 90%
 313 DRE. Recall the proportion of DRE is represented by $\sigma_1^2/(\sigma_1^2 + \sigma_2^2)$, where σ_1^2
 314 and σ_2^2 are the DRE variance and independent random error (IRE) variance from
 315 Equation 3, respectively. The total variance, $\sigma_1^2 + \sigma_2^2$, was always 2. The distance
 316 parameter was always $\sqrt{2}/3$, chosen so that the correlation in the DRE decayed
 317 to nearly zero at $\sqrt{2}$, the largest possible distance between two population units



(a) Histogram of a single realized population for the normal response. (b) Histogram of a single realized population for the skewed response.

Figure 3: Histograms of single realized populations simulated for the normal and skewed responses using the random layout and 50% DRE.

in the domain. For the skewed 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 skewed random variable whose total variance was 2. The skewed responses were used to evaluate performance of the sampling-inference approaches for data that were not normal but were still estimated using REML, which relies on a normal log-likelihood. Figure 3 shows an example of a realized population for the normal and skewed responses using the random layout and 50% DRE.

In each of the 36 simulation scenarios, there were 2000 independent simulation trials. Within each trial, a population was simulated according to the specifications of the particular simulation scenario (for the random location layout, locations were simulated separately for each trial). Next, SRS and GRTS samples were selected. Then, design-based and model-based inferences were used to estimate (design-based) or predict (model-based) the realized mean and construct 95% confidence (design-based) or 95% prediction (model-based) intervals. With model-based inference, covariance parameters and the realized mean were estimated (using REML) separately for each trial. After all 2000 trials, we

summarized the long-run performance of the sampling-inference combination in each scenario by calculating mean bias, root-mean-squared error, and interval coverage. Mean bias was taken as the average deviation between each trial's estimated (or predicted) mean ($\hat{\mu}_i$) and its realized mean (μ_i): $\frac{1}{n} \sum_{i=1}^{2000} (\hat{\mu}_i - \mu_i)$, where i indexes the simulation trials. Because each trial had different realized populations, μ_i changed with i . Root-mean-squared error was taken as the square root of the average squared deviation between each trial's estimated (or predicted) mean and its realized mean: $\sqrt{\frac{1}{n} \sum_{i=1}^{2000} (\hat{\mu}_i - \mu_i)^2}$. Interval coverage was taken as the proportion of simulation trials where the realized mean was contained in its 95% confidence (or prediction) interval. These intervals were constructed using the normal distribution – justification comes from the asymptotic normality of means via the central limit theorem (under some assumptions). Quantifying these metrics is important because together, they give us an idea of the accuracy (mean bias), spread (RMSE), and validity (interval coverage) of the sampling-inference combinations.

2.2. National Lakes Assessment Data

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 conterminous United States. One component of NARS is the National Lakes Assessment (NLA), which measures various aspects of lake health and water quality. We focus on analyzing zooplankton multi-metric indices (ZMMI) and mercury concentrations in parts per billion (Hg ppb) from the 2012 NLA. For ZMMI, data were collected at 1035 unique lakes. At less than 10% of lakes, two ZMMI replicates were collected. These were averaged for the purposes of our study so that each lake had one measurement for ZMMI. For Hg ppb, data were collected at 995 unique lakes (there were no replicates). The ZMMI and Hg ppb data are shown as spatial

maps and as histograms in Figure 4. The ZMMI data tend to be highest near the
coasts, lowest in the Central United States, are relatively symmetric, and have a
mean of 55.05. The Hg ppb data tend to be highest in the Northeastern United
States, lowest elsewhere, are skewed, and have a mean of 103.16 ppb. Also in
Figure 4 are separate spatial semivariograms for ZMMI and Hg ppb. The spatial
semivariogram quantifies the halved average squared differences (semivariance)
of responses whose separation (distance) falls within a separation class. The
spatial semivariance is closely related to the spatial covariance, and spatial
semivariograms are often used to gauge the strength of spatial dependence
in data. Both ZMMI and Hg ppb seem to have moderately strong spatial
dependence (Figure 4), as the semivariance increases steadily with distance
(meaning that observations nearby one another tend to be more similar than
observations far apart from one another).

We studied performance of the four sampling-inference combinations by
selecting 2000 SRS and GRTS samples of size $n = 50$, $n = 100$, and $n = 200$
from the realized ZMMI and Hg ppb populations and then analyzing the samples
using MB and DB inference. In total, there were six separate scenarios (two
responses crossed with three sample sizes). Within each SRS and GRTS sample,
design-based and model-based inferences were used to estimate or predict the
population mean and construct 95% coverage intervals. With model-based
inference, the exponential covariance was assumed, and covariance parameters
and the population mean were estimated using REML (separately for each SRS
and GRTS sample). We used the same evaluation metrics as for the simulated
data: mean bias, RMSE, and interval coverage. Mean bias was taken as the
average deviation between each sample's estimated (or predicted) mean ($\hat{\mu}_i$) and
the population mean (μ) (of ZMMI or Hg ppb): $\frac{1}{n} \sum_{i=1}^{2000} (\hat{\mu}_i - \mu)$, where i indexes
the simulation trials. Because each trial had the same realized population, μ did

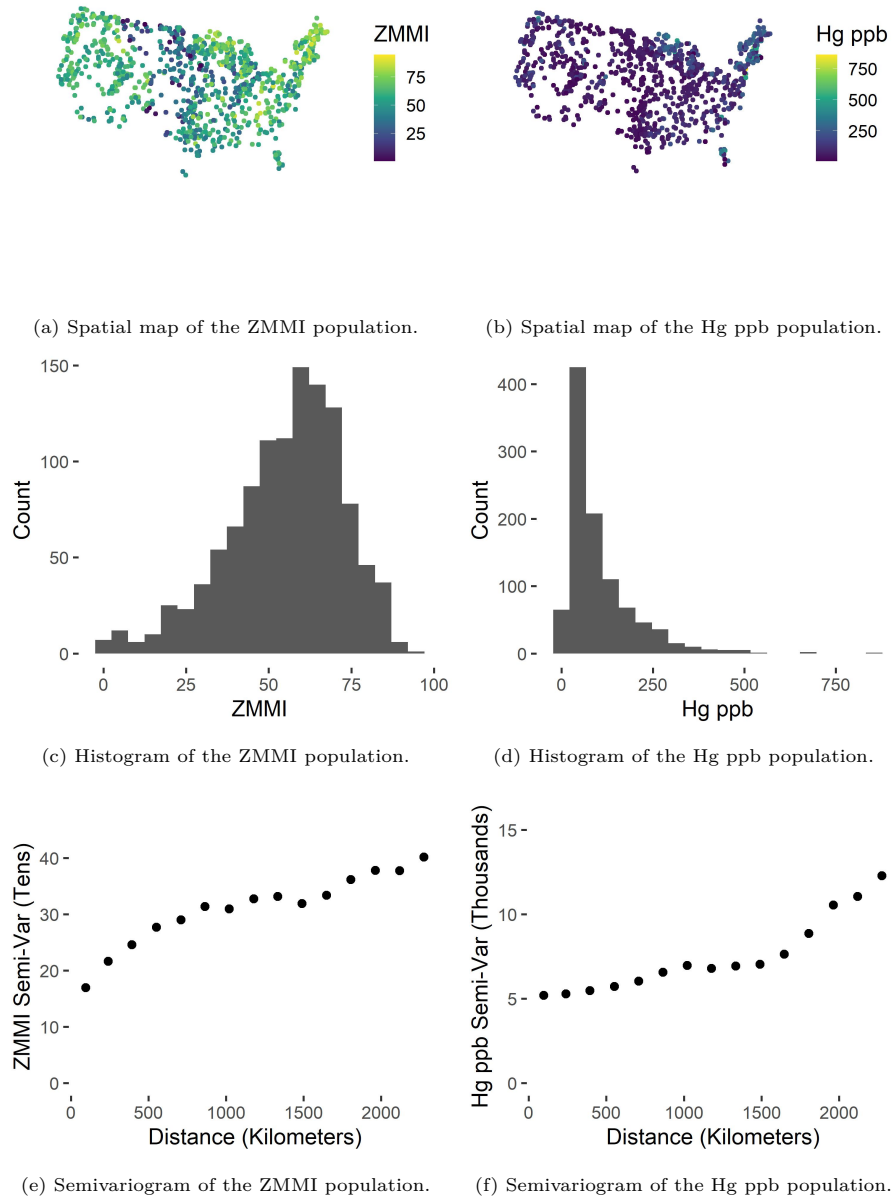


Figure 4: Exploratory graphics representing populations for the zooplankton multi-metric indices (ZMMI) and mercury concentration in parts per billion (Hg ppb) in the 2012 National Lakes Assessment (NLA) data.

not change with i (in contrast to the simulated data, where the realized mean changed with i). Root-mean-squared error was taken as the square root of the average squared deviation between each sample's estimated (or predicted) mean and its population mean: $\sqrt{\frac{1}{n} \sum_{i=1}^{2000} (\hat{\mu}_i - \mu)^2}$. Interval coverage was taken as the proportion of simulation trials where the population mean was contained in its 95% confidence (or prediction) interval. These intervals were constructed using the normal distribution.

3. Results

3.1. Simulated Data

Mean bias is nearly zero for all four sampling-inference 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.

We define the relative RMSE as a ratio with numerator given by the RMSE for a sampling-inference combination and the denominator given by the RMSE for SRS-DB. Relative RMSEs for the random location layout are provided in Fig. 5. When there is no spatial covariance (Fig. 5, "DRE%: 0%"), the four sampling-inference combinations have approximately equal RMSE. In these scenarios, using GRTS sampling or model-based inference does not generally increase efficiency compared to SRS-DB. When there is spatial covariance (Fig. 5, "DRE%: 50%" and "DRE%: 90%"), GRTS-MB tends to have the lowest RMSE, followed by GRTS-DB, SRS-MB, and finally SRS-DB. As the strength of spatial covariance increases, the gap in RMSE between SRS-DB and the other sampling-inference combinations widens. Finally we note that when there is spatial covariance, SRS-MB has a much lower RMSE than SRS-DB, suggesting that the lack of efficiency from SRS is largely mitigated by model-based inference.

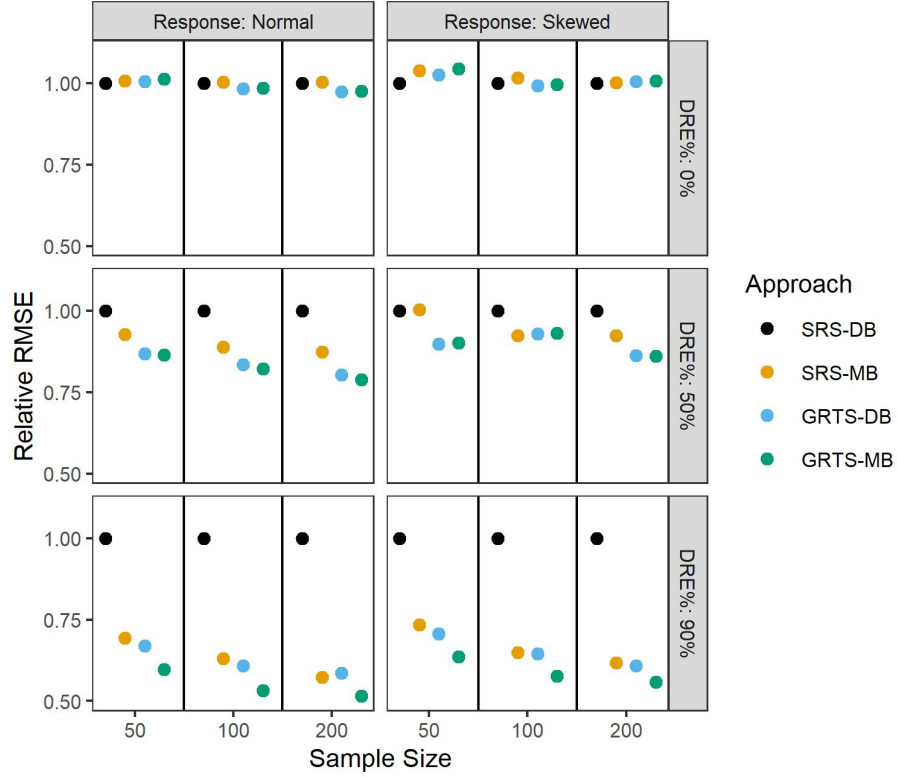


Figure 5: Simulated data relative RMSE for the four sampling-inference combinations and three sample sizes in the random location layout. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid, black lines separate the sample sizes.

415 These RMSE conclusions are similar to those observed in the grid location
 416 layout, so we omit a figure and discussion regarding the grid location layout here.
 417 Tables for RMSE in all 36 simulation scenarios are provided in the supporting
 418 information.

419 95% interval coverage for each of the four sampling-inference combinations
 420 in the random location layout is shown in Fig. 6. Within each simulation
 421 scenario, all sampling-inference combinations tend to have fairly similar interval
 422 coverage, though when $n = 50$ or $n = 100$, GRTS-DB coverage is usually a
 423 few percentage points lower than the other combinations, which suggests that

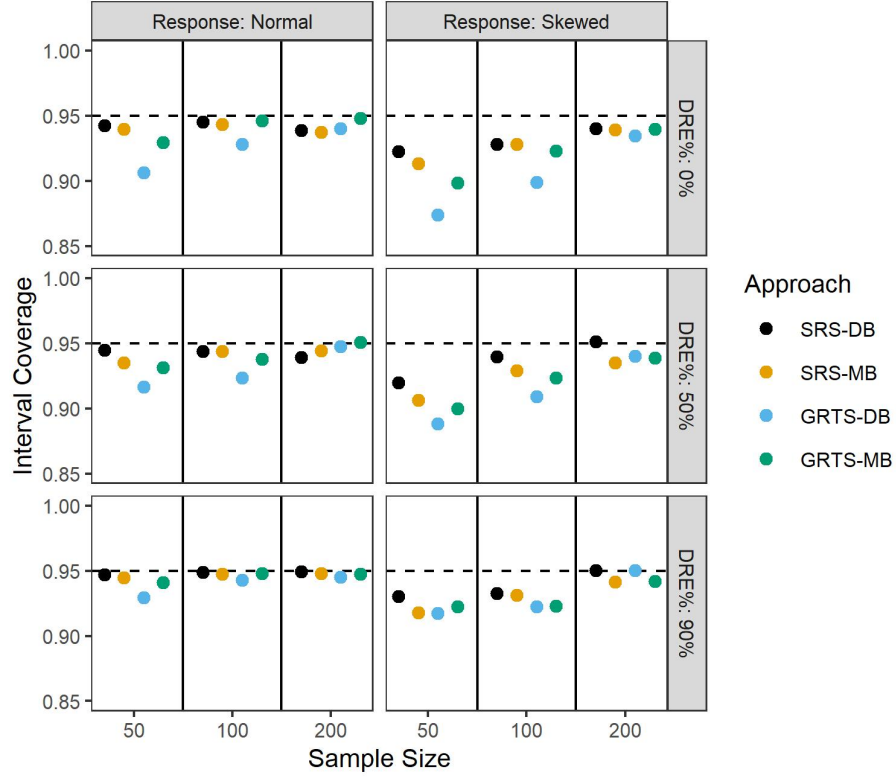


Figure 6: Simulated data interval coverage for the four sampling-inference combinations and three sample sizes in the random location layout. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid black lines separate the sample sizes and the dashed black lines represent 95% coverage.

the local neighborhood variance estimate may be slightly too small for small n . Coverage in the normal response scenarios is usually near 95%, while coverage in the skewed response scenarios usually varies from 90% to 95% but increases with the sample size. At a sample size of 200, all four sampling-inference combinations have approximately 95% interval coverage in both response scenarios for all DRE proportions. These interval coverage conclusions are similar to those observed in the grid location layout, so we omit a figure and discussion regarding the grid location layout here. Tables for interval coverage in all 36 simulation scenarios are provided in the supporting information.

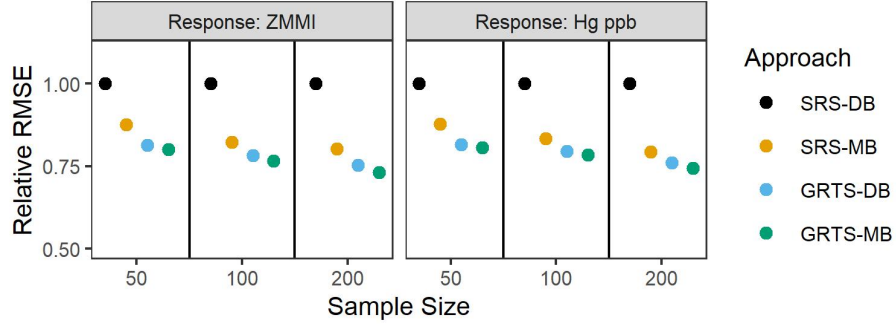


Figure 7: NLA data relative RMSE for the four sampling-inference combinations. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid, black lines separate the sample sizes.

3.2. National Lakes Assessment Data

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

The relative RMSE of both ZMMI (symmetric response) and Hg ppb (skewed response) for all four sampling-inference combinations are shown in Fig. 7. GRTS-MB has the lowest RMSE, followed by GRTS-DB, SRS-MB, and then SRS-DB. The difference in RMSE among GRTS-MB and GRTS-DB tends to be quite small. When $n = 50$, SRS-MB RMSE is approximately evenly between SRS-DB RMSE and GRTS-MB RMSE, but for the larger sample sizes ($n = 100$, $n = 200$), SRS-MB RMSE is closer to GRTS-MB RMSE. Lastly we note that GRTS-MB, GRTS-DB, and SRS-MB all have noticeably lower RMSE than SRS-DB. Tables for RMSE in all six scenarios are provided in the supporting information.

95% interval coverage of both ZMMI and Hg ppb for all four sampling-inference combinations is shown in Fig. 8. When $n = 50$, interval coverage for both responses is too low, though interval coverage is higher for ZMMI (symmetric response) than for Hg ppb (skewed response). When $n = 100$, ZMMI interval

coverage is approximately 95% except for GRTS-DB, which has coverage around 92%, while Hg ppb interval coverage ranges from approximately 90% (GRTS-DB) to 93% (GRTS-MB). When $n = 200$, ZMMI interval coverage is approximately 95% while Hg ppb interval coverage ranges from approximately 93% (GRTS-DB) to 95% (GRTS-MB). As with the simulated data, coverages for the NLA data tend to increase with the sample sizes, coverages tend to be higher for symmetric responses than for skewed responses, and the local neighborhood variance was slightly too small for small n , yielding slightly lower interval coverages than the other sampling-inference combinations. Recall that model-based inference defines interval coverage properties across realized populations. With the simulated data, we evaluated interval coverage across realized populations, but for the NLA data, we evaluated interval coverage within a single realized population. We did find that model-based coverages were similar to the design-based coverages, however, suggesting that for some realized populations it is reasonable to heuristically view data from separate random samples as being from approximately separate realized populations. But generally, if model-based intervals constructed from many random samples of a single realized population show improper coverage, this does not necessarily imply a deficiency in model-based inference. Tables for interval coverage in all six simulation scenarios are provided in the supporting information.

4. Discussion

The design-based and model-based approaches to frequentist statistical inference rest on fundamentally different foundations. Design-based approaches rely on random sampling to estimate population parameters. Model-based approaches rely on distributional assumptions to predict realized values of a data-generating stochastic process. Though model-based approaches do not rely on random

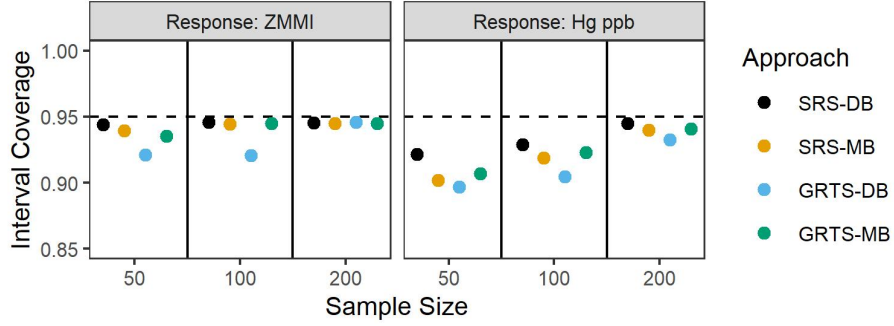


Figure 8: NLA data interval coverage for the four sampling-inference combinations. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid black lines separate the sample sizes and the dashed black lines represent 95% coverage.

477 sampling, random sampling can still be beneficial as a way to guard against pref-
 478 erential sampling. While design-based and model-based approaches have often
 479 been compared in the literature from theoretical and analytical perspectives,
 480 our contribution lies in studying them for finite population spatial data while
 481 implementing GRTS sampling and the local neighborhood variance estimator.
 482 Aside from the theoretical differences described throughout the manuscript, a
 483 few analytical findings from the simulated and real data studies were particularly
 484 notable. All sampling-inference combinations had approximately zero mean bias.
 485 Independent of the inference approach, the GRTS samples yielded lower RMSE
 486 than their SRS counterparts. Though GRTS-DB and GRTS-MB generally had
 487 very similar RMSE, SRS-MB tended to have much lower RMSE than SRS-DB,
 488 suggesting that the model-based inference mitigated much of the inefficiency in
 489 RMSE from SRS. As the proportion of dependent random error in the simulated
 490 data increased, SRS-MB, GRTS-DB, and GRTS-MB become increasingly more
 491 efficient (lower RMSE) than SRS-DB. Interval coverage tended to be higher for
 492 the symmetric responses than skewed responses and tended to increase with the
 493 sample size. At a sample size of $n = 200$, generally all interval coverages were
 494 near the desired value of 95%.

There are several benefits and drawbacks of the design-based and model-based approaches for finite population spatial sampling and inference. Some we have discussed, but others we have not, and they are worthy of consideration in future research. First, we discuss advantages of the design-based approach. Design-based inference is often computationally efficient, while model-based inference can be computationally burdensome, especially for likelihood-based estimation methods like REML that rely on the inverse of a covariance matrix. Design-based inference easily handles binary data through a straightforward application of the Horvitz-Thompson estimator. In contrast, analyzing binary data using model-based inference generally requires a logistic mixed regression model, the parameters of which can be difficult to estimate and interpret (Bolker et al., 2009). An advantage of design-based inference is that interval coverage is valid (has the proper coverage rate) as long as 1) the sample is sufficiently large to ensure the statistic's sampling distribution is approximately normal and 2) the variance estimator is consistent (Brus and De Gruijter, 1997; Särndal et al., 2003). This is because with the design-based approach, the sampling plan and inclusion probabilities are specified directly by the researcher. An advantage of SRS-DB not previously mentioned is that it is likely to be valid given the consistency of its variance estimator (Särndal et al., 2003). With the model-based approach, however, interval coverage is unlikely to be valid if the model assumptions made do not accurately reflect reality. Whether model assumptions accurately reflect reality can be a challenging and sometimes impossible question to answer definitively.

Now, we discuss advantages of the model-based approach. The model-based approach can more naturally quantify the relationship between covariates (predictor variables) and the response variable than design-based approaches. Model-based inference also yields estimated spatial covariance parameters, which

522 help better understand the dependence structure of the process in study. Model
523 selection is also possible using model-based inference and criteria such as cross
524 validation, likelihood ratio tests, or AIC (Akaike, 1974). Model-based inference
525 is capable of more efficient small-area estimation than design-based inference
526 because model-based inference can leverage distributional assumptions in areas
527 with few observed population units. Model-based approaches also accommodate
528 unit-by-unit predictions at unobserved locations that can be used to construct
529 informative visualizations like smoothed maps. Brus and De Gruijter (1997)
530 provide a more thorough discussion regarding the benefits and drawbacks of the
531 two approaches. In short, when deciding whether the design-based or model-
532 based approach is more appropriate to implement, these benefits and drawbacks
533 should be considered alongside the particular goals of the study.

534 There are many extensions of this research worthy of future consideration that
535 include sampling with unequal inclusion probabilities, using different spatially
536 balanced sampling approaches (instead of GRTS), using different spatial data
537 configurations, using different spatial domains like stream networks (Ver Hoef
538 and Peterson, 2010), using different response or covariance structures, and using
539 spatial or external mean trends (which can be defined through covariates).

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552 **Conflict of Interest Statement**

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

554 **Author Contribution Statement**

555 All authors conceived the ideas; All authors designed the methodology; MD
556 and MH performed the simulations and analyzed the data; MD and MH led the
557 writing of the manuscript; All authors contributed critically to the drafts and
558 gave final approval for publication.

559 **Data and Code Availability**

560 This manuscript has a supplementary **R** package that contains all of the
561 data and code used in its creation. The supplementary **R** package is hosted on
562 GitHub. Instructions for download are available at
563 <https://github.com/michaeldumelle/DvMsp>.

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

565 **Supporting Information**

566 In the supporting information, we provide tables of summary statistics for
567 all 36 simulation scenarios and all six real data scenarios.

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