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

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3 Abstract

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- 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 in a finite population spatial context.
- 2. We provide relevant background for the design-based and model-based approaches and then study their performance using simulated data and real data. The real data is from the United States Environmental Protection Agency's 2012 National Lakes Assessment. A variety of sample sizes, location layouts, dependence structures, and response types are considered.

 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 simulated and real data, we found that regardless of the strength of spatial dependence in the data, the generalized random tessellation stratified (GRTS) algorithm, which explicitly incorporates spatial locations into sampling, tends to outperform the simple random

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- 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.

44 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) esti-
- 48 mation; Spatially balanced sampling; Spatial covariance

49 1. Introduction

- When data cannot be collected for all units in a population (population units),
- $_{51}$ 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
- 53 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 (random sampling). Alternatively, in the model-based approach, inference relies on distributional assumptions about the underlying data-generating stochastic process (superpopulation). Each paradigm has a deep 57 historical context (Sterba, 2009) and its own set of benefits and drawbacks (Brus and De Gruijter, 1997; Hansen et al., 1983). In this manuscript, we compare 59 design-based and model-based approaches for finite population spatial sampling and inference. Spatial data are data that have some sort of spatial index (usually specified via coordinates). De Gruijter and Ter Braak (1990) and Brus and DeGruijter (1993) give early comparisons 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). Cooper (2006) 68 reviews the two approaches in an ecological context before introducing a "modelassisted" variance estimator that combines aspects from each approach. In addition to Cooper (2006), there has been substantial research and development 71 into estimators that use both design-based and model-based principles (see e.g., 72 Sterba (2009) and Cicchitelli and Montanari (2012), and for Bayesian approaches, 73 see Chan-Golston et al. (2020) and Hofman and Brus (2021)). While comparisons between design-based and model-based approaches have 75 been studied in spatial contexts, our contribution is comparing design-based approaches specifically built for spatial data to model-based approaches. Though 77 the broad comparisons we draw between design-based and model-based approaches generalize to finite and infinite populations, we focus on finite populations. 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 conterminous United States.
- An infinite population contains an infinite number of population units an
- 84 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 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
- 99 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

- 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

- 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 probability of selection to each sample (subset of
- 102 population units). Some examples of commonly used sampling designs include
- simple random sampling, stratified random sampling, and cluster sampling.
- 104 The inclusion probability of a population unit is calculated by summing each
- sample's probability of selection over all samples that contain the population unit.
- 106 Inclusion probabilities are often used when selecting samples and estimating
- population parameters.

When samples are chosen in a manner such that the layout of sampled units 108 reflects the layout of the population units, we call the resulting sample spatially 109 balanced. By "reflecting the layout of the population units", we mean that if 110 population units are concentrated in specific areas, the units in the sample should 111 be concentrated in the same areas. Because spatially balanced samples reflect 112 the layout of the population units, they are not necessarily spread out in space 113 in some equidistant manner. One method of selecting spatially balanced samples 114 is the generalized random tessellation stratified (GRTS) algorithm (Stevens and 115 Olsen, 2004), which we discuss in more detail in Section 1.1.2. To quantify the spatial balance of a sample, Stevens and Olsen (2004) proposed loss metrics 117 based on Voronoi polygons (i.e., Dirichlet Tessellations). Fundamentally, the design-based approach combines the randomness of the 119 sampling design with the data collected via the sample to justify the estimation and uncertainty quantification of fixed, unknown parameters of a population (e.g., 121 a population mean). Treating the data as fixed and incorporating randomness 122 through the sampling design yields estimators having very few other assumptions. 123 Confidence intervals for these types of estimators are typically derived using 124 limiting arguments that incorporate all possible samples. Sample means, for 125 example, are asymptotically normal (Gaussian) by the central limit theorem 126 (under some assumptions). If we repeatedly select samples from the population, 127 then 95% of all 95% confidence intervals constructed from a procedure with 128 appropriate coverage will contain the true fixed population mean. Särndal et al. (2003) and Lohr (2009) provide thorough reviews of the design-based approach. 130 The model-based approach assumes the population is a random realization of a data-generating stochastic process. Randomness is formally incorporated through 132

distributional assumptions on this process. Strictly speaking, randomness need

not be incorporated through random sampling, though Diggle et al. (2010)

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warn against preferential sampling. Preferential sampling occurs when the 135 process generating the data locations and the process being modeled are not 136 independent of one another. To guard against preferential sampling, model-137 based approaches can implement some form of random sampling. It is common, 138 however, for model-based approaches to sample non-randomly. When model-139 based approaches do implement random sampling, the inclusion probabilities are 140 ignored when analyzing the sample (in contrast to the design-based approach, which relies on these inclusion probabilities to analyze the sample). 142 Instead of estimating fixed, unknown population parameters, as in the designbased approach, often the goal of model-based inference is to predict the value 144 of a realized variable. For example, suppose the realized mean of all population units (the realized population mean) is the variable of interest. Instead of a fixed, 146 unknown mean, we are predicting the value of the mean, a random variable. Prediction intervals are then derived using assumptions of the data-generating 148 stochastic process. If we repeatedly generate realizations from the same process and select samples, then 95% of all 95% prediction intervals constructed from a 150 procedure with appropriate coverage will contain their respective realized means. 151 Cressie (1993) and Schabenberger and Gotway (2017) provide thorough reviews 152 of model-based approaches for spatial data. In Fig. 1, we provide a visual 153 comparison of the design-based and model-based approaches (Ver Hoef (2002) 154 and Brus (2021) provide similar figures). Fig. 1 contrasts the design-based 155

1.1.2. Spatially Balanced Design and Analysis

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

approach with a fixed population and random sampling to the model-based

approach with random populations and non-random sampling.

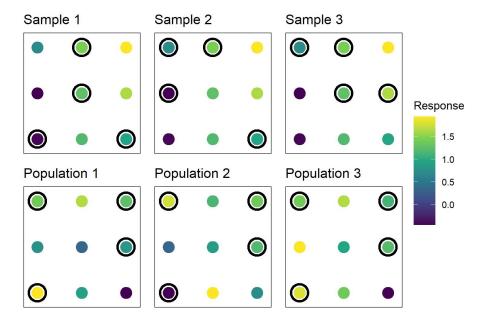


Figure 1: A visual comparison of the design-based and model-based approaches. In the top row, the design-based approach is highlighted. There is one fixed population with nine population units and three random samples of size four (points circled are those sampled). The response values at each site are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

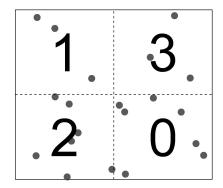
from samples lacking spatial balance (Barabesi and Franceschi, 2011; Benedetti 162 et al., 2017; Grafström and Lundström, 2013; Robertson et al., 2013; Stevens and 163 Olsen, 2004; Wang et al., 2013). The first spatially balanced sampling algorithm 164 to see widespread use was the generalized random tessellation stratified (GRTS) 165 algorithm (Stevens and Olsen, 2004). After the GRTS algorithm was devel-166 oped, several other spatially balanced sampling algorithms emerged, including 167 stratified sampling with compact geographical strata (Walvoort et al., 2010), 168 the local pivotal method (Grafström et al., 2012; Grafström and Matei, 2018), 169 spatially correlated Poisson sampling (Grafström, 2012), balanced acceptance sampling (Robertson et al., 2013), within-sample-distance sampling (Benedetti 171 and Piersimoni, 2017), and Halton iterative partitioning sampling (Robertson et al., 2018). In this manuscript, we select spatially balanced samples using 173 the GRTS algorithm because it is readily available in the spsurvey R package Dumelle et al., 2022) and naturally accommodates finite and infinite sampling 175 frames, unequal inclusion probabilities, and replacement units. Replacement 176 units are additional population units that can be sampled when a population 177 unit originally selected can no longer be sampled. A couple of reasons why 178 an originally selected site can no longer be sampled include its location being 179 physically inaccessible or it is on private land that the researcher does not have 180 permission to access. 183 The GRTS algorithm selects samples by utilizing a particular mapping 182 between two-dimensional and one-dimensional space that preserves proximity 183 relationships. First, the bounding box of the domain is split up into four 184 distinct, equally sized squares called level-one cells. Each level-one cell is 185 randomly assigned a level-one address of 0, 1, 2, or 3. The set of level-one 186

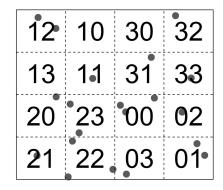
cells is denoted by A_1 and defined as $A_1 \equiv \{a_1 : a_1 = 0, 1, 2, 3\}$. Within

each level-one cell, the inclusion probability for each population unit (which is

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(a) Assignment of level-one cells to the spatial (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 cells 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 190 sized squares called level-two cells. Each level-two cell is randomly assigned 191 a level-two address of 0, 1, 2, or 3. The set of level-two cells is denoted by 192 A_2 and defined as $A_2 \equiv \{a_1a_2 : a_1 = 0, 1, 2, 3; a_2 = 0, 1, 2, 3\}$. The inclusion 193 probabilities within each level-two cell are summed, and if any of these sums 194 exceed one, a third level of cells is added. This process continues for k steps, 195 until all level-k cells have inclusion probability sums no larger than one. Then 196 $A_k \equiv \{a_1...a_k : a_1 = 0, 1, 2, 3; ...; a_k = 0, 1, 2, 3\}$. Figure 2 provides some intuition 197 regarding the assignment of level-one and level-two cells. 198 After determining A_k , the set is placed into hierarchical order. Hierar-199 chical order is a numeric order that first sorts A_k by the level-one addresses 200 from smallest to largest, then sorts A_k by the level-two addresses from small-201 est to largest, and so on. For example, A_2 in hierarchical order is the set 202 $\{00, 01, 02, 03, 10, ..., 13, 20, ..., 23, 30, ..., 33\}$. Because hierarchical ordering sorts 203 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 206 each population unit's inclusion probability equals its line-length. If a level-k207 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 209 [0,1] and a systematic sample is selected on the line, yielding n sample points for 210 a sample size n. Each of these sample points falls on some population unit's line 211 segment, and thus that population unit is selected in the sample. For further 212 details regarding the GRTS algorithm, see Stevens and Olsen (2004). 213

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

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

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

Grundy, 1953) variance estimators are often used to estimate $Var(\hat{\tau}_{ht})$, 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 226 neighborhood variance estimator does not rely on π_{ij} and estimates the variance 227 of $\hat{\tau}$ conditional on the random properties of the GRTS sample – the idea being 228 that this conditioning should yield a more precise estimate of $\hat{\tau}$. They show that 229 the contribution from each sampled population unit to the overall variance is 230 dominated by local variation. Thus the local neighborhood variance estimator 231 is a weighted sum of variance estimates from each sampled population unit's 232 local neighborhood. These local neighborhoods contain the sampled population 233 unit itself and its three nearest neighbors (among all other sampled population 234 units). For more details, see Stevens and Olsen (2003). 235

236 1.1.3. Finite Population Block Kriging

Finite population block kriging (FPBK) is a model-based approach that 237 expands the geostatistical Kriging framework to the finite population setting (Ver Hoef, 2008). Instead of developing inference based on a specific sampling 239 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) 241 for technical details and see Higham, Ver Hoef, Madsen, et al. (2021) for an extension to cases of imperfect detection among population units. Let 243 $\mathbf{z} \equiv \{\mathbf{z}(s_1), \mathbf{z}(s_2), ..., \mathbf{z}(s_N)\}\$ be an $N \times 1$ response vector at locations s_1, s_2, \ldots 244 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, $f(\mathbf{z}) = \mathbf{b}'\mathbf{z}$, 246 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 248 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 250

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

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.

FPBK assumes δ 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 δ . 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 δ (Cressie, 1993) – one example is the exponential covariance function. Cressie (1993) provides a thorough list of spatial covariance functions. The i, jth element of the exponential covariance matrix, $cov(\delta)$, is

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

where σ_1^2 is the variance parameter that quantifies the spatially dependent (correlated) variability, σ_2^2 is the variance parameter the quantifies that spatially independent (not correlated) variability, ϕ is the distance parameter that measures the distance-decay rate of the covariance, and $h_{i,j}$ is the Euclidean distance between population units i and j. In geostatistical literature, σ_1^2 is called the partial sill, σ_2^2 is called the nugget, and ϕ is called the range. We denote θ as the

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 β and θ (Patterson and Thompson, 1971). Minus twice the REML log-likelihood of the sampled sites is given by

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

where $\tilde{\beta} = (X_s^T \Sigma_{ss}^{-1} X_s)^{-1} X_s^T \Sigma_{ss}^{-1} z_s$ and Σ_{ss} is the covariance matrix of the sampled sites. Minimizing Equation 4 yields $\hat{\theta}_{reml}$, the REML estimates of 263 $\boldsymbol{\theta}$. Then $\hat{\boldsymbol{\beta}}_{reml}$, the REML estimate of $\boldsymbol{\beta}$, is given by $(\boldsymbol{X}_s^T \hat{\boldsymbol{\Sigma}}_{ss}^{-1} \boldsymbol{X})^{-1} \boldsymbol{X}_s^T \hat{\boldsymbol{\Sigma}}_{ss}^{-1} \boldsymbol{z}_s$ where $\hat{\Sigma}_{ss}$ is Σ_{ss} evaluated at $\hat{\theta}_{reml}$. 265 With the model formulation in Equation 2, the best linear unbiased predictor (BLUP) of $f(\mathbf{b}'\mathbf{z})$ and its prediction variance can be computed. While details 267 of the derivation are in Ver Hoef (2008), we note here that the predictor and 268 its variance are both moment-based, meaning that they do not rely on any distributional assumptions. Distributional assumptions are used, however, when 270 constructing prediction intervals. Other approaches, such as k-nearest-neighbors (Fix and Hodges, 1989; Ver 272 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 274 spatial data. Compared to the k-nearest-neighbors and random forest approach, 275 we prefer FPBK because it is model-based and relies on theoretically-based 276

variance estimators leveraging the model's spatial covariance structure, whereas

k-nearest-neighbors and random forests use ad-hoc variance estimators (Ver Hoef

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and Temesgen, 2013). Additionally, Ver Hoef and Temesgen (2013) compared FPBK, k-nearest-neighbors, and random forest in a variety of spatial data 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

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

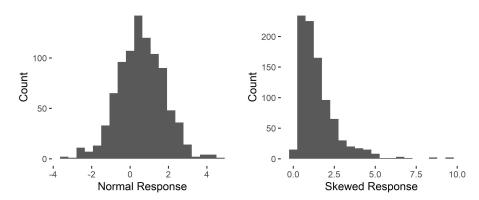
where z_i is the response value of the *i*th sampled population unit, \bar{z} is the mean of all z_i , n is the sample size, N is the population size, and f = (1 - n/N) (f is often called the finite population correction factor). For GRTS-DB, the Horvitz-Thompson estimator was used to estimate means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

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

The simulated and real data were used in distinct ways to answer distinct 292 questions. We used the simulated data to compare the sampling-inference 293 combinations across many realized populations (from the same data-generating 294 stochastic process) and random samples. We used the real data to compare 295 the sampling-inference combinations within a single realized population but 296 across random samples. With the simulated data, we were in control of the data-generating stochastic process and the random sampling process. With the 298 real data, we were only in control of the random sampling process, which is typically the case in reality. 300

301 2.1. Simulated Data

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 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, 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 31 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



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

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

to nearly zero at $\sqrt{2}$, the largest possible distance between two population units 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 335 summarized the long-run performance of the sampling-inference combination in 336 each scenario by calculating mean bias, root-mean-squared error, and interval 337 coverage. Mean bias was taken as the average deviation between each trial's 338 estimated (or predicted) mean $(\hat{\mu}_i)$ and its realized mean (μ_i) : $\frac{1}{n} \sum_{i=1}^{2000} (\hat{\mu}_i - \mu_i)$, 339 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 342 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 344 contained in its 95% confidence (or prediction) interval. These intervals were constructed using the normal distribution – justification comes from the asymp-346 totic normality of means via the central limit theorem (under some assumptions). Quantifying these metrics is important because together, they give us an idea of 348 the accuracy (mean bias), spread (RMSE), and validity (interval coverage) of the sampling-inference combinations.

351 2.2. National Lakes Assessment Data

The United States Environmental Protection Agency (USEPA), states, and 352 tribes periodically conduct National Aquatic Research Surveys (NARS) to assess the water quality of various bodies of water in the conterminous United States. 354 One component of NARS is the National Lakes Assessment (NLA), which measures various aspects of lake health and water quality. We focus on analyzing 356 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 358 unique lakes. At less than 10% of lakes, two ZMMI replicates were collected. 359 These were averaged for the purposes of our study so that each lake had one 360 measurement for ZMMI. For Hg ppb, data were collected at 995 unique lakes 361

(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 363 coasts, lowest in the Central United States, are relatively symmetric, and have a 364 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 366 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 369 spatial semivariance is closely related to the spatial covariance, and spatial semivariograms are often used to gauge the strength of spatial dependence 371 in data. Both ZMMI and Hg ppb seem to have moderately strong spatial 372 dependence (Figure 4), as the semivariance increases steadily with distance 373 (meaning that observations nearby one another tend to be more similar than observations far apart from one another). 375

We studied performance of the four sampling-inference combinations by 376 selecting 2000 SRS and GRTS samples of size n = 50, n = 100, and n = 200377 from the realized ZMMI and Hg ppb populations and then analyzing the samples 378 using MB and DB inference. In total, there were six separate scenarios (two 379 responses crossed with three sample sizes). Within each SRS and GRTS sample, 380 design-based and model-based inferences were used to estimate or predict the 38: population mean and construct 95% coverage intervals. With model-based 382 inference, the exponential covariance was assumed, and covariance parameters and the population mean were estimated using REML (separately for each SRS 384 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 388

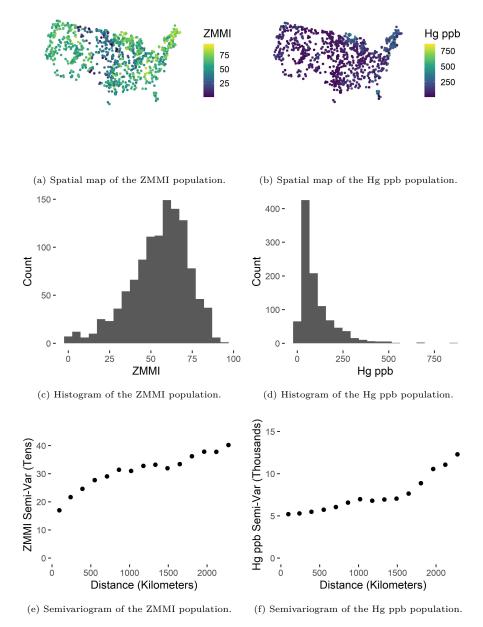


Figure 4: Exploratory graphics representing populations for the zooplankton multi-metric indices (ZMMI) and mercury concentration in parts per billion (Hg ppb) in the 2012 National Lakes Assessment (NLA) data.

the simulation trials. Because each trial had the same realized population, μ did 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.

Mean bias is nearly zero for all four sampling-inference combinations in all

397 3. Results

399

398 3.1. Simulated Data

36 scenarios, so we omit a more detailed summary of those results here. Tables 400 for mean bias in all 36 simulation scenarios are provided in the supporting 401 information. 402 We define the relative RMSE as a ratio with numerator given by the RMSE 403 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 405 Fig. 5. When there is no spatial covariance (Fig. 5, "DRE%: 0%"), the four 406 sampling-inference combinations have approximately equal RMSE. In these 407 scenarios, using GRTS sampling or model-based inference does not generally 408 increase efficiency compared to SRS-DB. When there is spatial covariance (Fig. 409 5, "DRE%: 50%" and "DRE%: 90%"), GRTS-MB tends to have the lowest 410 RMSE, followed by GRTS-DB, SRS-MB, and finally SRS-DB. As the strength 411 of spatial covariance increases, the gap in RMSE between SRS-DB and the other 412 sampling-inference combinations widens. Finally we note that when there is spatial covariance, SRS-MB has a much lower RMSE than SRS-DB, suggesting 414

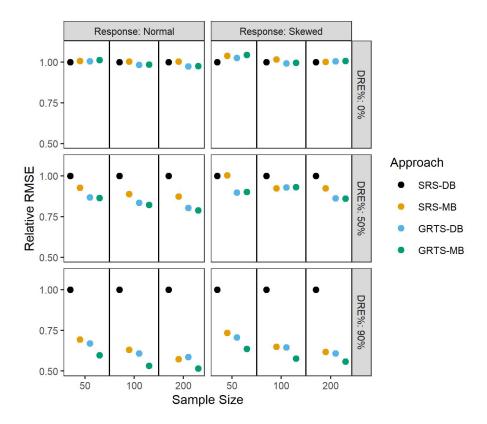


Figure 5: Simulated data relative RMSE for the four sampling-inference combinations and three sample sizes in the random location layout. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid, black lines separate the sample sizes.

- that the lack of efficiency from SRS is largely mitigated by model-based inference.
- 416 These RMSE conclusions are similar to those observed in the grid location
- layout, so we omit a figure and discussion regarding the grid location layout here.
- $_{418}$ Tables for RMSE in all 36 simulation scenarios are provided in the supporting
- 419 information.
- 95% interval coverage for each of the four sampling-inference combinations
- $_{\rm 421}$ $\,$ in the random location layout is shown in Fig. 6. Within each simulation
- scenario, all sampling-inference combinations tend to have fairly similar interval
- coverage, though when n = 50 or n = 100, GRTS-DB coverage is usually a

few percentage points lower than the other combinations, which suggests that 424 the local neighborhood variance estimate may be slightly too small for small n. 425 Coverage in the normal response scenarios is usually near 95%, while coverage in 426 the skewed response scenarios usually varies from 90% to 95% but increases with 427 the sample size. At a sample size of 200, all four sampling-inference combinations 428 have approximately 95% interval coverage in both response scenarios for all DRE 429 proportions. These interval coverage conclusions are similar to those observed in 430 the grid location layout, so we omit a figure and discussion regarding the grid 431 location layout here. Tables for interval coverage in all 36 simulation scenarios are provided in the supporting information. 433

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 samplinginference 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

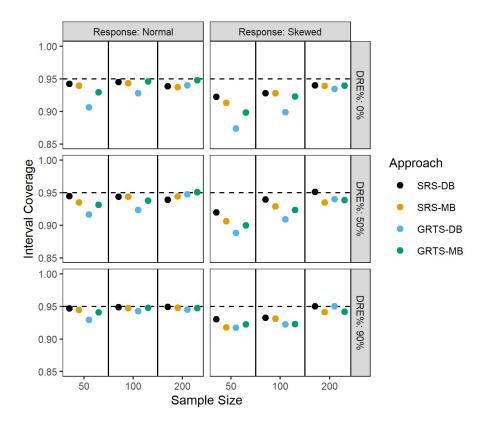


Figure 6: Simulated data interval coverage for the four sampling-inference combinations and three sample sizes in the random location layout. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid black lines separate the sample sizes and the dashed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

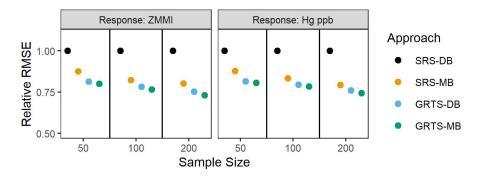


Figure 7: NLA data relative RMSE for the four sampling-inference combinations. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid, black lines separate the sample sizes.

response) than for Hg ppb (skewed response). When n = 100, ZMMI interval 451 coverage is approximately 95% except for GRTS-DB, which has coverage around 452 92%, while Hg ppb interval coverage ranges from approximately 90% (GRTS-DB) 453 to 93% (GRTS-MB). When n = 200, ZMMI interval coverage is approximately 454 95% while Hg ppb interval coverage ranges from approximately 93% (GRTS-DB) 455 to 95% (GRTS-MB). As with the simulated data, coverages for the NLA data 456 tend to increase with the sample sizes, coverages tend to be higher for symmetric 457 responses than for skewed responses, and the local neighborhood variance was 458 slightly too small for small n, yielding slightly lower interval coverages than the 459 other sampling-inference combinations. Recall that model-based inference defines 460 interval coverage properties across realized populations. With the simulated data, we evaluated interval coverage across realized populations, but for the NLA data, 462 we evaluated interval coverage within a single realized population. We did find that model-based coverages were similar to the design-based coverages, however, 464 suggesting that for some realized populations it is reasonable to heuristically 465 view data from separate random samples as being from approximately separate 466 realized populations. But generally, if model-based intervals constructed from 467 many random samples of a single realized population show improper coverage, 468 this does not necessarily imply a deficiency in model-based inference. Tables for 469 interval coverage in all six simulation scenarios are provided in the supporting 470 information. 471

472 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

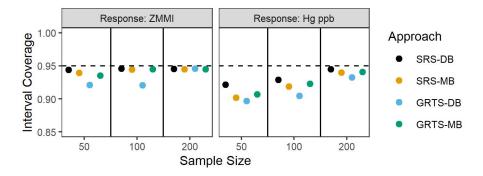


Figure 8: NLA data interval coverage for the four sampling-inference combinations. The rows indicate the proportion of dependent error and the columns indicate the response type. The solid black lines separate the sample sizes and the dashed black lines represent 95% coverage.

stochastic process. Though model-based approaches do not rely on random 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 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

near the desired value of 95%.

521

There are several benefits and drawbacks of the design-based and modelbased approaches for finite population spatial sampling and inference. Some we 497 have discussed, but others we have not, and they are worthy of consideration 498 in future research. First, we discuss advantages of the design-based approach. 499 Design-based inference is often computationally efficient, while model-based 500 inference can be computationally burdensome, especially for likelihood-based 501 estimation methods like REML that rely on the inverse of a covariance matrix. 502 Design-based inference easily handles binary data through a straightforward application of the Horvitz-Thompson estimator. In contrast, analyzing binary 504 data using model-based inference generally requires a logistic mixed regression model, the parameters of which can be difficult to estimate and interpret (Bolker 506 et al., 2009). An advantage of design-based inference is that interval coverage valid (has the proper coverage rate) as long as 1) the sample is sufficiently 508 large to ensure the statistic's sampling distribution is approximately normal and 509 2) the variance estimator is consistent (Brus and De Gruijter, 1997; Särndal 510 et al., 2003). This is because with the design-based approach, the sampling 511 plan and inclusion probabilities are specified directly by the researcher. An 512 advantage of SRS-DB not previously mentioned is that it is likely to be valid 513 given the consistency of its variance estimator (Särndal et al., 2003). With 514 the model-based approach, however, interval coverage is unlikely to be valid 515 if the model assumptions made do not not accurately reflect reality. Whether model assumptions accurately reflect reality can be a challenging and sometimes 517 impossible question to answer definitively. 518 Now, we discuss advantages of the model-based approach. The model-519 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 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) provide a more thorough discussion regarding the benefits and drawbacks of the 531 two approaches. In short, when deciding whether the design-based or modelbased approach is more appropriate to implement, these benefits and drawbacks 533 should be considered alongside the particular goals of the study.

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

Acknowledgments

We would like to thank the editors and anonymous reviewers for their hard work and time spent providing us with thoughtful, valuable feedback which greatly improved the manuscript.

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553 Conflict of Interest Statement

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

555 Author Contribution Statement

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

Data and Code Availability

- $_{561}$ This manuscript has a supplementary R package that contains all of the
- data and code used in its creation. The supplementary R package is hosted on
- 563 GitHub. Instructions for download are available at
- https://github.com/michaeldumelle/DvMsp.
- If the manuscript is accepted, this repository will be archived in Zenodo.

566 Supporting Information

- In the supporting information, we provide tables of summary statistics for
- ⁵⁶⁸ all 36 simulation scenarios and all six real data scenarios.

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