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

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Abstract

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1. Introduction

There are two general approaches for using data to make statistical inferences about a population: design-based approaches and model-based approaches. When data cannot be obtained for all units in a population (population units), data on a subset of the population units is collected in a sample. In the design-based approach, inferences about the underlying population are informed from a probabilistic process in which population units are selected to be in the sample. Alternatively, in the model-based approach, inferences are made from specific assumptions about the underlying process that generated the data. Each paradigm has a deep historical context (Sterba, 2009) and its own set of general advantages (Hansen et al., 1983).

Though the design-based and model-based approaches apply to statistical inference in a broad sense, we focus on comparing these approaches for spatial data. We define spatial data as variables measured at specific geographic locations. De Gruijter and Ter Braak (1990) give an early comparison of design-based and model-based approaches for spatial data, quashing the belief that design-based

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approaches could not be used for spatially correlated data. Thereafter, several comparisons between design-based and model-based for spatial data have been considered, but they tend to compare design-based approaches that ignore spatial locations to model-based approaches (Brus and De Gruijter, 1997; Ver Hoef, 2002; Ver Hoef, 2008). Cooper (2006) review the two approaches in an ecological context before introducing a "model-assisted" variance estimator that combines aspects from each approach. In addition to Cooper (2006), there has been substantial research and development into estimators that use both design and model-based principles (see e.g. Cicchitelli and Montanari (2012), Chan-Golston et al. (2020) for a Bayesian approach, and Sterba (2009)). More recent overviews include Brus (2020) and Wang et al. (2012), but no numerical comparison has been made between design-based approaches that incorporate spatial locations and model-based approaches.

The rest of this paper is organized as follows. In Section 2, we compare sampling and estimation procedures between the design-based approach and the model-based approach. In Section 3, we use simulated and real data to study the the behavior of both approaches. And in Section 5, we end with a discussion and provide directions for future research.

2. Background

The design-based and model-based approaches incorporate randomness in fundamentally different ways. In this section, we describe the role of randomness and its effects on subsequent inferences. We then discuss specific inference methods for the design-based and model-based approaches for spatial data.

2.1. Comparing Design-Based vs. Model-Based

The design-based approach assumes the data are fixed. Randomness is incorporated in the selection of population units according to a sampling design. A sampling design assigns a positive probability of inclusion in the sample (inclusion probability) to each population unit. Some examples of commonly used sampling designs include independent random sampling (IRS), stratified random sampling, and cluster sampling. The goal is to use the sampling design and the sampled data to estimate population parameters like means and totals. These population parameters are typically assumed to be fixed but unknown.

Treating the data as fixed and incorporating randomness through the sampling design yields estimators having very few other assumptions. Confidence intervals for these types of estimators are typically derived using limiting arguments. Means and totals, for example, are asymptotically normally distributed by the Central Limit Theorem. Särndal et al. (2003) and Lohr (2009) provide thorough reviews of the design-based approach.

The model-based approach assumes the data are a random realization of a data-generating process. Randomness is often incorporated through distributional assumptions on this process. Instead of estimating fixed but unknown parameters (as in the design-based approach), the goal of model-based inference

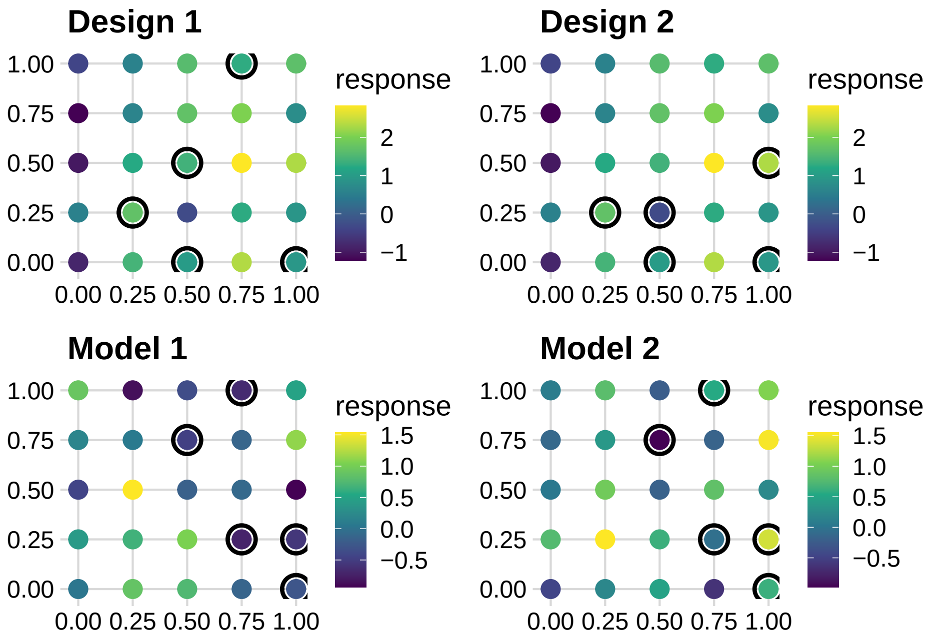


Figure 1: A comparison of sampling under the design-based and model-based frameworks. In the top row, we have one fixed population, and two random samples. In the bottom row, we have two realizations of the same spatial process sampled at the same locations.

in the spatial context is often *prediction* of an unknown quantity. For example, suppose the realized mean of all population units is the quantity of interest. Instead of *estimating* a fixed unknown mean, we are *predicting* the value of the mean, a random variable. We know that if we sampled all population units, we would have an exact prediction for the mean of our one realized process, without any uncertainty. But we are typically not interested in the true, unknown mean of the underlying process.

Assuming the data is a realization of a specific data-generating process yields predictors that are linked to distributional assumptions. These distributional assumptions are used to derive prediction intervals. The distributional assumptions allow the prediction intervals to be more precise. Cressie (1993) and Schabenberger and Gotway (2017) provide reviews of model-based approaches for spatial data.

Description of Figure 1 goes here.

2.2. Spatially Balanced Design and Analysis

The design-based approach can use spatial locations to obtain spatially balanced samples. First we discuss spatial balance with respect to the population (Stevens Jr and Olsen, 2004). A sample is spatially balanced with respect to the population if the sampled population units are a miniature of the population units. A sample is a miniature of the population if the distribution of the sampled population units mirrors the density of all population units. Spatial balance with respect to the population is different than spatial balance with respect to geography. A sample that is spatially balanced with respect to geography is spread out in some type of equidistant manner over geographical space and is not meant to be miniatures of the population. When we refer to spatial balance henceforth, we mean spatial balance with respect to the population.

Spatially balanced samples are useful because they tend to yield estimates that have lower variance than estimates constructed from sampling designs lacking spatial balance (Barabesi and Franceschi, 2011; Benedetti et al., 2017; Grafström and Lundström, 2013; Robertson et al., 2013; Stevens Jr and Olsen, 2004; Wang et al., 2013). To quantify spatial balance, Stevens Jr and Olsen (2004) proposed loss functions based on Voroni polygons. The first spatially balanced sampling algorithm that saw widespread use was the Generalized Random Tessellation Stratified (Stevens Jr and Olsen, 2004). Since GRTS was developed, several other spatially balanced sampling algorithms have emerged, including 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 (Benedetti and Piersimoni, 2017), and Halton Iterative Partitioning (Robertson et al., 2018). We focus on the Generalized Random Tessellation Stratified (GRTS) algorithm to select spatially balanced sampling because it has several attractive properties detailed by Stevens Jr and Olsen (2004) and Dumelle et al. (2021).

The GRTS algorithm is used to sample from finite and infinite populations and works by utilizing a mapping between two-dimensional and one-dimensional space. The population units in two-dimensional space are divided into cells using a hierarchical index. Population units are then mapped to a one-dimensional line via the hierarchical indexing. The line length of each population unit equals its inclusion probability. A systematic sample is conducted on the line and these samples are linked to a population unit in two-dimensional space, which results in the desired sample. Stevens Jr and Olsen (2004) provide and Dumelle et al. (2021) provide further details.

After collecting a sample using the GRTS algorithm, the data are used to estimate population parameters. The Horvitz-Thompson estimator (Horvitz and Thompson, 1952) yields unbiased estimates of population means and totals. For example, if τ is a population total, then the Horvitz-Thompson estimator of 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 and π_i are the observed value and inclusion probability of the ith population unit selected in the sample. A similar formula exists for estimating the mean, μ. Horvitz and Thompson (1952) and Sen (1953) provide variance estimators for $\hat{\tau}_{ht}$, but they have two drawbacks. First, they rely on calculating π_{ij}, the probability that population unit i and population unit j are included in the sample, and this can be very difficult to calculate. Second, they ignore the spatial locations of the population units. To address these drawbacks, Stevens Jr and Olsen (2003) proposed a local neighborhood variance estimator. The local neighborhood variance estimator does not rely on π_{ij}, and it incorporates spatial locations by assigning higher weights to nearby observations. Stevens Jr and Olsen (2003) show this variance estimators tends to reduce the estimated standard error of $\hat{\tau}$, yielding narrower confidence confidence intervals for τ.

2.3. 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 basing inference off of a specific sampling design, we assume the data are generated by a spatial process. Ver Hoef (2008) gives details on the theory of FPBK, but some of the basic principles are summarized below. Let $\mathbf{z} \equiv \{\mathrm{z}(s_1), \mathrm{z}(s_2), ..., \mathrm{z}(s_N)\}$ be a response variable that can be measured at the N population units and is represented as an $N \times 1$ vector. Suppose we want 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. For example, if we want to predict the population total across all population units, then we would use a vector of 1's for the weights.

Typically, however, we only have a sample of the N population units. 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,

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

where $\mathbf{X}_s$ and $\mathbf{X}_u$ are the design matrices for the sampled and unsampled population units, respectively; β is the parameter vector of fixed effects; and $\boldsymbol{\delta}_s$ and $\boldsymbol{\delta}_u$ are random errors for the sampled and unsampled population units, respectively. Denoting $\boldsymbol{\delta} \equiv [\boldsymbol{\delta}_s \ \boldsymbol{\delta}_u]'$, we assume the expectation of $\boldsymbol{\delta}$ equals $\mathbf{0}$.

We also typically assume that there is spatial correlation in $\boldsymbol{\delta}$, which can be modeled using a covariance function. It is common to assume the covariance function is second-order stationary and isotropic (Cressie, 1993), and that the spatial covariance decreases as the separation between population units increases. Many spatial covariance functions exist, but the primary function we use throughout the simulations and applications in this manuscript is the exponential covariance function: the i, j^{th} entry for $\mathrm{cov}(\boldsymbol{\delta})$ is

$$\mathrm{cov}(\delta_i, \delta_j) = \theta_1 \exp(-3h_{i,j}/\theta_2) + \theta_3 \mathbb{1}\{\mathbf{h}_{i,j} = 0\}, \tag{3}$$

where $h_{i,j}$ is the distance between population units i and j, and $\boldsymbol{\theta}$ is a vector of spatial covariance parameters of the partial sill θ_1, the range θ_2, and the nugget θ_3, and $\mathbb{1}$ is an indicator function. However, any spatial covariance function could be used in the place of the exponential, including functions that allow for non-stationarity or anisotropy (Chiles and Delfiner, 1999, pp. 80–93).

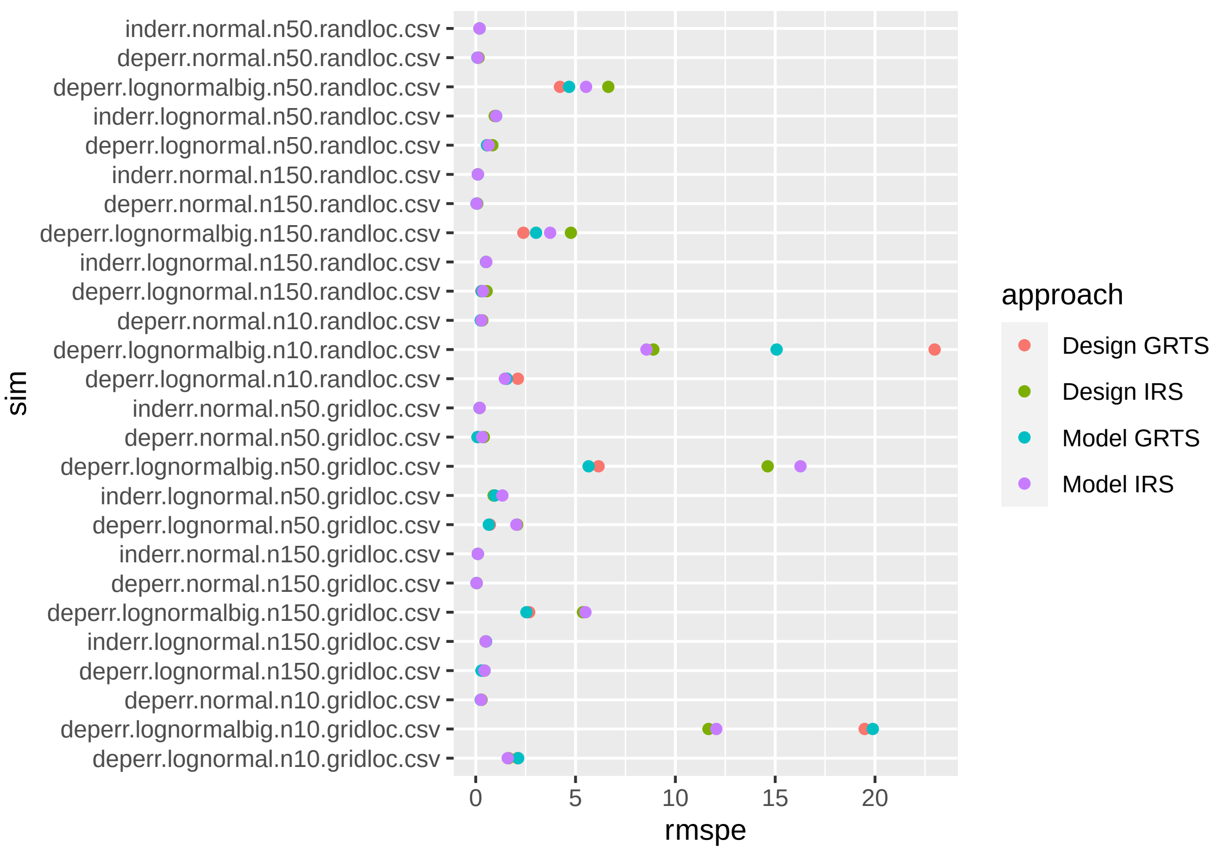
With the above model formulation, the Best Linear Unbiased Predictor (BLUP) for $f(\mathbf{b}'\mathbf{z})$ and its prediction variance can be computed. While details of the derivation are in (Ver Hoef, 2008), we note here that the predictor and its variance are both moment-based.

We note that we only use FPBK in this paper in order to focus more on comparing the design-based and model-based approaches. However, k-nearest-neighbors (Fix and Hodges, 1951; Ver Hoef and Temesgen, 2013), random forest (Breiman, 2001), Bayesian models (Chan-Golston et al., 2020), among others, can also be used to obtain predictions for a mean or total from spatially correlated responses in a finite population setting.

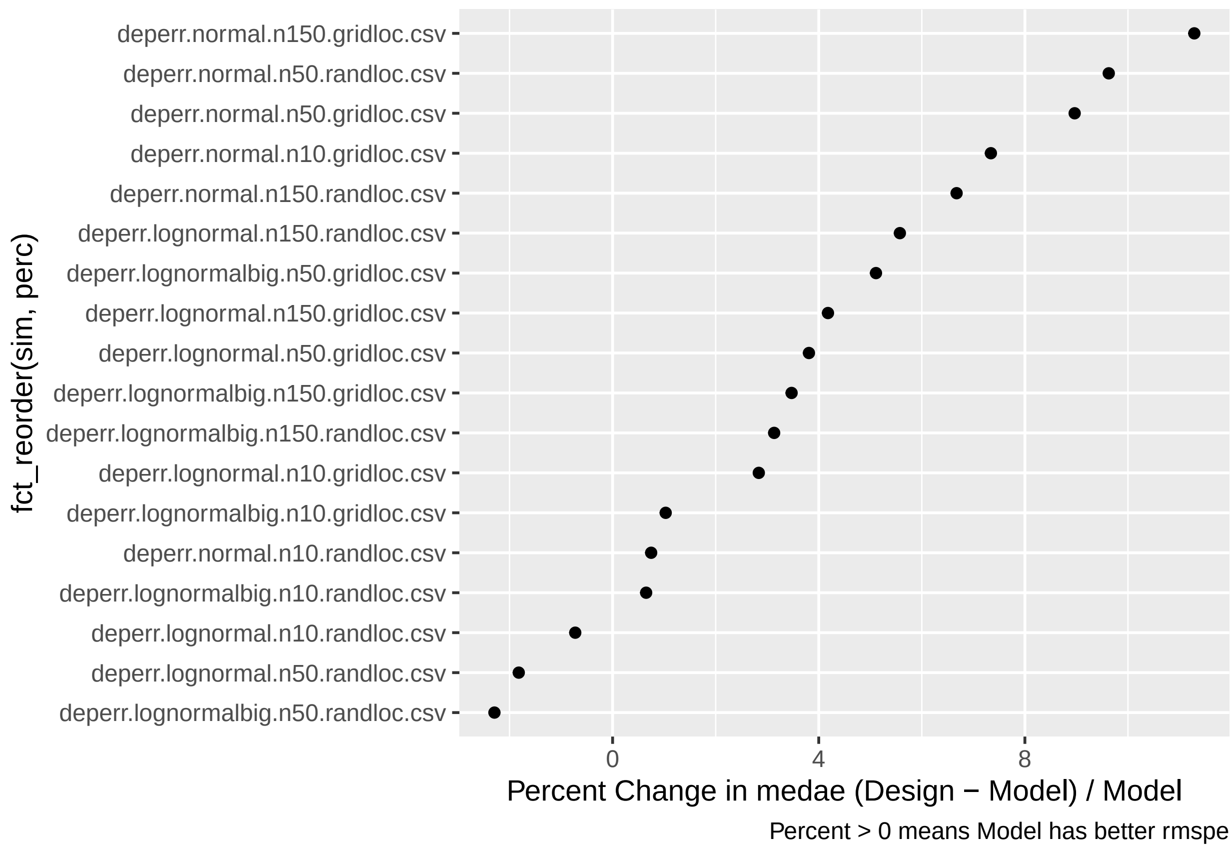
3. Numerical Study

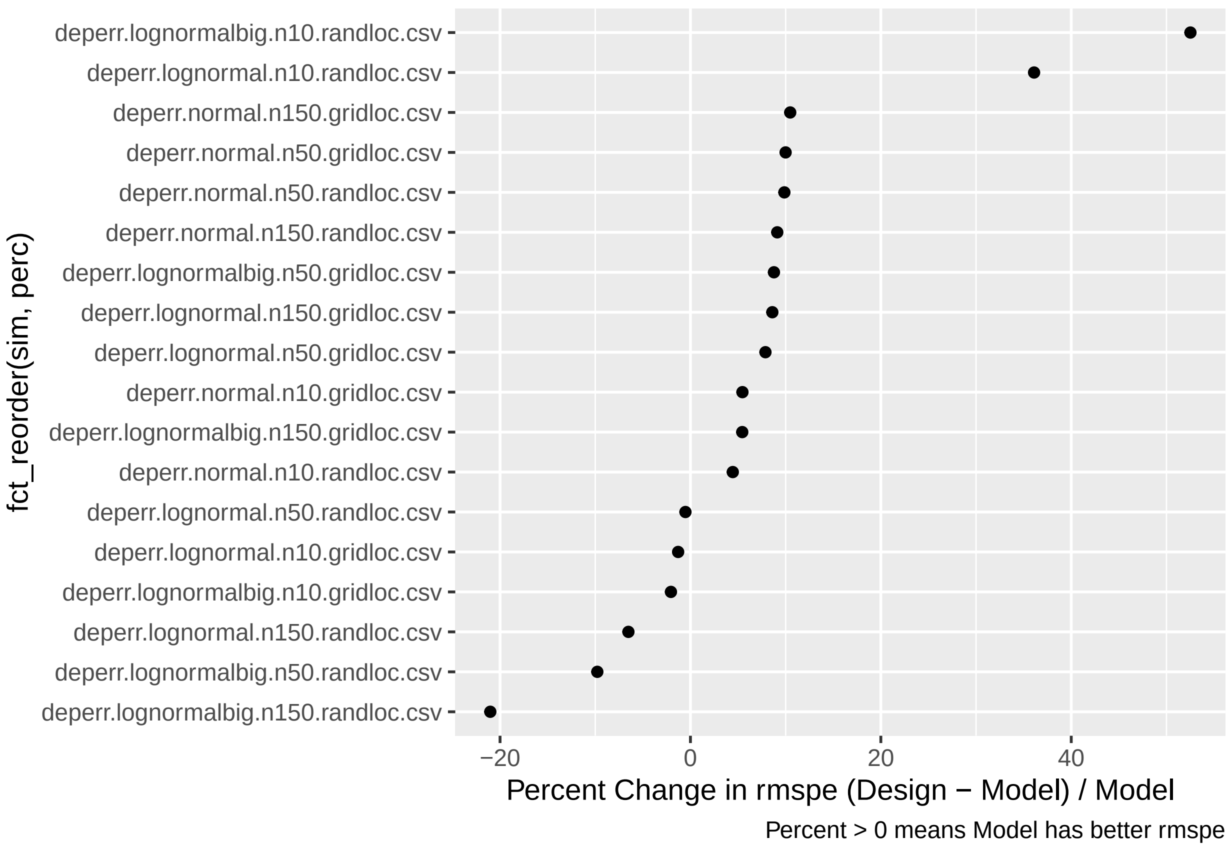
Major Points from August 3 Simulations:

1. In most of the dependent error simulation settings, either all four approahces (IRS-Design, IRS-Model, GRTS-Design, and GRTS-Model) perform equally or GRTS-Design and GRTS-Model outperform IRS-Design and IRS-Model. Exceptions to this are a couple of the settings with very small sample sizes (n = 10), in which the IRS does better than GRTS. In the independent error settings, it usually doesn't matter much which approach is used, which makes sense.

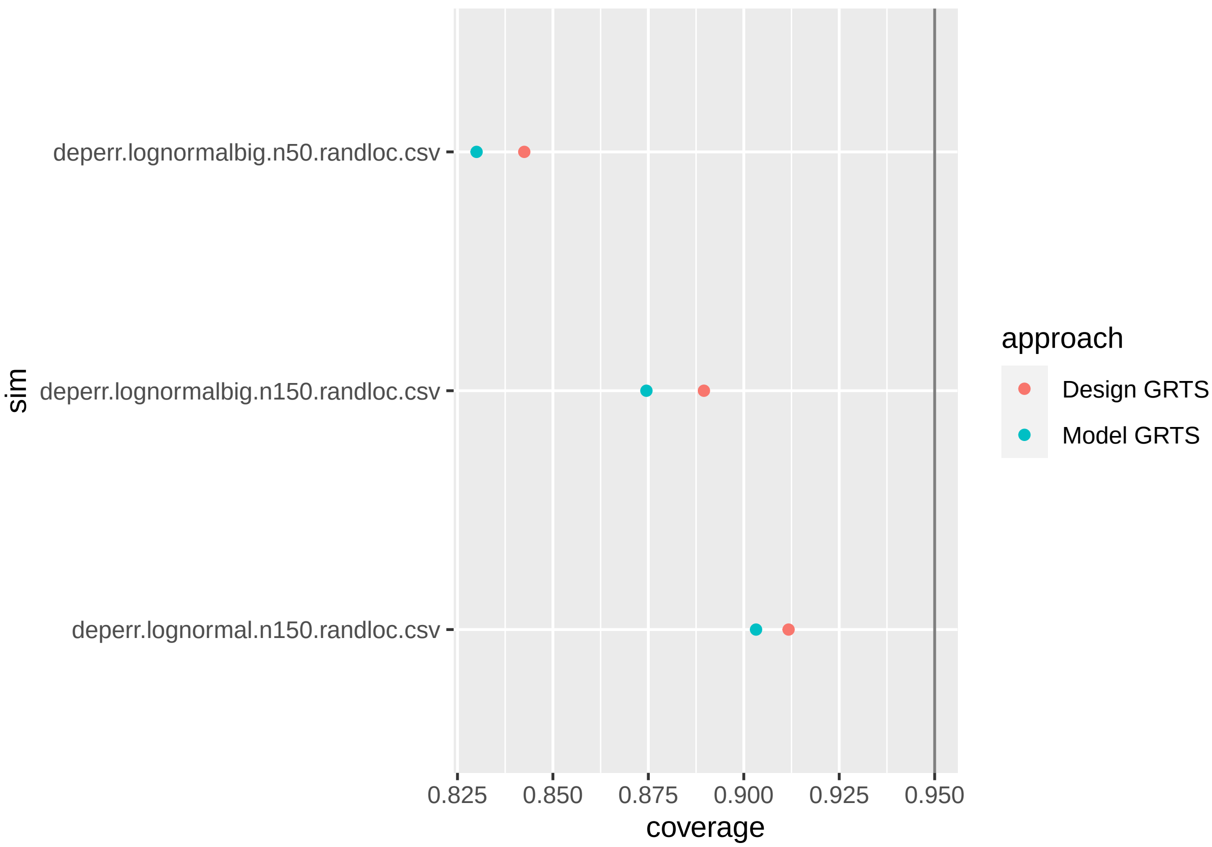


2. We will now focus in a bit more on comparing Design-GRTS to Model-GRTS, the two best approaches for any reasonable sample size. In the independent error settings, the two approaches perform very similarly, so those results are omitted in the following graph. In the dependent error settings, using rmspe as the performance criterion, Model-GRTS outperforms Design-GRTS in 12 of the 18 settings, the two approaches perform very similarly in 3 settings, and Design-GRTS outperforms Model-GRTS in 3 settings.





3. Focusing in on the three settings where Design-GRTS outperforms Model-GRTS, we see that, in two of the settings, the log-normal response has a large variance, corresponding to a large right-skew after exponentiation. All three settings have sites in random locations. However, in only one of these settings would we recommend actually using Design-GRTS. In the other two settings, the data are sufficiently skewed that a practitioner should not use either approach, though it is "safer" to use Design-GRTS.



4. Take-home messages

- In terms of rmspe, a model-based analysis on a GRTS design yields an rmspe similar to or lower than a design-based analysis on a GRTS design, as long as the response variable is not "too skewed."
- If the response variable is very skewed, then neither analysis is appropriate, but, the design-based analysis is quicker.
- a spatially balanced GRTS sample outperforms IRS in nearly all dependent error settings, as expected.
- methods that use spatial correlation generally perform better on random location points than they do on gridded points. This makes some intuitive sense because (1) on average, the minimum distance between an unobserved point and its nearest observed neighbor should be lower for random points and (2) the span of the study area is maximized for a grid based on the way that we set up the simulations (with the random points being drawn as uniform random variables within the boundary of the grid).
- comparison of Design-GRTS and Model-GRTS between two settings with different locations of points, but otherwise the same simulation parameters, should really be done on the same surface realization. One very strange

realized response vector could drastically alter the results, especially on the exponentiated log data. In the same way that we compare the four approaches on the same realized data, we should also try to do the same with the locations, if they are of interest. (The realized mean won't be exactly the same but should be close).

Sample Simulation

For the following simulation results, we simulated 1040 different gridded populations, each of size 900 (on the unit square) with sample size 150. For the design-based approach, population units were selected via GRTS, the Horvitz-Thompson estimator was used,and the local mean variance was used. For the model-based approach (FPBK), population units were selected via Independent Random Sampling (IRS) and the appropriate prediction and prediction variance formulas were used.

The response was normally distributed with an exponential covariance function with partial sill of 0.9, effective range of $\sqrt{2}$, and a nugget of 0.1. For model-based, we assumed the correct form of the covariance function (exponential), but estimated the spatial parameters with REML.

Base Simulations

- both good: correctly specified model with high correlation (we did this in Table **??**)
- break model: highly non-normal errors with small sample size
- break design: small area estimation

Simulation Discussion Questions

- model-based: how should sample be drawn? should locations be fixed?
- change n or sampling fraction?

Other Base Settings?

- both good?: misspecified covariance model with high correlation
- break both? non-gaussian areas with smaller sample size

3.1. Software

The GRTS algorithm and the local neighborhood variance estimator are available in the **R** package `spsurvey` (Dumelle et al., 2021). FPBK can be readily performed in `R` with the `sptotal` package (Higham et al., 2020). We use `sptotal` for both the simulation analysis and the application, estimating parameters with Restricted Maximum Likelihood (REML).

4. Application

The Environmental Protection Agency (EPA), states, and tribes periodically conduct National Aquatic Research Surveys (NARS) in the United States to assess the water quality of various bodies of water. We will use the 2012 National

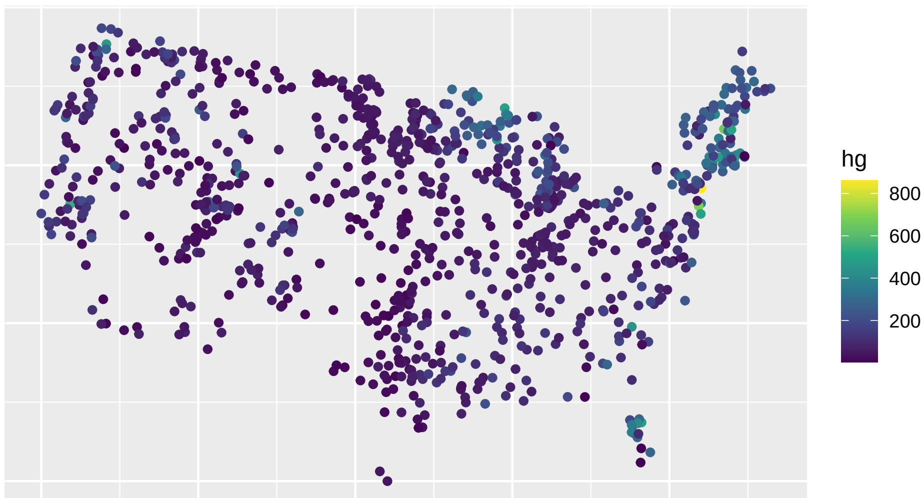


Figure 2: Population distribution of mercury concentration for 986 lakes in the contiguous United States. Thirty-five lakes were dropped from the analysis because they were missing mercury concentration.

Lakes Assessment (NLA), which measures various aspects of lake health and quality in lakes in the contiguous United States, to obtain an interval for mean mercury concentration. Although all lakes in the survey were measured in 2012, there may not always be enough time or money to do so. Therefore, we will explore whether or not we can still obtain a relatively precise estimate for the realized mean mercury concentration if we only take a sample of 100 of the 986 lakes.

Figure 2 shows that mercury concentration is right-skewed, with most lakes having a low value of mercury concentration but a few having a much higher concentration. Mercury concentration exhibits some spatial correlation, with high mercury concentrations in lakes in the northeast and north central United States. Because we are considering these lakes to be our entire population, we know that the realized mean mercury concentration is 103.03 ng / g.

Table 1: Table XXX. Application of design-based and model-based approaches to the NLA data set on mercury concentration.

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

Table 1 shows the application of a design-based analysis on an IRS, a model-based analysis on an IRS, a design-based analysis on a GRTS sample, and a model-based analysis on a GRTS sample. We see that, for all four analyses, the true realized mean mercury concentration is within the bounds of the 95% intervals. However, we should not generalize the results of this particular realization to any other data set or even to other potential samples of this data set.

But, we do note a couple of patterns. The design-based IRS analysis shows the largest standard error: a likely reason is that this is the only approach that does not use the spatial correlation in mercury concentration across the contiguous United States. We also see that, for the samples drawn, the both analyses with the GRTS sampling design have a lower standard error than the

5. Discussion

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