A comparison of design-based and model-based approaches for finite population 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 and model-based. When data cannot be obtained for all units in a population (population units), data on a subset of the population units is collected and called 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 data that incorporates the specific locations of the population units into either the design or estimation process. De Gruijter and Ter Braak (1990) give an early comparison of design-based and model-based

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approaches for spatial data, quashing the belief that design-based approaches could not be used for spatially correlated data. Thereafter, several comparisons between design-based and model-based for spatial data have been considered (Brus and De Gruijter, 1997; Ver Hoef, 2002, 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).

Though comparisons between design-based and model-based approaches to spatial data have been studied, no numerical comparison has been made between design-based approaches that incorporate spatial locations and model-based approaches. In this manuscript, we compare design-based approaches that incorporate spatial locations to model-based approaches for spatial data. Though these comparisons generalize to both finite populations (e.g. point resources) and infinite populations (e.g. linear and areal resources), we focus on applications to finite populations. The rest of the manuscript is organized as follows. In Section 2, we compare sampling and estimation procedures between the design-based approach and the model-based approach for spatial data. In Section 3, we use a simulation approach to study the behavior and performance of both approaches. In Section 4, we use both approaches to analyze real data. 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 and Model-Based Approaches

The design-based approach assumes the population is fixed. Randomness is incorporated via the selection of units in a sampling frame according to a sampling design. A sampling frame is the set of all units available to be sampled. A sampling design assigns a positive probability of inclusion (inclusion probability) to each unit in the sampling frame. Some examples of commonly used sampling designs include simple random sampling, stratified random sample, and cluster sampling. These sampling designs tend to select units from the sampling frame independently of other units, so we call them "Independent Random Sampling" (IRS) designs. Sampling designs incorporating the spatial locations of units in the sample frame are called spatially balanced designs. Spatially balanced designs can be obtained using the Generalized Random Tessellation Stratified (GRTS) algorithm (Stevens and Olsen, 2004), which we discuss in more detail

in Section 2.2. The design-based approach combines the randomness of the sampling design and the data collected via the sample to estimate parameters (e.g. means and totals) of a population. Generally, these population parameters are assumed to be fixed, unknown constants.

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 that incorporate all possible randomizations of sampling units selected via the sampling design. Means and totals, for example, are asymptotically Gaussian by the Central Limit Theorem (under some assumptions). If we repeatedly sample the surface, then 95% of all 95% confidence intervals constructed from a procedure with appropriate coverage will contain the true, fixed mean. 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 incorporated through distributional assumptions on this process. Strictly speaking, randomness need not be incorporated through random sampling, though Diggle et al. (2010) warn against preferential sampling Preferential sampling occurs when the process generating the data locations and the process being modeled are not independent of one another. To guard against preferential sampling, model-based approaches often still implement random sampling.

Instead of estimating fixed but unknown parameters (as in the design-based approach), the goal of model-based inference in the spatial context is often to predict a realized variable, or value. For example, suppose the realized mean of all population units is the value of interest. Instead of *estimating* a fixed, unknown mean, we are *predicting* the value of the mean, a random variable. Prediction intervals are then derived leveraging assumptions of the data generating process. If we repeatedly generate the response values from a fixed spatial process and obtained a sample, then 95% of all 95% prediction intervals constructed from a procedure with appropriate coverage will contain their respective realized means. Cressie (1993) and Schabenberger and Gotway (2017) provide reviews of model-based approaches for spatial data. A visual comparison of the design-based and model-based assumptions is provided in Figure 1 (Brus (2020) provides a similar figure).

2.2. Spatially Balanced Design and Analysis

Spatially balanced samples can be obtained using the design-based approach. Spatially balanced samples are useful because parameter estimates from these samples tend to vary less than parameter estimates from samples that are not spatially balanced (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 that saw widespread use was the Generalized Random Tessellation Stratified (GRTS) algorithm (Stevens and Olsen, 2004). To quantify the spatial balance of a

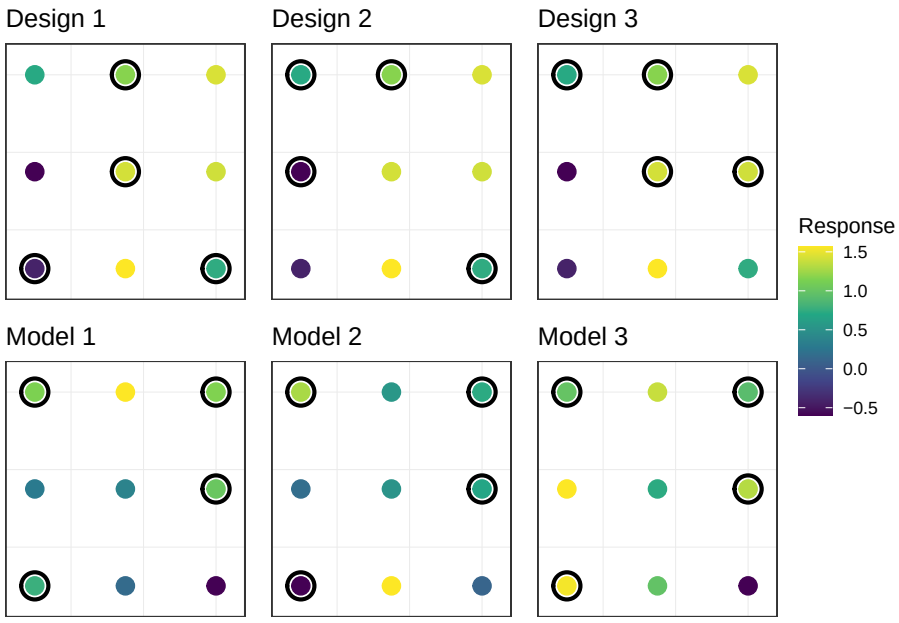

Figure 1: A comparison of sampling under the design-based and model-based frameworks. Points circled are those that are sampled. In the top row, we have one fixed population, and three random samples of n = 4. The response values at each site are fixed, but we obtain different estimates for the mean response because the randomly sampled sites vary from sample to sample. In the bottom row, we have three realizations of the same spatial process sampled at the same locations. The spatial process generating the response values has a single mean, but the realized mean is different in each of the three panels.

sample, Stevens and Olsen (2004) proposed loss metrics based on Voroni polygons. 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 Sampling (Benedetti and Piersimoni, 2017), and Halton Iterative Partitioning Sampling (Robertson et al., 2018). In this manuscript, we use Generalized Random Tessellation Stratified (GRTS) sampling because it has several attractive properties: GRTS sampling accommodates finite and infinite sampling frames; accommodates equal, unequal, and proportional (to) size inclusion probabilities; accommodates legacy (historical) sampling; accommodates a minimum distance between units in a sample; accommodates reverse hierarchically ordered replacement units in a sample (replacement units are units available to be sampled if an original unit cannot be sampled); and is available in the spsurvey R package Dumelle et al. (2021).

The GRTS algorithm samples from finite and infinite populations by utilizing a mapping between two-dimensional and one-dimensional space. The units in the two-dimensional sampling frame are divided into cells using a hierarchical address. This hierarchical address is then used to map the units from two-dimensional space to a one-dimensional line where each unit's line length equals its inclusion probability. A systematic sample is conducted on the line and linked back to a unit in two-dimensional space, which results in the desired sample. Stevens and Olsen (2004) and Dumelle et al. (2021) provide further details.

After selecting a GRTS sample, data are collected and used to estimate population parameters. To unbiasedly estimate population means and totals from sample data, one can use the Horvitz-Thompson estimator (Horvitz and Thompson, 1952). If τ is a population total, the Horvitz-Thompson estimate of τ, denoted by $\hat{\tau}_{ht}$, is 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 ith unit in the sample and π_i is the inclusion probability of the ith unit in the sample. An estimate of the population mean is obtained by dividing $\hat{\tau}_{ht}$ by the population size.

While the Horvitz-Thompson estimator is unbiased for population means and totals, it is also important to quantify the uncertainty in these estimates. Horvitz and Thompson (1952) and Sen (1953) provide variance estimators for $\hat{\tau}_{ht}$, but they have two drawbacks. First, these estimators rely on calculating π_{ij}, the probability that unit i and unit j are both in the sample – this quantity can be challenging if not impossible to calculate analytically. Second, these estimators ignore the spatial locations of the units in the sampling frame. 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 incorporates spatial locations – for technical details see Stevens and Olsen (2003). Stevens and Olsen (2003) show the local neigborhood

variance estimator tends reduce $\text{Var}(\hat{\tau})$ compared to variance estimators ignoring spatial locations, yielding narrower 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 $\mathbf{z} \equiv \{\text{z}(s_1), \text{z}(s_2), ..., \text{z}(s_N)\}$ be a response vector at locations s_1, s_2, . . . , s_N 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.

We often 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 $\mathbf{0}$.

In addition to assuming the expectation of $\boldsymbol{\delta}$ equals $\mathbf{0}$, we also assume that there is spatial correlation in $\boldsymbol{\delta}$ that 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, jth entry for $\text{cov}(\boldsymbol{\delta})$ is

$$\text{cov}(\delta_i, \delta_j) = \begin{cases} \sigma^2_{ps} \exp(-h_{i,j}/\phi) & h_{i,j} > 0 \\ \sigma^2_{ps} + \sigma^2_n & h_{i,j} = 0 \end{cases}, \tag{3}$$

where σ^2_{ps} is the partial sill measuring coarse-scale (correlated) variability, σ^2_n is the nugget measuring fine-scale (indepenent) variability, ϕ is the range parameter measuring the distance-decay rate of the covariance, and $h_{i,j}$ is the Euclidean distance between population units i and j. Any spatial covariance function could be used in the place of the exponential, however, 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, meaning they don't rely on any distributional assumptions.

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 of a finite population. We choose to use FPBK because it is faster than a Bayesian approach and random forest and because Ver Hoef and Temesgen (2013) showed that the method outperforms k-nearest-neighbors in many scenarios.

3. Numerical Study

We used a numerical simulation study to investigate performance of four design-analysis combinations, summarized in Table 1.

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

Table 1: Types of Sampling Design and Analysis combinations considered in the simulation study. The rows give the two types of sampling designs while the columns give the two types of analyses.

We used a crossed design with the simulation parameters given in Table 2 for a total of 36 scenarios. All scenarios used exponential correlation with an effective range of $\sqrt{2}$ for $N = 900$ response values simulated on the unit square in either random locations (Site Locations = Random) or gridded locations (Site Locations = Gridded). The mean for the spatial process generating the response was set to zero.

For the lognormal scenarios, the response values were simulated using the specified correlation parameters using a normal distribution and were subsequently exponentiated. A total variance of 2 and a mean of 0 on the normal scale is equivalent to a total variance of 47 and a mean of 2.72 after exponentiation. Therefore, when the model-based methods were used for lognormal response, the correlation was mis-specified. We chose to simulate values with a lognormal distribution so that we could test the model-based analysis approach with a mis-specified model and so that we could test both analysis approaches on data that exhibits a large amount of skewness.

There were 2000 simulation trials for each of the 36 parameter combinations. In each trial, response values were generated from a spatial process with the specified parameters, and a GRTS sample and an IRS sample were selected. For the GRTS sample, the design-based approach using the local neighborhood variance (GRTS-Design) and a model-based approach were applied (GRTS-Model). For the IRS sample, the design-based approach using the simple random

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

Table 2: Simulation parameters. Total variability for all scenarios was 2 so that the partial sill was 0, 1, or 1.8.

sample variance (IRS-Design) and a model-based approach were applied (IRS-Model).

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).

Figure 2 shows the relative efficiency of the four approaches from Table 1 with "IRS-Design" as the baseline:

$$\text{E} = \frac{\text{rMSPE of approach}}{\text{rMSPE of IRS-Design}},$$

where rMSPE is the root-Mean-Squared-Prediction-Error. When there is no spatial correlation (top row), the four approaches have approximately equal rMSPE, even when the assumptions of the model-based approaches are violated. So, using GRTS or using a spatial model does not result in much loss in efficiency even if the response variable is not spatially correlated. When there is high spatial correlation (bottom row), the GRTS-Model approach tends to perform best, but difference in relative efficiency between GRTS-Model and GRTS-Design is not very big. In the lognormal, high partial sill settings (bottom-right facet), GRTS-Design outperforms IRS-Model by a large margin, suggesting that the design decision (whether to use IRS or GRTS) is more important than the analysis decision (whether to analyze using model assumptions or not).

Unsurprisingly, Figure 2 also shows that, when the assumptions for GRTS-Model are satisfied, the approach outperforms GRTS-Design. However, even when the model that generates the data is different than the model used to fit the data, as in the lognormal response, the model-based approach still outperforms the design-based approach when there is a high amount of spatial correlation.

Plot Note: change colours and think about shape think about legend going on graph

Figure 3 shows the coverage for each of the four approaches. We see that the four approaches have somewhat similar coverages in all settings, with GRTS-Design having slightly lower coverage when the response is normal.

In the normal response settings, where assumptions for the model-based approaches and the design-based approaches are satisfied, all approaches have coverage around the nominal 0.95. Because the intervals are symmetric, normal-based intervals, the coverages are generally lower than the nominal 95%. We see that, because the sampling distribution of the mean is asymptotically normal

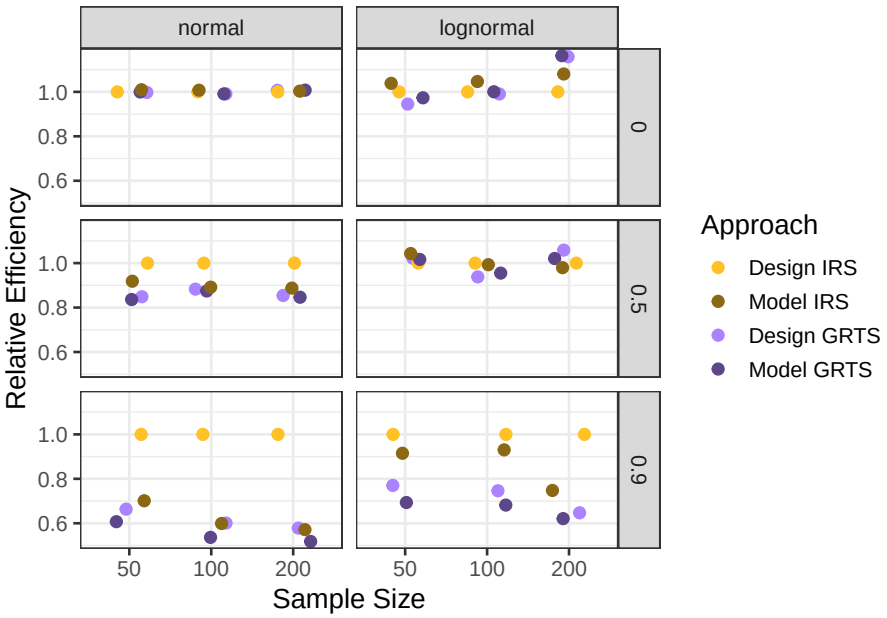

Figure 2: Relative Efficiency of the four design-analysis approaches. The plot is faceted by the type of response on the columns and the partial-sill to total-variance ratio on the rows.

(reference for this? a spatial version of CLT), the coverages when the sample size is 200 are much closer to the nominal 95% than the coverages when the sample size is 50. In general, the more skewed the distribution of the response, the larger the sample size needed to ensure proper coverage of these normal-based intervals.

Do we want to mention stuff like what's in these next bullet points or no?

- for the model-based approach, the more skewed the population is, the higher the sample size needed to satisfy CLT for predicting a mean. The derivation of the BLUP is entirely moment-based (no distribution assumed) but we still need to assume a distribution to estimate spatial parameters and to generate bounds of a prediction interval.
- many confidence intervals generated for design-based approaches also rely on the CLT and the normal distribution to generate the interval. Again, for highly skewed data with a small sample size, this assumption is violated even though all of the assumptions for generating the estimator are valid.

4. Application

The Environmental Protection Agency (EPA), states, and tribes periodically conduct National Aquatic Research Surveys (NARS) in the United States to

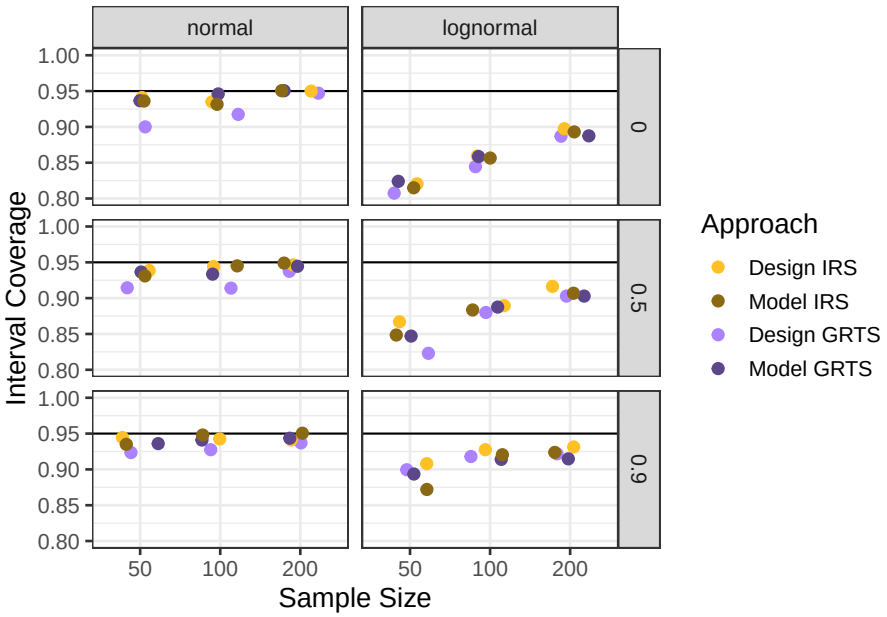

Figure 3: Coverage of the four design-analysis approaches. All confidence intervals are normal-based and have a nominal confidence level of 0.95, marked with a horizontal line. The plot is faceted by the type of response on the columns and the partial-sill to total-variance ratio on the rows.

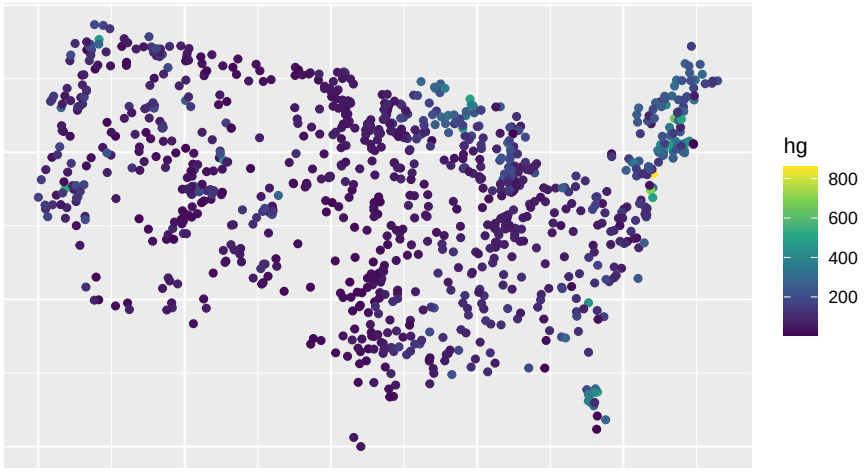

Figure 4: Population distribution of mercury concentration for 986 lakes in the contiguous United States. Thirty-five lakes were dropped from the analysis because they were missing mercury concentration.

assess the water quality of various bodies of water. We will use the 2012 National 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 an adequately precise estimate for the realized mean mercury concentration if we only take a sample of 100 of the 986 lakes.

Figure 4 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 103.2 ng / g.

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

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

Table 3 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 analyses with the IRS sampling design. We would expect this to be the case for most samples because mercury concentration exhibits spatial correlation so a spatially balanced sample should usually yield a lower standard error. If it is acceptable to have an interval for mean mercury concentration of about 25 ng / g and if we ignore the other variables that the EPA collects information on in these NLA surveys, then the EPA could consider sampling just 50 lakes to save time and money.

5. Discussion

- Pros of Design-Based (items we are not exploring): computationally efficient, few assumptions, more naturally handles binary data,
- Pros of Model-Based (items we are not exploring): covariate inference, more efficient small-area estimation, model selection?, estimated spatial parameters to better understand spatial structure, site-by-site predictions/prediction map

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