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

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Abstract

This is the 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).

Tony O.: Should this paragraph address that spatial information can be incorporated in the design stage or in the analysis stage (or both). In general, it's not clear whether we are referring to site selection process or the estimation process

Though the design-based and model-based approaches apply to statistical inference in a broad sense, we focus on comparing these approaches for spatial

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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 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, but they tend to compare design-based approaches that ignore spatial locations to model-based approaches (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), but no numerical comparison has been made between design-based approaches that incorporate spatial locations and model-based approaches.

Lisa M.: Add paragraph describing contribution of manuscript.

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 population is 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 simple random sampling, stratified random sample, and cluster sampling, which we refer to as Independent Random Sampling (IRS) survey designs. The goal is to use the sampling design and the sampled data to estimate population parameters like means and totals. These population parameters are traditionally assumed to be fixed but unknown.

Treating the data as fixed and incorporating randomness through the sampling design (top row of Figure 1 ((cite Brus 2021 here since our figure is similar?))) 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. 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.

Jay VH: I think it is important to stress that the limiting distribution is over all possible randomizations, constrained by whatever design is used.

Jay VH: quantity is vague. We should stick with variables, or realized variables (we might also call these values, but we should define and establish a consistent terminology early on.) **Matt H**: I think, though this comment is for this paragraph, we should establish the terminology earlier.

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 and need not be incorporated through random sampling (bottom row of Figure 1). 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 *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.

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. If we repeatedly generate the response values from a fixed spatial process and obtain 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.

Tony O.: Before this section is it useful to have a section that lays out the general site selection and general analysis options. Thinking about site selection as design-based IRS, design-based GRTS, Arbitrary set of sites, selection for model-based. Then general analysis options as design-based no spatial, design-based spatial, model-based. This four by three table would show that model-based analyses are possible for all selection options. Design-based options with no spatial info possible for IRS-based and GRTS-based. Design-based options with spatial info possible for GRTS-based.

Jay VH: What about the design for model-based inference? Strictly speaking, it is fixed – there is no probabilistic use of a randomized design. However, we are going to have to deal with Diggle et al. (2010).

2.2. Spatially Balanced Design and Analysis

Lisa M.: Need a more precise definition of “miniature” in this context, and need an example.

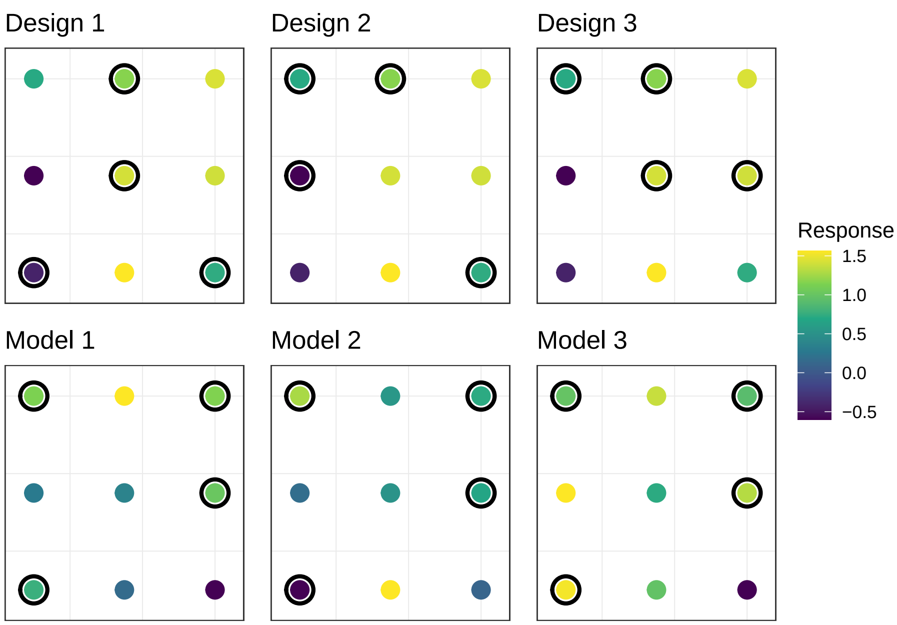

Figure 1: A comparison of sampling under the design-based and model-based frameworks. Points circled are those that are sampled. In the top row, we have one fixed population, and three random samples of n = 4. The response values at each site are fixed, but we obtain different estimates for the mean 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.

Jay VH: Saying "the distribution of the sampled population units mirrors the density of..." is confusing to me. Are these formal statistical definitions of distribution (cumulative distribution function) and density (probability density function)? Wouldn't IRS sample be a miniature, as it should, on average, mirror a population?

The design-based approach can use spatial locations to obtain spatially balanced samples. First we discuss spatial balance with respect to the population (Stevens 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 and Olsen, 2004; Wang et al., 2013). To quantify spatial balance, Stevens 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 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, including **Lisa M.**: List major attractive properties, and detailed by Stevens 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 and Olsen (2004) 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 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 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 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.

However, 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,

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

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 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 $\text{cov}(\boldsymbol{\delta})$ is

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

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 equal to 1 when distance h_i, j is equal to 0, and equal to 0 otherwise. 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).

Lisa M. : Include formulas. Perhaps, but, these are very heavy in notation and matrix algebra. We might consider, however, adding the formulas to an Appendix.

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. 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.

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

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

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.

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

Sample Size (n)	50	100	200
Site Locations	Random	Gridded	
Partial Sill / Total Variance	0	0.5	0.9
Response Type	Normal	Lognormal	

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 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:

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

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

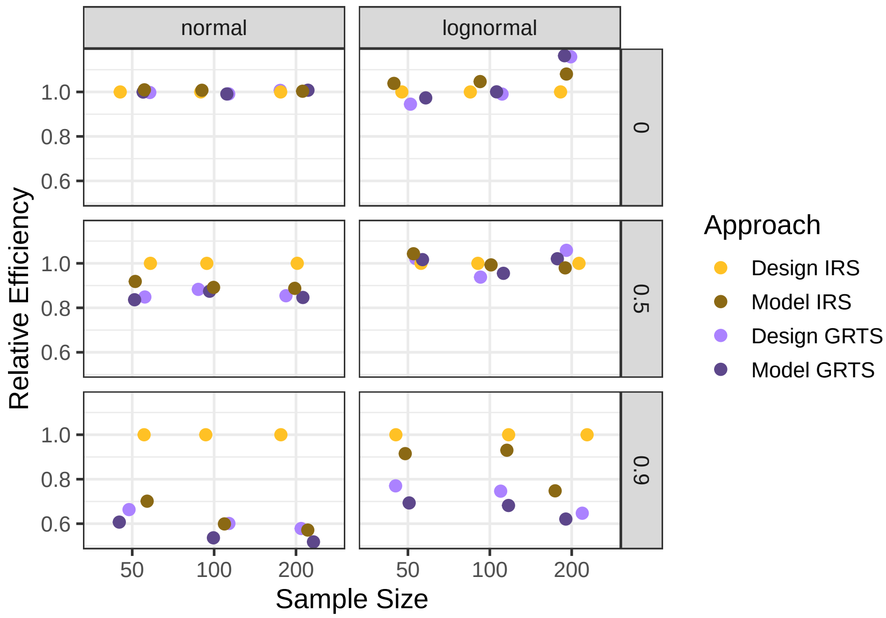

Figure 2: Relative Efficiency of the four design-analysis approaches. The plot is faceted by the type of response on the columns and the partial-sill to total-variance ratio on the rows.

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 (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

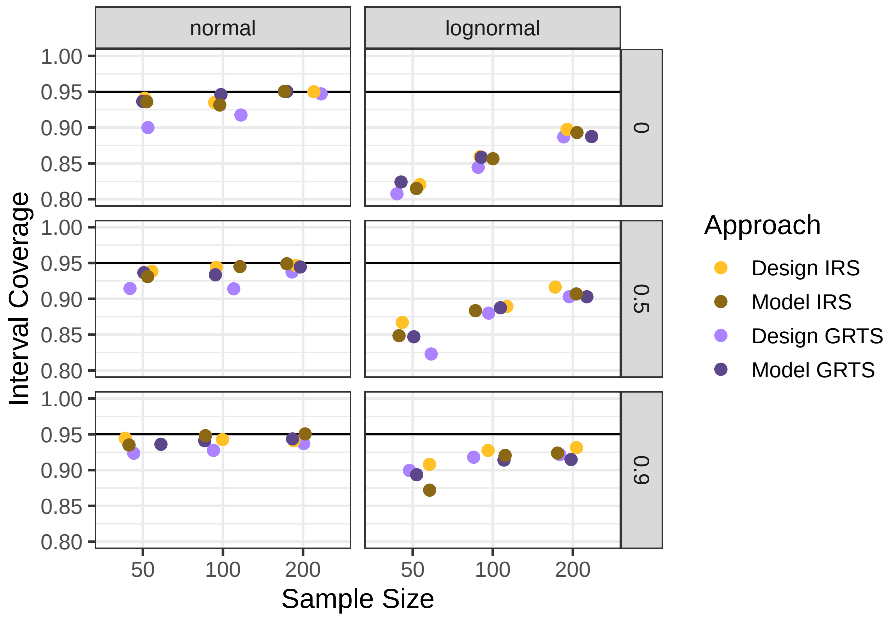

Figure 3: Coverage of the four design-analysis approaches. All confidence intervals are normal-based and have a nominal confidence level of 0.95, marked with a horizontal line. The plot is faceted by the type of response on the columns and the partial-sill to total-variance ratio on the rows.

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

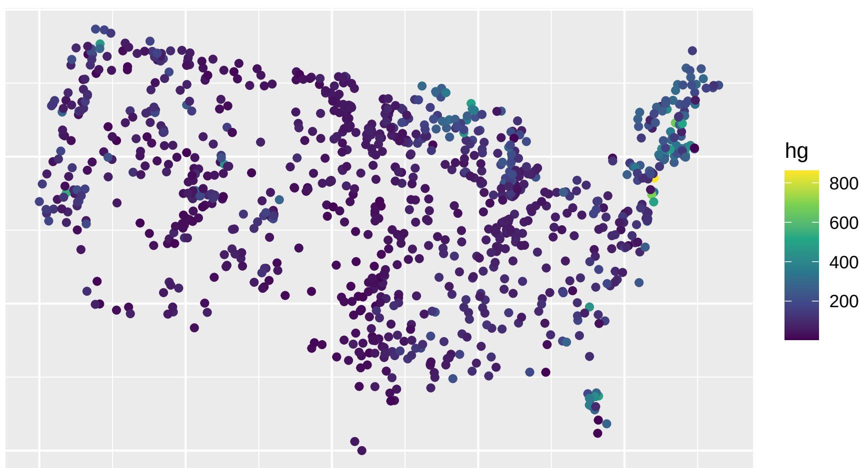

Figure 4: Population distribution of mercury concentration for 986 lakes in the contiguous United States. Thirty-five lakes were dropped from the analysis because they were missing mercury concentration.

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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