

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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- Ecological Applications
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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; 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.

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 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 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

80 Central Limit Theorem. Särndal et al. (2003) and Lohr (2009) provide thorough
81 reviews of the design-based approach.

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

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

88 The model-based approach assumes the data are a random realization of a
89 data-generating process. Randomness is often incorporated through distribu-
90 tional assumptions on this process. Instead of estimating fixed but unknown
91 parameters (as in the design-based approach), the goal of model-based inference
92 in the spatial context is often *prediction* of an unknown quantity. For example,
93 suppose the realized mean of all population units is the quantity of interest.
94 Instead of *estimating* a fixed unknown mean, we are *predicting* the value of the
95 mean, a random variable. We know that if we sampled all population units, we
96 would have an exact prediction for the mean of our one realized process, without
97 any uncertainty. But we are often not interested in the true, unknown mean of
98 the underlying process.

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

105 Description of Figure 1 goes here.

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

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

117 2.2. Spatially Balanced Design and Analysis

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

120 **Jay VH:** Saying “the distribution of the sampled population units mirrors
121 the density of...” is confusing to me. Are these formal statistical definitions of
122 distribution (cumulative distribution function) and density (probability density
123 function)? Wouldn’t IRS sample be a miniature, as it should, on average, mirror
124 a population?

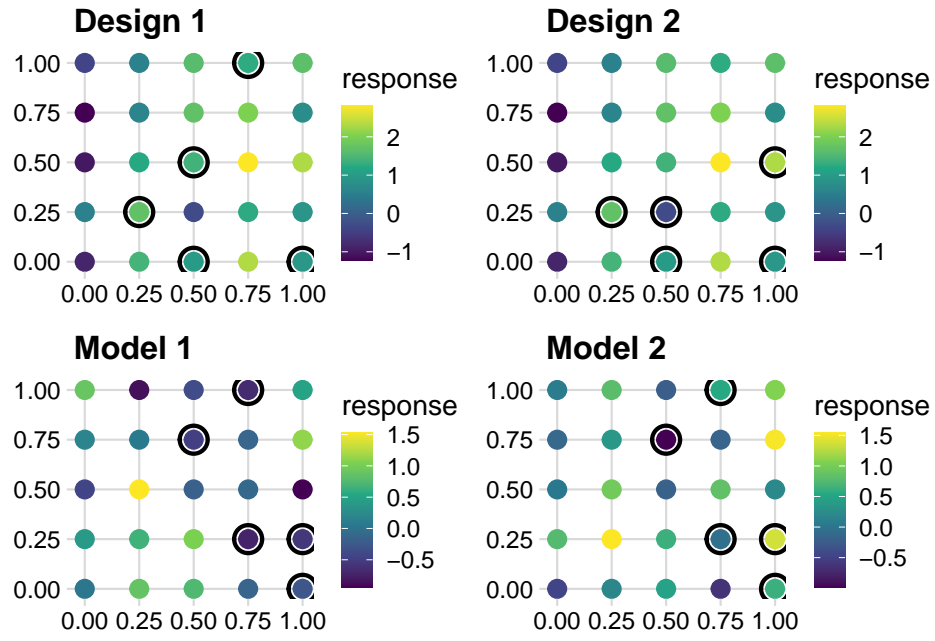


Figure 1: A comparison of sampling under the design-based and model-based frameworks. Points circled are those that are sampled. In the top row, we have one fixed population, and two random samples. In the bottom row, we have two realizations of the same spatial process sampled at the same locations.

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

136 Spatially balanced samples are useful because they tend to yield estimates
137 that have lower variance than estimates constructed from sampling designs
138 lacking spatial balance (Barabesi and Franceschi, 2011; Benedetti et al., 2017;
139 Grafström and Lundström, 2013; Robertson et al., 2013; Stevens and Olsen,
140 2004; Wang et al., 2013). To quantify spatial balance, Stevens and Olsen (2004)
141 proposed loss functions based on Voroni polygons. The first spatially balanced
142 sampling algorithm that saw widespread use was the Generalized Random
143 Tessellation Stratified (Stevens and Olsen, 2004). Since GRTS was developed,
144 several other spatially balanced sampling algorithms have emerged, including
145 the Local Pivotal Method (Grafström et al., 2012; Grafström and Matei, 2018),
146 Spatially Correlated Poisson Sampling (Grafström, 2012), Balanced Acceptance
147 Sampling (Robertson et al., 2013), Within-Sample-Distance (Benedetti and
148 Piersimoni, 2017), and Halton Iterative Partitioning (Robertson et al., 2018).
149 We focus on the Generalized Random Tessellation Stratified (GRTS) algorithm
150 to select spatially balanced sampling because it has several attractive properties,
151 including **Lisa M.**: List major attractive properties, and detailed by Stevens
152 and Olsen (2004) and Dumelle et al. (2021).

153 The GRTS algorithm is used to sample from finite and infinite populations
154 and works by utilizing a mapping between two-dimensional and one-dimensional
155 space. The population units in two-dimensional space are divided into cells using
156 a hierarchical index. Population units are then mapped to a one-dimensional
157 line via the hierarchical indexing. The line length of each population unit equals
158 its inclusion probability. A systematic sample is conducted on the line and these
159 samples are linked to a population unit in two-dimensional space, which results
160 in the desired sample. Stevens and Olsen (2004) and Dumelle et al. (2021)
161 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

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

where Z_i and π_i are the observed value and inclusion probability of the i th 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 estimator tends to reduce the estimated standard error of $\hat{\tau}$, 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 $\mathbf{z} \equiv \{z(s_1), z(s_2), \dots, z(s_N)\}$ be a response vector at locations s_1, s_2, \dots, 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 ,

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

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

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

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

There were several variables to alter in the simulations, and the names of the scenarios in future plots mirror these variables

- correlation type: dependent errors or independent errors
- error type:
 - normal: mean 0, variance 2
 - lognormal: log scale mean 0, log scale variance 2 (total variance 47)
 - lognormalbig: log scale mean 0, log scale variance 4 (total variance 2,926)
- sample sizes: $n = 10, 50, 150$; $N = 900$
- layout: gridded vs random uniform population locations confined to a 1 x 1 unit square

So for example, the `inderror.normal.n50.randloc` is the simulation having independent random errors that are normal, a sample size of 50, and random population locations.

There were 2000 trials for each simulation. The original response (before exponentiating if applicable) for the dependent error cases was normally distributed with an exponential covariance function with partial sill of 0.9, effective

233 range of $\sqrt{2}$, and a nugget of 0.1. For the independent error cases, the partial
 234 sill was 0 and the nugget was 1.

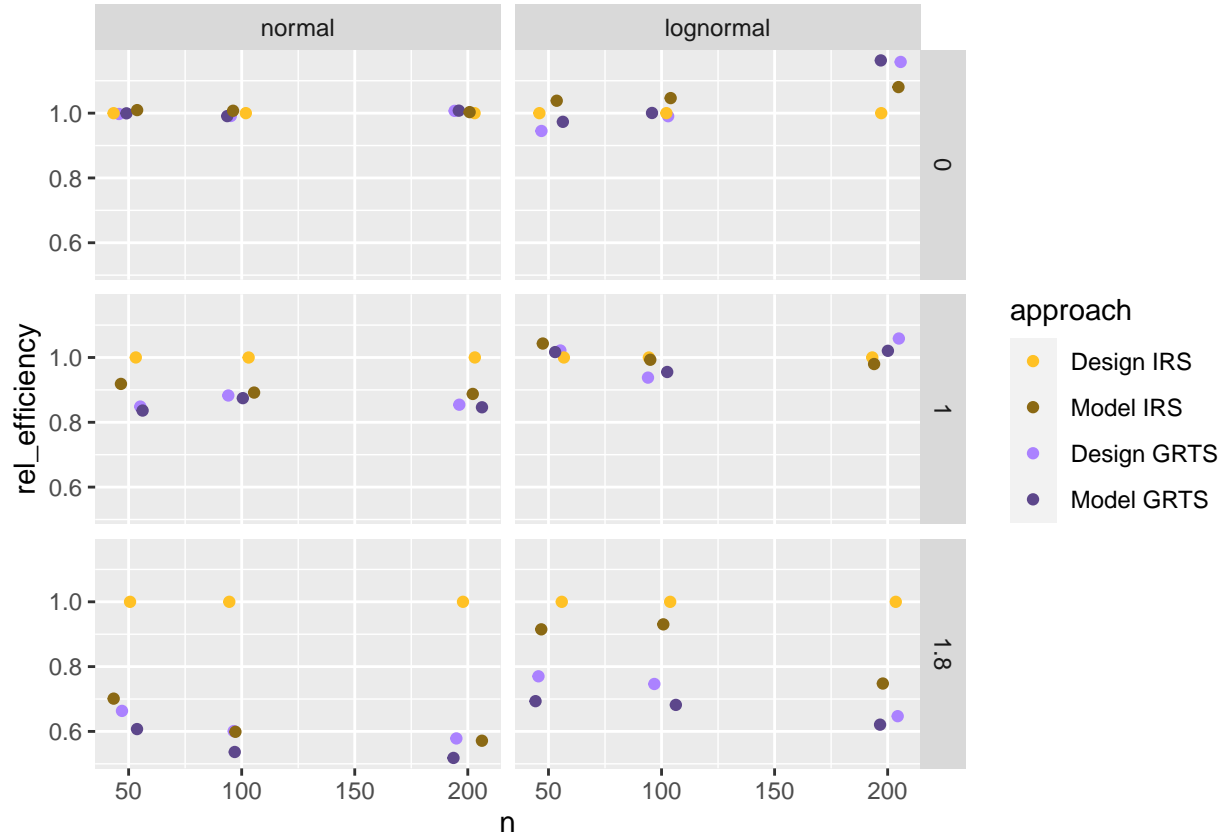
235 **Lisa M.** Notes: adding an intermediate level of spatial dependency? Transfer
 236 simulation scenarios to a table Explain what the effective range is Fill in the
 237 details of what exactly each approach means (perhaps a table would be a good
 238 way to do this) Reorder the sims in the first figure by some criterion. Think
 239 about what would be a “reasonable sample size” instead of 10. Define medae If
 240 the data has a large right-skew, wouldn’t one consider a transformation before
 241 the analysis? We should address this by stating that the BLUP for the log
 242 response does not mean that $e^{\log \text{BLUP}}$ is the BLUP for the response on the
 243 original scale.

244 In each simulated data set, a GRTS sample and an IRS sample were selected.
 245 Then for the GRTS sample, the design-based approach using the local neighbor-
 246 hood variance (Design GRTS) and a model-based approach were applied (Model
 247 GRTS). Then for the IRS sample, the design-based approach using the simple
 248 random sample variance (Design IRS) and a model-based approach were applied
 249 (Model IRS).

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

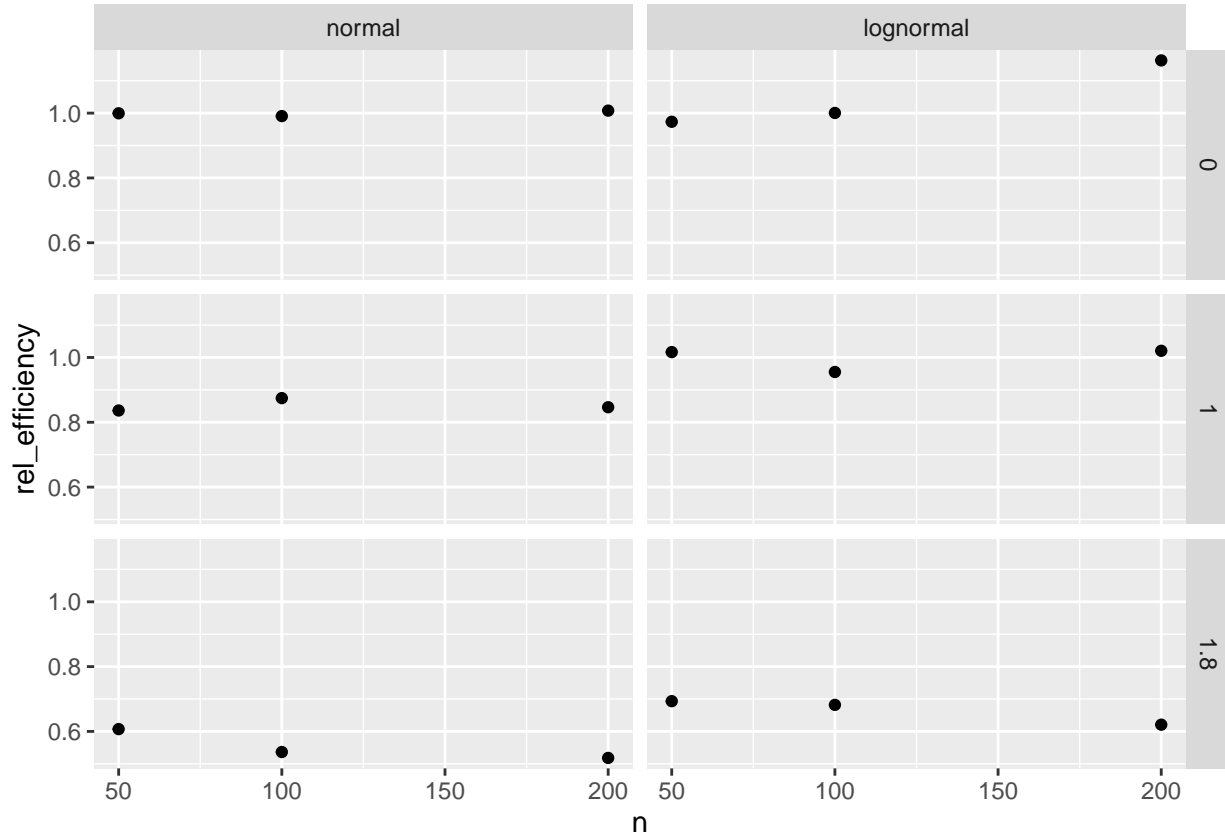
255 MAJOR POINTS for the following Figure, which has relative efficiency
 256 ($\text{rmspe} / \text{Design IRS rmspe}$): We see that

- 257 • When there is no spatial correlation (top row), we aren’t losing that much
 258 by using a spatial method over Design IRS, even if assumptions are violated.
- 259 • When there is a lot of spatial correlation Model GRTS tends to perform
 260 best, but difference in relative efficiency between Model GRTS and Design
 261 GRTS is not very big. In many settings Design GRTS outperforms Model
 262 IRS by a large margin, suggesting that the design decision (whether to use
 263 IRS or GRTS) is much more important than the analysis decision (whether
 264 to analyze using model assumptions or not).
- 265 • If there is a large amount of spatial correlation, we should **not** use IRS.
 266 Even though it’s assumptions are satisfied, the resulting estimator is much
 267 worse than an estimator using a spatially balanced sample.
- 268 • If we are comparing design-based and model-based methods, we should
 269 not use a poor design to compare with (give examples?).



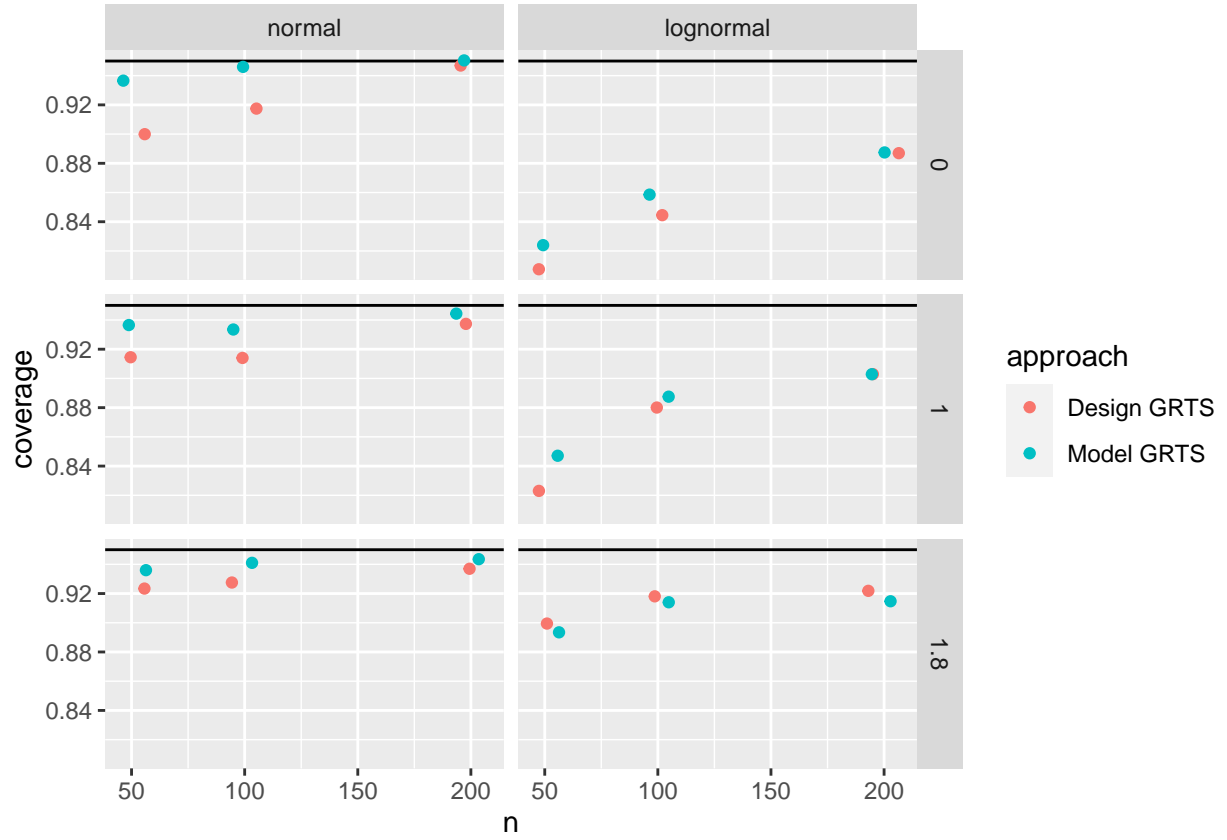
MAJOR POINTS for the following Figure:

- when we drop the IRS samples to compare the GRTS samples more closely (looking at the relative efficiency of model rmspe / design rmspe), we see that the model-based approach is usually better than the design-based approach (but, keep in mind that the improvement was small compared to the improvement of both methods over Design IRS).
- when the model used is the same model that generated the data, the Model-based approach far outperforms the Design-based approach, especially when there is a lot of spatial correlation (bottom-left facet). The methods perform similarly when there is no spatial correlation.
- even when the model that generates the data is different than the model used to fit the data (lognormal), the model-based approach still outperforms the design-based approach when there is a high amount of spatial correlation.



MAJOR POINTS for the following Figure:

- coverage for the model-based estimator is slightly higher than coverage for the design-based estimator in the normal settings. Coverages are about equal in the lognormal settings with a slight edge to model-based (this is the point that will be tougher to explain: I would have expected the design-based estimator to have better coverage in the lognormal settings because it has fewer assumptions).
- coverage is at or near the nominal 95% in all of the normal settings, where assumptions for the model approach and the design approach are satisfied.
- 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.



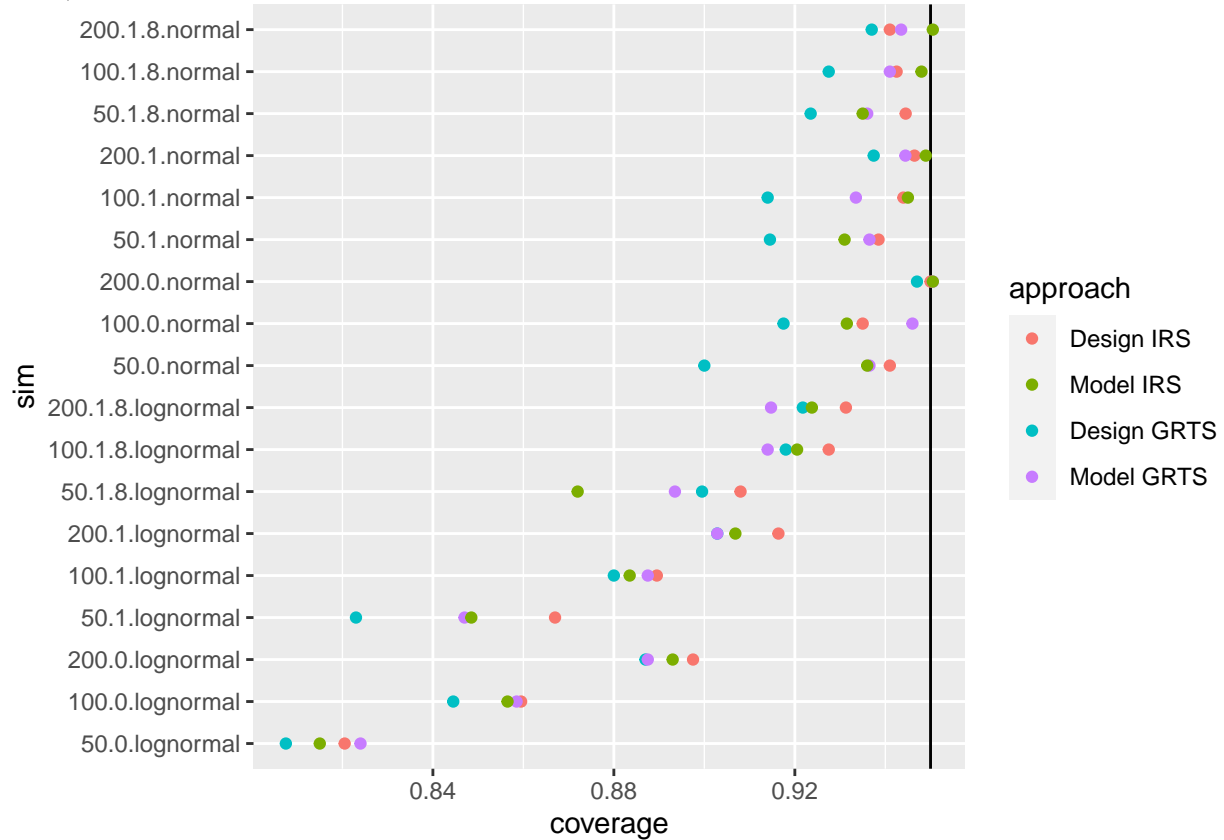
Major Points from August 3 Simulations:

1. In most of the dependent error simulation settings, either all four approaches (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 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. Coverage

For Gaussian errors, coverage for all approaches tended to be near 0.95. There was less between-approach deviation in coverages for random locations compared to grid locations. Generally, the larger the skew, the worse the coverage, and the larger the sample size, the better the coverage. Design GRTS (local neighborhood variance) tended to slightly undercover, a result Tony was familiar with.



333

5. 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 better.
- a spatially balanced GRTS sample outperforms IRS in nearly all dependent error settings, as expected.

341

- 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).

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 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 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 103.2 ng / g.

Table 1: Application of design-based and model-based approaches to the NLA data set on mercury concentration. The true mean concentration is 103.2 ng / g

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

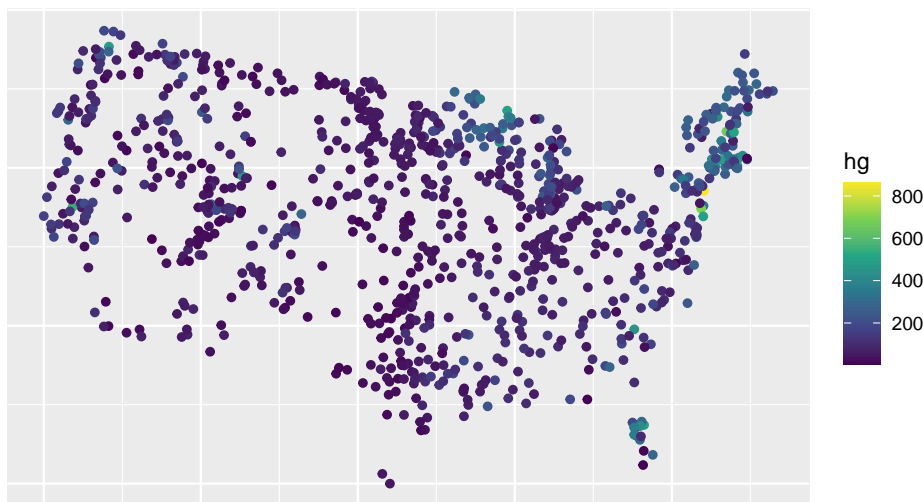


Figure 2: Population distribution of mercury concentration for 986 lakes in the contiguous United States. Thirty-five lakes were dropped from the analysis because they were missing mercury concentration.

374 Table 1 shows the application of a design-based analysis on an IRS, a model-
 375 based analysis on an IRS, a design-based analysis on a GRTS sample, and a
 376 model-based analysis on a GRTS sample. We see that, for all four analyses,
 377 the true realized mean mercury concentration is within the bounds of the
 378 95% intervals. However, we should not generalize the results of this particular
 379 realization to any other data set or even to other potential samples of this data
 380 set.

381 But, we do note a couple of patterns. The design-based IRS analysis shows
 382 the largest standard error: a likely reason is that this is the only approach
 383 that does not use the spatial correlation in mercury concentration across the
 384 contiguous United States. We also see that, for the samples drawn, the both
 385 analyses with the GRTS sampling design have a lower standard error than the
 386 analyses with the IRS sampling design. We would expect this to be the case for
 387 most samples because mercury concentration exhibits spatial correlation so a
 388 spatially balanced sample should usually yield a lower standard error. If it is
 389 acceptable to have an interval for mean mercury concentration of about 25 ng /
 390 g and if we ignore the other variables that the EPA collects information on in
 391 these NLA surveys, then the EPA could consider sampling just 50 lakes to save
 392 time and money.

393 5. Discussion

- 394 • Pros of Design-Based (items we are not exploring): computationally effi-
 395 cient, 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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