

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

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12 **Abstract**

 This is the abstract.

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21 **1. Introduction**

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

32 Though the design-based and model-based approaches apply to statistical
33 inference in a broad sense, we focus on comparing these approaches for spatial
34 data. We define spatial data as variables measured at specific geographic locations.
35 De Gruijter and Ter Braak (1990) give an early comparison of design-based and
36 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 location in sampling 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 sampling 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 properties of parameter estimates from both approaches. And in Section 4, 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 process. Randomness is often incorporated through distributional assumptions on the data-generating process. Instead of estimating fixed but unknown parameters (as in the design-based approach), the goal of model-based inference in the spatial

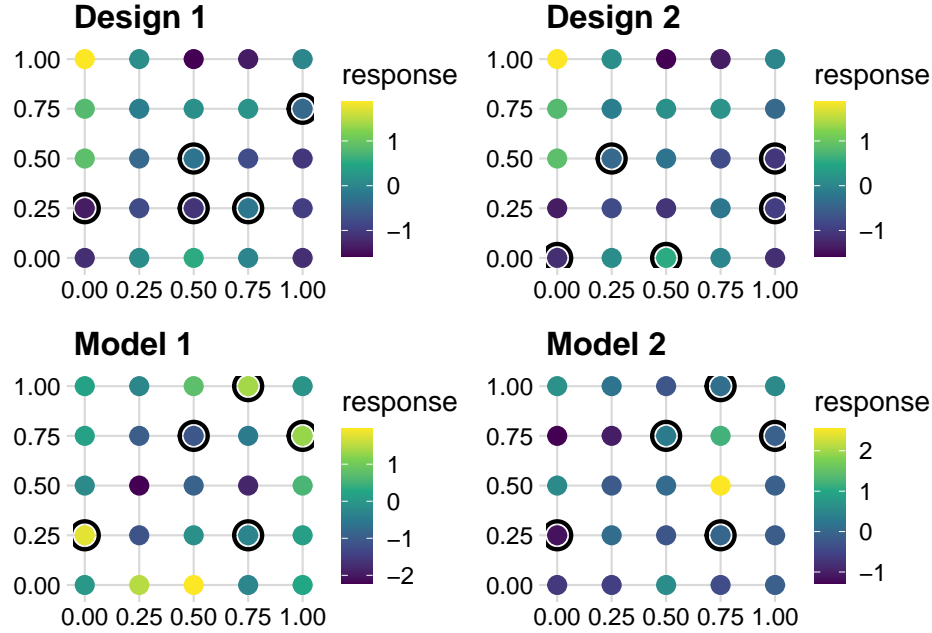


Figure 1: A comparison of sampling under the design-based and model-based frameworks. In the top row, we have one fixed population, and two random samples. In the bottom row, we have two realizations of the same spatial process sampled at the same locations.

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 the true mean of the spatial process that generated our realized data is still not known. When predicting the realized mean, we typically are not interested in the underlying process' true mean.

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 can be more precise. Cressie (1993) and Schabenberger and Gotway (2017) provide reviews of model-based approaches for spatial data.

2.2. Spatially Balanced Design and Analysis

Sampling designs can incorporate spatial locations to obtain samples that are spatially balanced with respect to the population (Stevens Jr and Olsen, 2004). A sample is spatially 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 are 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) algorithms. We focus on the Generalized Random Tessellation Stratified (GRTS) algorithm to select spatially balanced sampling because the algorithm 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 size. Stevens Jr and Olsen (2004) provide and Dumelle et al. (2021) provide further details. The GRTS algorithm is available in the **R** package `spsurvey` (Dumelle et al., 2021).

After collecting a sample, the data are used to estimate population parameters. The Horvitz-Thompson estimator (Horvitz and Thompson, 1952) and its continuous analog (Cordy, 1993) yield unbiased estimates of population means and totals. 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. 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, which can be very difficult to

136 calculate. Second, they ignore the spatial locations of the population units.
 137 To address these drawbacks, Stevens Jr and Olsen (2003) proposed a local
 138 neighborhood variance estimator. The local neighborhood variance estimator
 139 does not rely on π_{ij} , and it incorporates spatial locations by assigning higher
 140 weights to nearby observations. Stevens Jr and Olsen (2003) show this variance
 141 estimators tends to reduce the variability associated with estimating τ . This
 142 yields confidence intervals for τ that are narrower than confidence intervals
 143 constructed from variance estimators ignoring spatial locations.

144 2.3. Finite Population Block Kriging

145 We only use FPBK in this paper in order to focus more on comparing the
 146 design-based and model-based approaches. However, k-nearest-neighbors (Fix
 147 and Hodges, 1951; Ver Hoef and Temesgen, 2013), random forest (Breiman,
 148 2001), Bayesian models (Chan-Golston et al., 2020), among others, can also be
 149 used to obtain predictions for a mean or total from spatially correlated responses
 150 in a finite population setting.

151 Finite Population Block Kriging (FPBK) is an alternative to sampling-based
 152 methods (Ver Hoef, 2008). FPBK expands the geostatistical kriging framework
 153 to the finite population setting. Instead of basing inference off of a specific
 154 sampling design, we assume the data were generated by a spatial process with
 155 parameters that can be estimated using the framework of a model.

156 Ver Hoef (2008) gives details on the theory of FPBK, but some of the basic
 157 principles are summarized below. For a response variable \mathbf{z} that can be measured
 158 on a finite number of N sites, we want to predict some linear function of the
 159 response variable, $\tau(\mathbf{z}) = \mathbf{b}'\mathbf{z}$, where \mathbf{b} is a vector of weights. For example, if we
 160 want to predict the total abundance across all sites, then we would use a vector
 161 of 1's for the weights.

162 Typically, however, we only have a sample of the N sites. Denoting quantities
 163 that are part of the sampled sites with a subscript s and quantities that are part
 164 of the unsampled sites with a subscript u ,

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

165 where \mathbf{X}_s and \mathbf{X}_u are the design matrices for the sampled and unsampled sites,
 166 respectively, and $\boldsymbol{\delta}_s$ and $\boldsymbol{\delta}_u$ are random errors for the sampled and unsampled
 167 sites. Denoting $\boldsymbol{\delta} \equiv [\boldsymbol{\delta}_s \ \boldsymbol{\delta}_u]'$, we assume that $E(\boldsymbol{\delta}) = \mathbf{0}$.

We also typically assume that there is spatial correlation in $\boldsymbol{\delta}$, which can be
 modeled using a covariance function. Many common choices for this function
 assume that spatial covariance decreases with increasing Euclidean distance
 between sites. The primary function used throughout the simulations and
 applications of this manuscript is the Exponential covariance function: the i, j^{th}
 entry for $\text{var}(\boldsymbol{\delta})$ 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 sites 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 . However, any spatial covariance function could be used in the place of the Exponential, including functions that allow for anisotropy [pg. 80 - 93](Chiles and Delfiner, 1999).

With the above model formulation, the Best Linear Unbiased Predictor (BLUP) for $\tau(\mathbf{b}'\mathbf{z})$ is vague 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. Neither require a particular distribution for \mathbf{z} .

3. Numerical Study

For the following simulation results, we simulated 1040 different gridded populations, each of size 900 with sample size 150. For the model-based approach (FPBK), sites were selected via Independent Random Sample. For GRTS, the local mean variance was 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.

Approach	Bias	RMSE	MedAE	Coverage	PClose	MedIL
Design	0.0003	0.0353	0.0251	0.9461	0.4889	0.1362
Model	-0.0001	0.0362	0.0253	0.9480	0.5111	0.1430

Table 1: Approach, mean bias (Bias), root-mean-squared error (RMSE), median absolute error (MedAE), 95 percent interval coverage (Coverage), proportion of times the approach was closer to the true value (PClose), and median interval length (MedIL)

Base Simulations

- both good: correctly specified model with high correlation
- break model: non-gaussian errors
- break design: small area estimation
- both good?: misspecified covariance model with high correlation
- break both? non-gaussian areas with smaller sample size
- change n or sampling fraction
- model-based: how should sample be drawn? should locations be fixed?

3.1. Software

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).

199 3.2. *Applied Example*

200 Potential Data Sets:

- 201 • National Lakes Assessment
- 202 • Moose in Alaska
- 203 • Temperature Data from NOAA

204 4. Discussion

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