

Comparison of Estimators for the National Resources Inventory Calibration Study

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Abstract

The National Resources Inventory (NRI) is a longitudinal survey of non-federal lands in the U.S. A new protocol for measuring the extent of developed land was implemented in 2003. In 2005, an experiment was conducted to estimate the relation between measurements obtained from the new and former procedures. We propose a model for the data from the calibration experiment and evaluate estimators of model parameters through simulation.

The estimation procedure requires an estimator of the unknown covariance matrix of a vector of moments. One way to estimate this covariance matrix is to use the moments of the normal distribution. The delete-one jackknife provides a non-parametric alternative. The results of the simulation study indicate that both estimators of model parameters are approximately unbiased and that the estimator based on the jackknife covariance matrix is more variable than the estimator based on the normal moment covariance matrix.

We construct two estimators of the variance of the estimator based on the normal moment covariance matrix. The first continues to use the moments of the normal distribution to estimate the unknown covariance matrix. The second variance estimator uses the jackknife estimator in conjunction with the normal moment estimator. Both estimators are approximately unbiased for variances of estimators of the slope and intercept in the linear calibration equation. Skewness leads to a downward bias in the normal-based variance estimator for variance components.

KEY WORDS: Measurement Error, Calibration, Sandwich Variance Estimator

1. Introduction

We consider the problem of calibrating a new instrument for measuring developed land in the National Resources Inventory (NRI) against a standard procedure. The NRI is a large-scale longitudinal survey of nonfederal lands in the U.S. The NRI provides estimates of land cover, land use, and conservation practices from 1982 through the present. A new protocol for measuring the extent of developed land – urbanized areas and transportation infrastructure – was implemented in 2003. It is important that measurements under the new protocol are consistent with measurements from the old protocol because a primary objective of the NRI is to estimate change. To retain the interpretability of NRI's trend estimates, it is

essential that physical changes are not confounded with the impacts of new procedures. In 2005, a special study was conducted to obtain data that can be used to estimate the relation between measurements from the new and former procedures. We propose a linear calibration equation for the data from the 2005 calibration experiment.

To estimate model parameters, we apply generalized least squares to a vector of first and second sample moments. We consider two ways to estimate the covariance matrix of the vector of sample moments. The first uses the moments of the normal distribution and the second is the delete-one jackknife. The normal moment estimator is inconsistent if the observations are not normal, while the jackknife estimator is consistent in the absence of parametric assumptions (Shao, 2003).

We compare two estimators of the variance of the estimator based on the normal moment covariance matrix. The first variance estimator continues to use the normal moments to estimate the unknown covariance matrix. The second variance estimator is akin to the “sandwich” or “heteroscedasticity-consistent” variance estimator of generalized estimating equations (Carroll and Kauer- mann, 2001).

In Section 2, we describe the protocol used in the NRI and the structure of the 2005 calibration experiment. A model is presented in Section 3 for the data collection procedure. In Section 4, we describe the estimators of model parameters and the variance estimators. In Section 5, we discuss the simulation study used to evaluate the effects of skewness and sample size on properties of the estimators.

2. The Calibration Experiment

2.1 Recent Protocol Changes in the NRI

Sampling units in the NRI are sections of land called “segments.” Approximate areas of segments range from 40 to 640 acres, with a typical size of 160 acres. Much of the NRI data are based on aerial photographs of sampled segments. Before 2000, photo interpretation was recorded on a transparent overlay placed over the segment photo. Now, all of the photographs are digitized, which enables computer-assisted data collection.

In 2003, an additional change to the procedure for measuring developed land was implemented. Developed land includes residential and urban areas as well as transportation infrastructure. Under the original procedure, data collectors manually outlined the developed area on

a transparent overlay placed on the segment photo. Data gatherers needed to make some difficult judgments with respect to boundaries of residential areas when implementing this method. The new procedure involves a combination of manual and computerized delineation in an effort to eliminate some of the variability due to inherent differences between data collectors. Under the new procedure, the data collector clicks on the roof of a residence with a mouse on the digitized segment photo. A computer program then uses these locations to define the developed area. Each residence defines the center of a hexagon. Hexagons are linked if the distance between centers is below a certain threshold. A region is deemed “built-up” if it is composed of hexagons of a pre-specified total area.

2.2 Measurement of Developed Land

Under both the new and old protocols, measurement of developed land involves several steps. In a given year, the data collector first reexamines the photograph of the segment from the previous year to determine the developed land features for that year. He/she then measures changes that have occurred. Consequently, a determination of level in any given year requires imagery from the current year and from the previous or “base” year.

2.3 The 2005 Calibration Study

Since it was no longer possible to implement the old protocol in 2005, the data collection component of the calibration study applied new methods to photo images of segments from 2001 and 2003 for which measurements from the old procedure already existed. The 2002 data were not used because the available NRI sample size for 2002 is smaller than those of 2001 and 2003. Three Remote Sensing Laboratories (RSL), the East, Central, and West, oversee data collection in the NRI. Due to differences in the character of land use in the three regions, we analyze the data from each RSL separately. In the 2005 calibration experiment, the East RSL had 1036 segments, the Central RSL had 1055 segments, and the West RSL had 608 segments. Images from 2001 serve as the “base year” and those from 2003 function as the “current year”. Therefore, measurements of interest are 2003 level and change for the 2001 to 2003 interval.

Two independent determinations are made on each segment using the new protocol. (Without this replication, we would not be able to identify important sources of variability). To ensure that the calibration experiment provides a valid representation of the real data collection process, each of these replicates requires two data collectors. The first data collector measures 2001 level using the photo image from 1997. The second data collector uses this first data collector’s determination as the starting point for measurements of 2003 level and 2001 to 2003 change. The first data collector’s determination of 2001 level is not used in the statistical analysis be-

cause it is directly influenced by the 1997 measurement, which is based on the old protocol. The four data collectors involved in this process (two for each replicate) are randomly assigned to segments and to tasks.

The data of interest consist of the following variables for each segment:

- one measurement of 2003 level from the old procedure
- one measurement of 2001-2003 change from the old procedure
- two independent measurements of 2003 level from the new procedure
- two independent measurements of 2001-2003 change from the new procedure.

3. Model Specification

The model that we propose for the data from the calibration study reflects the data collection process. In this section, we first specify a model for the individual observations on each segment. We then define the vector of first and second sample moments of the observations, which serves as the response variable in the estimation procedure. We conclude this section with a discussion of some of the properties of the theoretical covariance matrix of this vector of sample means and covariances.

3.1 A Model for Individual Measurements of Acres of Developed Land

Let i be the index for the segment, where $i = 1, \dots, n$, and let t be the index for the two time points. Here $t = 1$ stands for 2001 and $t = 2$ denotes 2003. For each segment i , two sets of data collectors make independent measurements of both 2003 level and 2001 to 2003 change using the new protocol. Let $j = 1, 2$ represent these replicates.

The statistical conceptualization consists of three main parts: 1) a model for the population of true segment values, 2) a model for the measurements from the old protocol, and 3) a model for the measurements from the new procedure.

Let x_{ti} denote the true, unobserved, acres of developed land on segment i in year t . We treat these true values as a random sample from a population:

$$x_{ti} = \mu_t + \gamma_{ti}, \text{ where } E[\gamma_{ti}] = 0, \text{ and } \text{Var}(\gamma_{ti}) = \sigma_x^2. \quad (1)$$

We also assume that the true values on a given segment at the two time points are correlated:

$$x_{2i} - x_{1i} = d_i, \quad (2)$$

where $E[d_i] = \mu_2 - \mu_1$, and $\text{Var}(d_i) = \sigma_d^2$.

Second, we specify a model for the measurements of both 2003 level and 2001 to 2003 change based on the old protocol. Let X_{ti} be the measurement of developed land

on segment i in year t obtained from the old procedure, and let u_{ti} be the associated measurement error. We assume $E[u_{ti}] = 0$ and $Var(u_{ti}) = \sigma_{ui}^2$. Then, 2003 level is

$$X_{2i} = x_{2i} + u_{2i}, \quad (3)$$

and 2001 to 2003 change is

$$\Delta X_i := X_{2i} - X_{1i} = d_i + b_i, \quad (4)$$

where $E[b_i] = 0$ and $Var(b_i) = \sigma_{bi}^2$.

Third, we specify a linear relation between the true values associated with the new protocol and the unobserved measurands. Let Y_{tij} denote the measured acres of developed land using the new protocol. Let e_{tij} be the random measurement error in the new procedure. Assume $E[e_{tij}] = 0$, and $Var(e_{tij}) = \sigma_{ei}^2$. The model for 2003 level is

$$Y_{2ij} = \delta + \alpha x_{2i} + e_{2ij}. \quad (5)$$

For 2001 to 2003 change, we specify

$$\Delta Y_{ij} = Y_{2ij} - Y_{1ij} = \alpha d_i + a_{ij}, \quad (6)$$

where a_{ij} have $E[a_{ij}] = 0$ and $Var(a_{ij}) = \sigma_{ai}^2$. Ideally, $\delta = 0$ and $\alpha = 1$. Because Y_{tij} is generated by a computer program, adjustments will be made to the program until these target values are attained.

We make two assumptions regarding independence relationships. First, because the four data collectors work independently, we assume e_{ti1} and e_{ti2} are independent for all t and i . Likewise, we assume a_{i1} and a_{i2} are independent for all i . Second, we assume (u_{ti}, b_i) and (e_{tij}, a_{ij}) are independent for all i, t , and j .

3.2 Summary Statistics Used in Estimation

We summarize the information in the data from each segment through a vector of statistics. For each segment i , let

$$\mathbf{z}_i = \left(\frac{1}{2}(\Delta Y_{i1} + \Delta Y_{i2}), \Delta X_i, \frac{1}{2}(Y_{2i1} + Y_{2i2}), X_{2i}, Y_{2i2} - Y_{2i1}, \Delta Y_{i2} - \Delta Y_{i1} \right)'. \quad (7)$$

Let $\bar{\mathbf{Z}}$ and $\mathbf{m}_{\mathbf{ZZ}}$ be the sample mean and covariance matrix of the vectors \mathbf{z}_i , respectively. Let \bar{Z}_i denote the i^{th} entry of $\bar{\mathbf{Z}}$, and let m_{ij} denote the entry in row i and column j of $\mathbf{m}_{\mathbf{ZZ}}$ (where $i, j = 1, \dots, 6$). Let $\sigma_{ij} = E[m_{ij}]$ denote the corresponding population moments. By the model assumptions in (1) – (6), there are seventeen first and second order sample moments with non-zero expectations. Let \mathbf{W} denote the vector of seventeen sample moments, and let β denote the vector of ten model parameters. Then,

$$\mathbf{W} = (\bar{Z}_1, \bar{Z}_2, \bar{Z}_3, \bar{Z}_4, m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{33}, m_{34}, m_{44}, m_{55}, m_{56}, m_{66}), \quad (8)$$

and

$$\beta = (\delta, \alpha, \mu_1, \mu_2, \sigma_x^2, \sigma_d^2, \sigma_u^2, \sigma_b^2, \sigma_e^2, \sigma_a^2). \quad (9)$$

The variances in β are average variances. The mean of \mathbf{W} is a nonlinear function of the ten model parameters. Specifically,

$$E[\mathbf{W}] := \mathbf{g}(\beta) \quad (10)$$

$$= [\alpha(\mu_2 - \mu_1), \mu_2 - \mu_1, \delta + \alpha\mu_2, \mu_2, \alpha^2\sigma_d^2 + \frac{\sigma_a^2}{2}, \alpha\sigma_d^2, \frac{\alpha^2\sigma_d^2}{2} + \frac{\sigma_a^2}{4}, \frac{\alpha\sigma_d^2}{2}, \sigma_d^2 + \sigma_b^2, \frac{\alpha\sigma_d^2}{2}, \frac{\sigma_d^2}{2} + \frac{\sigma_b^2}{2}, \alpha^2\sigma_x^2 + \frac{\sigma_e^2}{2}, \alpha\sigma_x^2, \sigma_x^2 + \sigma_u^2, 2\sigma_e^2, \sigma_a^2, 2\sigma_a^2]. \quad (11)$$

We assume that \mathbf{W} has a finite variance, $\mathbf{V}_{\mathbf{ww}}$.

Observe that some of the entries of \mathbf{W} provide direct unbiased estimators of certain model parameters. For example, the 15th, 16th and 17th components of \mathbf{W} are unbiased estimators of $2\sigma_e^2$, σ_a^2 and $2\sigma_a^2$ respectively. Similarly, the second and fourth elements of \mathbf{W} are unbiased for μ_2 and $\mu_2 - \mu_1$ respectively. Because the method of moments produces several consistent estimators of the elements β , we use generalized least squares with \mathbf{W} as the response in estimating β .

We write $\mathbf{V}_{\mathbf{ww}}$ in partitioned form to clarify the structure of this covariance matrix:

$$\mathbf{V}_{\mathbf{ww}} = \begin{pmatrix} \Omega_{11} & \Omega_{12} & \Omega_{13} \\ \Omega_{12}' & \Omega_{22} & \Omega_{23} \\ \Omega_{13}' & \Omega_{23}' & \Omega_{33} \end{pmatrix}. \quad (12)$$

With no distributional assumptions, $\mathbf{V}_{\mathbf{ww}}$ has 153 unconstrained parameters. The entries of the 4x4 matrix Ω_{11} are covariances of sample means. The 14x14 matrix Ω_{22} has covariances of sample second moments of the four elements of \mathbf{z}_i with nonzero expectations. The 3x3 matrix Ω_{33} contains covariances of second moments of measurement errors from the new protocol.

4. Estimation

To apply generalized least squares to the vector of sample moments \mathbf{W} to estimate β requires a working covariance value for $\mathbf{V}_{\mathbf{ww}}$. We compare estimators of β arising from two choices for the working matrix. To construct the first estimator $\hat{\beta}_1$, we employ the moments of the normal distribution to obtain the working covariance matrix for \mathbf{W} . We refer to $\hat{\beta}_1$ as the “estimator based on the normal-moments.” We denote the elements of $\hat{\beta}_1$ by $\hat{\alpha}_1, \hat{\delta}_1$, etc. For the second estimator $\hat{\beta}_2$, we use the delete-one jackknife to estimate $\mathbf{V}_{\mathbf{ww}}$. We refer to $\hat{\beta}_2$ as the “estimator based on the jackknife” and denote the elements of $\hat{\beta}_2$ by $\hat{\alpha}_2, \hat{\delta}_2$, etc. In both procedures, we alter extreme observations in an attempt to stabilize the covariance matrices used in estimation.

We compare two estimators of the variance of $\hat{\beta}_1$. We adopt the terminology and notation of Carroll and Kauer mann (2001) to label these two estimators. The first variance estimator continues to use the moments of the normal distribution for the covariance of \mathbf{W} . We call this variance estimator the model based estimator. We denote the model based estimator by $\hat{\mathbf{V}}_{\mathbf{M}}(\hat{\beta}_1)$. We incorporate

the jackknife estimator of the covariance of \mathbf{W} into the second estimator of the variance of $\hat{\beta}_1$ in sandwich form. We denote this sandwich variance estimator by $\hat{\mathbf{V}}_{\mathbf{S}}(\hat{\beta}_1)$.

We investigate an estimator for the variance of β_2 that uses the same jackknife estimator of $\mathbf{V}_{\mathbf{ww}}$ used to construct $\hat{\beta}_2$.

4.1 Estimation of $\mathbf{V}_{\mathbf{ww}}$

Normal Moment Estimator of $\mathbf{V}_{\mathbf{ww}}$

If the populations of true values and measurement errors have normal distributions, then

$$\mathbf{V}_{\mathbf{ww}} = \text{block-diag}(\Omega_{11}, \Omega_{22}^*), \quad (13)$$

where Ω_{11} is as in (12) and Ω_{22}^* is the lower right 13x13 block of $\mathbf{V}_{\mathbf{ww}}$:

$$\Omega_{22}^* = \begin{pmatrix} \Omega_{22} & \Omega_{23} \\ \Omega_{23}' & \Omega_{33} \end{pmatrix}. \quad (14)$$

In (14), the element of Ω_{22}^* corresponding to m_{ij} and m_{kl} is

$$(\sigma_{ik}\sigma_{jl} + \sigma_{il}\sigma_{jk}). \quad (15)$$

Replacing theoretical moments σ_{ij} with sample moments m_{ij} produces the first estimator of $\mathbf{V}_{\mathbf{ww}}$, which we denote by $\hat{\mathbf{V}}_{\mathbf{ww},1}$. If the assumption of normality holds, then $\hat{\mathbf{V}}_{\mathbf{ww},1}$ is a consistent estimator of the covariance of \mathbf{W} . The normal moment estimator is consistent for covariances of sample means, Ω_{11} , provided the error variances are constant.

Jackknife Estimator of $\mathbf{V}_{\mathbf{ww}}$

An alternative estimator of $\mathbf{V}_{\mathbf{ww}}$ is the delete-one jackknife procedure. For $k = 1, \dots, n$, we omit segment k and let $\mathbf{W}^{(k)}$ be the vector of seventeen sample moments based on the $n-1$ remaining segments. Then, the jackknife estimator of $\mathbf{V}_{\mathbf{ww}}$ is

$$\hat{\mathbf{V}}_{\mathbf{ww},2} = \frac{n-1}{n} \sum_{i=1}^n (\mathbf{W}^{(i)} - \bar{\mathbf{W}}_{jk})(\mathbf{W}^{(i)} - \bar{\mathbf{W}}_{jk})', \quad (16)$$

where $\bar{\mathbf{W}}_{jk} = \frac{1}{n} \sum_{i=1}^n \mathbf{W}^{(i)}$. The jackknife procedure is consistent for $\mathbf{V}_{\mathbf{ww}}$ as long as fourth moments exist.

Modification to Largest Order Statistics

The vector \mathbf{W} is essentially a sample mean of n 17x1 vectors

$$\begin{aligned} \mathbf{W}_i = & (Z_{i1}, Z_{i2}, Z_{i3}, Z_{i4}, (Z_{i1} - \bar{Z}_1)^2, (Z_{i1} - \bar{Z}_1)(Z_{i2} - \bar{Z}_2), \\ & (Z_{i1} - \bar{Z}_1)(Z_{i3} - \bar{Z}_3), (Z_{i1} - \bar{Z}_1)(Z_{i4} - \bar{Z}_4), \\ & (Z_{i2} - \bar{Z}_2)^2, (Z_{i2} - \bar{Z}_2)(Z_{i3} - \bar{Z}_3), \\ & (Z_{i2} - \bar{Z}_2)(Z_{i4} - \bar{Z}_4), (Z_{i3} - \bar{Z}_3)^2, (Z_{i3} - \bar{Z}_3)(Z_{i4} - \bar{Z}_4), \\ & (Z_{i4} - \bar{Z}_4)^2, (Z_{i5} - \bar{Z}_5)^2, (Z_{i5} - \bar{Z}_5)(Z_{i6} - \bar{Z}_6), (Z_{i6} - \bar{Z}_6)^2). \end{aligned} \quad (17)$$

For $j = 1, \dots, 17$, let W_{ij} be the j^{th} entry of the vector \mathbf{W}_i . If the upper tail of the distribution of $\{W_{ij}\}_{i=1}^n$ is more skewed than the exponential, then the estimator described below is better than the sample mean for estimation of the population mean (Fuller, 1991).

Let $W_{(k),j}$ be the k^{th} order statistic of the collection W_{ij} , $i = 1, \dots, n$. Under the exponential model for the largest 30 order statistics, the variables

$$z_{k,j} = (n-k+1)(W_{(k),j} - W_{(k-1),j}), \quad k = n-30, \dots, n \quad (18)$$

have independent, exponential distributions. Then, replace the largest three order statistics $W_{(k),j}$ by $W_{(k),j}^*$ for $k = n, n-1, n-2$, where

$$W_{(n-2),j}^* = W_{(n-3),j} + \min\left(\frac{1}{3}z_{j,n-3}, W_{(n-2),j} - W_{(n-3),j}\right), \quad (19)$$

$$W_{(n-1),j}^* = W_{(n-2),j} + \min\left(\frac{1}{2}z_{j,n-3}, W_{(n-1),j} - W_{(n-2),j}\right), \quad (20)$$

$$W_{(n),j}^* = W_{(n-1),j} + \min(z_{j,n-3}, W_{(n),j} - W_{(n-1),j}), \quad (21)$$

and \bar{Z}_{n-3} is the sample mean of the smallest $n-3$ values of $z_{k,j}$.

When we use sample moments based on the modified data set, we denote the normal moment estimator of the covariance of \mathbf{W} by $\hat{\mathbf{V}}_{\mathbf{ww},1}^*$. The jackknife estimator of $\mathbf{V}_{\mathbf{ww}}$ arising from the modified data set is denoted by $\hat{\mathbf{V}}_{\mathbf{ww},2}^*$. The intent of the modification is to stabilize estimates of the inverse of $\mathbf{V}_{\mathbf{ww}}$ when the sample size is small and the distribution of values skewed. Consequently, we use the estimates of $\mathbf{V}_{\mathbf{ww}}$ based on the modified data set in estimation of β but use the original n observations to estimate the variance of \mathbf{W} in variance estimation when we do not require an additional estimate of the inverse.

4.2 Definition of $\hat{\beta}_1$ and $\hat{\beta}_2$

The estimation procedure selects $\hat{\beta}_i$ to minimize the quadratic form

$$(\mathbf{W} - \mathbf{g}(\beta))' \hat{\mathbf{V}}_{\mathbf{ww},i}^{*-1} (\mathbf{W} - \mathbf{g}(\beta)), \quad (22)$$

where $\hat{\mathbf{V}}_{\mathbf{ww},i}^*$ for $i = 1, 2$ are defined in Section 4.1. In practice, estimates of $\mathbf{V}_{\mathbf{ww}}$ can be unstable when $n = 100$. Therefore, we compute $\hat{\mathbf{V}}_{\mathbf{ww},i}^{*-1}$ as

$$\hat{\mathbf{V}}_{\mathbf{ww},i}^{*-1} = [\hat{\mathbf{V}}_{\mathbf{ww},i}^* + 17n^{-1} \text{diag}(\hat{\mathbf{V}}_{\mathbf{ww},i}^*)]^{-1}, \quad (23)$$

where $\text{diag}(\hat{\mathbf{V}}_{\mathbf{ww},i}^*)$ is a diagonal matrix containing the diagonal elements of $\hat{\mathbf{V}}_{\mathbf{ww},i}^*$. The small additions to the diagonal elements of $\hat{\mathbf{V}}_{\mathbf{ww},i}^*$ help prevent the estimates of $\mathbf{V}_{\mathbf{ww}}$ from becoming too close to singular.

4.3 Variance Estimation

We consider two estimators of the variance of $\hat{\beta}_1$ that are in the spirit of the model-based and sandwich variance estimators of generalized estimating equations (Carroll, 2001). The model-based estimator continues to use the moments of the normal distribution for estimation of $\mathbf{V}_{\mathbf{ww}}$, as follows:

$$\begin{aligned} \hat{\mathbf{V}}_{\mathbf{M}}(\hat{\beta}_1) &= [\mathbf{D}(\hat{\beta}_1)' \hat{\mathbf{V}}_{\mathbf{ww},1}^{*-1} \mathbf{D}(\hat{\beta}_1)]^{-1} \mathbf{D}(\hat{\beta}_1)' \hat{\mathbf{V}}_{\mathbf{ww},1}^{*-1} \quad (24) \\ &\hat{\mathbf{V}}_{\mathbf{ww},1} \hat{\mathbf{V}}_{\mathbf{ww},1}^{*-1} \mathbf{D}(\hat{\beta}_1) [\mathbf{D}(\hat{\beta}_1)' \hat{\mathbf{V}}_{\mathbf{ww},1}^{*-1} \mathbf{D}(\hat{\beta}_1)]^{-1}, \end{aligned}$$

where $\hat{\mathbf{V}}_{\mathbf{ww},1}^{*-1}$ is defined in (23) and $\hat{\mathbf{V}}_{\mathbf{ww},1}$ is defined in (13)-(15) in Section 4.1.

Use of a sandwich variance estimator is more appropriate if we are willing to employ the normal model for estimation but are reluctant to believe that the variables are normally distributed. To construct the sandwich variance estimator, we replace $\hat{\mathbf{V}}_{\mathbf{ww},1}$ in (24) with $\hat{\mathbf{V}}_{\mathbf{ww},2}$ as given below:

$$\begin{aligned} \hat{\mathbf{V}}_{\mathbf{S}}(\hat{\beta}_1) &= [\mathbf{D}(\hat{\beta}_1)' \hat{\mathbf{V}}_{\mathbf{ww},1}^{*-1} \mathbf{D}(\hat{\beta}_1)]^{-1} \mathbf{D}(\hat{\beta}_1)' \hat{\mathbf{V}}_{\mathbf{ww},1}^{*-1} \quad (25) \\ &\hat{\mathbf{V}}_{\mathbf{ww},2} \hat{\mathbf{V}}_{\mathbf{ww},1}^{*-1} \mathbf{D}(\hat{\beta}_1) [\mathbf{D}(\hat{\beta}_1)' \hat{\mathbf{V}}_{\mathbf{ww},1}^{*-1} \mathbf{D}(\hat{\beta}_1)]^{-1}. \end{aligned}$$

An estimator of the variance of $\hat{\beta}_2$ is

$$\begin{aligned}\hat{\mathbf{V}}(\hat{\beta}_2) &= [\mathbf{D}(\hat{\beta}_2)' \hat{\mathbf{V}}_{\mathbf{w}\mathbf{w},2}^{*-1} \mathbf{D}(\hat{\beta}_2)]^{-1} \mathbf{D}(\hat{\beta}_2)' \hat{\mathbf{V}}_{\mathbf{w}\mathbf{w},2}^{*-1} \\ &\quad \hat{\mathbf{V}}_{\mathbf{w}\mathbf{w},2} \hat{\mathbf{V}}_{\mathbf{w}\mathbf{w},2}^{*-1} \mathbf{D}(\hat{\beta}_2) [\mathbf{D}(\hat{\beta}_2)' \hat{\mathbf{V}}_{\mathbf{w}\mathbf{w},2}^{*-1} \mathbf{D}(\hat{\beta}_2)]^{-1}.\end{aligned}\quad (26)$$

5. Simulation Study

We conducted a small simulation study to evaluate the estimators of β and the variance estimators under a variety of circumstances. In the data from the calibration experiment, both the true segment values and the measurement errors have skewed distributions. Therefore, we assess the effects of skewness on properties of estimators of error variances.

5.1 Conditions in Simulations

The model for simulation is the model defined in Section 3. We generate data sets with $n = 100, 500, \text{ and } 1000$ segments. The parameter vector used in the simulations is

$$\begin{aligned}\beta &= (\alpha, \delta, \sigma_u^2, \sigma_e^2, \sigma_x^2, \sigma_d^2, \sigma_b^2, \sigma_a^2, \mu_1, \mu_2) \\ &= (1, 0, 60, 50, 200, 35, 100, 80, 13, 12).\end{aligned}$$

The Monte Carlo sample size is 1000.

Simulation 1: Normal x_{ti}, e_{ti}, u_{ti}

The first simulation serves as a baseline. We generate populations of \mathbf{Z}_i composed of normally distributed true segment values and measurement errors. Under normality, $\mathbf{V}_{\mathbf{w}\mathbf{w}}$ is block diagonal. The submatrices Ω_{12} and Ω_{13} in (12), which contain covariances between sample means and sample second moments, are matrices of zeros. Because the measurement errors and true segment values are uncorrelated, Ω_{23} is a matrix of zeros as well.

Simulation 2: Skewed x_{ti}

In the second simulation, the x_{ti} and d_i are sums of multiples of independent $\chi_{(1)}^2$ random variables. Specifically,

$$x_{1i} = \sqrt{\frac{\sigma_d^2}{4} (\chi_{(1)1i}^2 - 1)} + \sqrt{\frac{\sigma_x^2}{2} - \frac{\sigma_d^2}{4} (\chi_{(1)2i}^2 - 1)} + \mu_1, \quad (27)$$

$$x_{2i} = \sqrt{\frac{\sigma_d^2}{4} (\chi_{(1)3i}^2 - 1)} + \sqrt{\frac{\sigma_x^2}{2} - \frac{\sigma_d^2}{4} (\chi_{(1)2i}^2 - 1)} + \mu_2 \quad (28)$$

and $d_i = x_{2i} - x_{1i}$, where $\chi_{(1)1i}^2, \chi_{(1)2i}^2,$ and $\chi_{(1)3i}^2$ are independent $\chi_{(1)}^2$ random variables. Several features of the population covariance matrix $\mathbf{V}_{\mathbf{w}\mathbf{w}}$ are the same when the population of true values is skewed as when the true values are normally distributed. As discussed in Section 3.2, the last three entries of \mathbf{W} correspond to sample variances and covariances of measurement errors from the new protocol. Consequently, the submatrix Ω_{33} defined in (12) does not change when skewness is introduced into the population of true values. The submatrices Ω_{13} and Ω_{23} in (12) contain population third moments of measurement errors. Because measurement errors are normal, Ω_{13} and Ω_{23} are matrices of zeros under the conditions of Simulation 2. The covariance matrix of sample means Ω_{11} is invariant to changes in the underlying distribution.

The only submatrices in (12) that differ between Simulations 1 and 2 are Ω_{12} and Ω_{22} . Inspection of the mean of the jackknife estimates of $\mathbf{V}_{\mathbf{w}\mathbf{w}}$ at $n = 1000$ suggests that the most substantial changes to Ω_{12} occur in the lower 3x2 block, which is associated with measurements of level from the new and old protocols. The magnitudes of the entries of Ω_{22} are consistently larger when the population of true segment values is skewed.

Simulation 3: Skewed x_{ti}, e_{ti}, u_{ti} :

The third simulation attempts to represent the data from the actual calibration experiment more closely than the other two. The true segment values are as in Simulation 2. The measurement errors are sums of multiples of independent $\chi_{(3)}^2$ random variables. For the old protocol,

$$u_{1i} = (\chi_{(3)1i}^2 - 3) \sqrt{\frac{\sigma_b^2}{12}} + (\chi_{(3)2i}^2 - 3) \sqrt{\frac{\sigma_u^2}{6} - \frac{\sigma_b^2}{12}} \quad (29)$$

$$u_{2i} = (\chi_{(3)3i}^2 - 3) \sqrt{\frac{\sigma_b^2}{12}} + (\chi_{(3)2i}^2 - 3) \sqrt{\frac{\sigma_u^2}{6} - \frac{\sigma_b^2}{12}}. \quad (30)$$

Errors associated with measurements from the new protocol are generated in the same way with σ_e^2 in place of σ_u^2 and σ_a^2 in place of σ_b^2 . The errors in measurements of change over time are generated as $a_i = e_{2i} - e_{1i}$ and $b_i = u_{2i} - u_{1i}$ for the new and old protocols respectively. In (29)-(30), $\chi_{(3)1i}^2, \chi_{(3)2i}^2,$ and $\chi_{(3)3i}^2$ are independent $\chi_{(3)}^2$ random variables.

Some characteristics of $\mathbf{V}_{\mathbf{w}\mathbf{w}}$ remain unchanged when the measurement errors are skewed. The upper left 4x4 block of covariances of sample means remains the same. Because measurement errors from the new and old protocols are still uncorrelated, covariances between the last three entries of \mathbf{W} and terms involving only the measurements from the old protocol are still zero.

5.2 Simulation Results

Relative Biases of the Estimators of β

Tables 1.a and 1.b give the Monte Carlo relative biases (the ratio of the Monte Carlo bias to the square root of the Monte Carlo variance) of $\hat{\beta}_1$ and $\hat{\beta}_2$ respectively at the sample size of $n = 500$. We note that $\hat{\beta}_2$, the estimator based on the jackknife covariance matrix, is unstable and may not have finite moments. Some extreme observations were observed at $n = 100$. As a consequence, the empirical biases and variances of $\hat{\beta}_2$ do not necessarily estimate population quantities. The Monte Carlo relative biases are consistently smaller for regression parameters than for variances. Regardless of the estimation procedure, sample size, or distribution of values, bias accounts for less than 1% of the mean square errors of the estimators of α and δ . A relatively larger proportion of the mean square errors associated with estimation of variance components are due to bias. A negative bias accounts for 2 – 4% of the mean square errors of both estimators of σ_e^2 and σ_u^2 . The addition of $17n^{-1} \text{diag}(\hat{\mathbf{V}}_{\mathbf{w}\mathbf{w},i}^*)$ to the diagonal elements of $\hat{\mathbf{V}}_{\mathbf{w}\mathbf{w},i}$ in expression (23) of Section 4.2 greatly reduces the bias of the estimators of variance components

at $n = 100$. Without the small adjustment to the diagonal elements of $\hat{\mathbf{V}}_{\mathbf{w}\mathbf{w},i}^*$, bias explains 10–20% of the mean square errors associated with estimation of σ_u^2 and σ_e^2 at $n = 100$. Because the addition of $17n^{-1}\text{diag}(\hat{\mathbf{V}}_{\mathbf{w}\mathbf{w},i}^*)$ has a larger impact at the smaller sample sizes, the magnitudes of the relative biases decrease at a rate slightly slower than \sqrt{n} . Skewness in x_{ti} worsens the relative bias of the estimator based on the jackknife covariance matrix for σ_x^2 . At the sample size $n = 500$, bias explains 5% and 6% of the mean square errors of $\hat{\sigma}_{x,2}^2$ under the conditions of Simulations 2 and 3, respectively.

Variances of the Estimators of β

Both sample size and skewness impact the variances of the two estimators of β . The relative variances also vary across the elements of the parameter vector β . Tables 2.a-2.c give the ratios of the empirical variances of $\hat{\beta}_2$ to those of $\hat{\beta}_1$ at the three sample sizes. We used a first-order Taylor series expansion to compute approximate standard errors for these ratios. The asterisks in Tables 2.a-2.c indicate which estimated relative variances differ from 1 by at least two standard errors.

The magnitudes of the relative variances in Tables 2.a-2.c are largest at $n = 100$, and the associated standard errors decrease as the sample size increases. For instance, at the sample size of $n = 100$, when the population of true values is normal, the standard error of the estimated relative variance corresponding to α in Table 2.a is .025. When we increase the sample size to $n = 500$ and $n = 1000$, the standard errors of the estimated relative variances associated with α decrease to .009 and .006 respectively. Similarly, when x_{ti} are skewed, the estimated relative variances associated with estimation of α decrease as the sample size increases. Simultaneously, our uncertainty associated with these estimated ratios decreases. The standard errors of the estimated relative variances for α under the conditions of Simulation 2 are .141, .026, and .015 for sample sizes of 100, 500, and 1000 respectively.

Skewness in the distribution of true segment values increases the magnitudes of the estimated relative variances associated with α , δ , and σ_u^2 and also heightens our uncertainty about these estimated relative variances. Despite the increase in the standard errors of estimated relative variances in the presence of skewness, the differences between columns 1 and 2 of Tables 2.a-2.c are large compared to their standard errors. For example, an approximate 95% confidence interval for the ratio of the variance of $\hat{\alpha}_2$ to that of $\hat{\alpha}_1$ at $n = 100$ is [1.10, 1.15]. An approximate 95% confidence interval for the variance of $\hat{\alpha}_2$ relative to that of $\hat{\alpha}_1$ at $n = 100$ when x_{ti} are skewed is [1.50, 2.06]. Among the simulations at $n = 500$ and $n = 1000$ when the x_{ti} are normal, only one of the empirical relative variances exceeds 1 by more than two estimated standard errors. In contrast, when the x_{ti} are skewed, the empirical relative variances associated with α , δ , and σ_u^2 exceed 1 by more than two standard errors.

The discrepancy between the variances of the two estimators is greater for α and σ_u^2 than for δ , σ_e^2 and σ_x^2 .

For example, the only estimated relative variances for σ_e^2 that differ from 1 by more than 2 standard errors occur in Simulations 1 and 2 at the sample sizes of $n = 100$ and $n = 500$. The estimated relative variances for σ_x^2 are less than 1 at the sample sizes of $n = 500$ and $n = 1000$ when the distribution of x_{ti} is skewed. Nonetheless, the data suggest that the estimator based on the normal moment covariance matrix is still superior.

Bias of $\hat{\mathbf{V}}_S(\hat{\beta}_1)$

Table 3.a gives ratios of the means of the sandwich variance estimators to the empirical variances of $\hat{\beta}_1$ under the various simulation conditions. We computed approximate standard errors for these ratios as in the previous section. The estimator $\hat{\mathbf{V}}_S(\hat{\beta}_1)$ consistently has a bias of less than 5%. The figures in Table 3.a do not differ from 1 by more than 2 standard errors. Skewness in the true values or measurement errors does not systematically increase the bias for any of the parameters of interest. As the last row of Table 3.a shows, the bias of the sandwich variance estimator remains negligible for σ_x^2 , even when the distribution of true values is skewed. For example, under the conditions of Simulation 2, at a sample size of $n = 100$, the ratio of the mean of the sandwich variance estimator of the variance of $\hat{\sigma}_{x,1}^2$ is 1.03. Similarly, the third and fourth rows of Table 3.a show that the sandwich variance estimator remains unbiased for variances of estimators of σ_e^2 and σ_u^2 when the measurement errors have skewed distributions.

Bias of $\hat{\mathbf{V}}_M(\hat{\beta}_1)$

Table 3.b gives ratios of the means of the model variance estimators to the empirical variances of $\hat{\beta}_1$ under the various simulation conditions. While the sandwich variance estimator is little affected by skewness in the distributions of true values and measurement errors, non-normality leads to a severe downward bias in the model estimator of the variance of $\hat{\beta}_1$ for consideration of variance components directly related to quantities with skewed distributions. For example, the last row of Table 3.b shows that when x_{ti} are skewed and the measurement errors are normal (as in Simulation 2), the means of the model based estimators of the variances of $\hat{\sigma}_{x,1}^2$ at the three sample sizes are only 21 – 25% of the corresponding Monte Carlo variances. The model variance estimator also exhibits a negative bias for the variance of $\hat{\sigma}_{d,1}^2$ under the conditions of Simulation 2. The means of the model variance estimators are approximately 60–70% of the empirical variances of $\hat{\sigma}_d^2$ at the three sample sizes. Skewness in the measurement errors does not further increase the biases related to σ_x^2 and σ_d^2 observed in the second simulation. The last two rows of Table 3.b demonstrate that skewness in measurement errors (Simulation 3) creates a negative bias in the model estimator for consideration of measurement error variances. The model estimator also consistently underestimates the variances of $\hat{\sigma}_{a,1}^2$ and $\hat{\sigma}_{b,1}^2$ (variances of the errors in measuring change over time with the new and old protocols respectively) under the conditions of Simulation 3.

Despite the bias in the model variance estimator for

certain variance components, $\hat{V}_M(\hat{\beta}_1)$ remains essentially unbiased for variances of $\hat{\alpha}_1$ and $\hat{\delta}_1$, even in the presence of skewness in x_{ti} , e_{ti} and u_{ti} . A comparison of the first two rows of Tables 3.a and 3.b reveals that the bias in the model variance estimator is similar to that of the sandwich estimator for variances of regression parameters.

Bias of $\hat{V}(\hat{\beta}_2)$

The mean of $\hat{V}(\hat{\beta}_2)$ is consistently smaller than the Monte Carlo variance of $\hat{\beta}_2$. The bias is typically most severe at the sample size of $n=100$. Within each sample size, the bias is relatively stable across the three simulations. The first three columns of Table 3.c show that when the true values and measurement errors are normally distributed, the downward bias decreases as the sample size increases. There does not appear to be a consistent relation between bias and sample size when either the true values or measurement errors are skewed.

6. Summary

The objective in the National Resources Inventory calibration study is to calibrate a new measurement procedure against a standard method. The model in Section 3 permits estimation of the linear calibration equation and of measurement error variances. Simulation results indicate that two estimators of model parameters are nearly unbiased. The estimator based on the jackknife covariance matrix has a higher variance than the estimator based on the normal moments. One explanation for the robustness of the estimator based on the normal moments to mild skewness is that the normal-moment covariance matrix preserves much of the structure of the theoretical covariance matrices under the simulation conditions considered. We conjecture that both estimation procedures perform similarly with respect the variance of measurements from the new protocol, σ_e^2 , because both rely heavily on the unbiased estimator of σ_e^2 in the last element of the original vector of sample covariances. The normal-based estimator of the variance of the estimator based on the normal moments is biased downward for variances of estimators of variance components when distributions are skewed. The consistent downward bias of the estimator of the variance of the estimator based on the jackknife covariance matrix is most severe at the smallest sample size.

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Table 1: Relative Bias at $n = 500$.

Ratios of Monte Carlo biases to square roots of Monte Carlo variances.

1.a Estimators Based on Normal Moments.			
	Normal x_{ti}	Skewed x_{ti}	Skewed x_{ti}, e_{ti}, u_{ti}
$\alpha = 1$	0.02	0.03	0.01
$\delta = 0$	0.06	-0.06	0.00
$\sigma_u^2 = 60$	-0.13	-0.15	-0.10
$\sigma_e^2 = 50$	-0.08	-0.10	-0.24
$\sigma_x^2 = 200$	-0.11	-0.06	-0.08

1.b Estimators Based on Jackknife.			
	Normal x_{ti}	Skewed x_{ti}	Skewed x_{ti}, e_{ti}, u_{ti}
$\alpha = 1$	0.03	0.02	0.06
$\delta = 0$	0.06	-0.06	-0.04
$\sigma_u^2 = 60$	-0.12	-0.16	-0.10
$\sigma_e^2 = 50$	-0.08	-0.10	-0.15
$\sigma_x^2 = 200$	-0.10	-0.23	-0.26

Table 2: Relative Variances: Ratios of variances of estimators based on the jackknife to variances of estimators based on the normal moments.

2.a n=100			
Parameter	Normal x_{ti}	Skewed x_{ti}	Skewed x_{ti}, e_{ti}, u_{ti}
$\alpha = 1$	1.14*	1.73*	2.12*
$\delta = 0$	1.08*	1.33*	1.43*
$\sigma_u^2 = 60$	1.12*	2.20*	1.88*
$\sigma_e^2 = 50$	1.10*	1.07*	1.03
$\sigma_x^2 = 200$	1.10*	0.99	0.97

2.b n=500			
Parameter	Normal x_{ti}	Skewed x_{ti}	Skewed x_{ti}, e_{ti}, u_{ti}
$\alpha = 1$	1.01	1.21*	1.19*
$\delta = 0$	1.02	1.10*	1.08*
$\sigma_u^2 = 60$	1.02	1.41*	1.34*
$\sigma_e^2 = 50$	1.01	1.03*	1.01
$\sigma_x^2 = 200$	1.02	0.97	0.98

2.c, n=1000			
Parameter	Normal x_{ti}	Skewed x_{ti}	Skewed x_{ti}, e_{ti}, u_{ti}
$\alpha = 1$	1.01	1.07*	1.11*
$\delta = 0$	1.01	1.03*	1.03*
$\sigma_u^2 = 60$	1.01	1.20*	1.11*
$\sigma_e^2 = 50$	1.00	1.01	1.02
$\sigma_x^2 = 200$	1.01*	1.02	0.98

Entries with asterisks differ from one by more than two standard errors.

Table 3: Ratios of means of variance estimators to variances of estimators.

3.a Ratios of means of sandwich variance estimators to variances of estimators based on the normal moment covariance matrix. $(E[\hat{\mathbf{V}}_2(\hat{\beta}_1)]/\mathbf{V}(\hat{\beta}_1))$

Parameter	Normal x_{ti}			Skewed x_{ti}			Skewed x_{ti}, u_{ti}, e_{ti}		
	n=100	n=500	n=1000	n=100	n=500	n=1000	n=100	n=500	n=1000
$\alpha = 1$	1.10	0.96	1.02	0.96	0.98	1.00	1.07	0.94	1.01
$\delta = 0$	1.00	1.01	1.00	1.00	0.96	0.99	1.02	0.97	.99
$\sigma_u^2 = 60$	0.99	1.02	0.98	0.97	0.96	1.02	0.99	0.99	1.07
$\sigma_e^2 = 50$	0.99	1.00	1.05	1.02	1.01	0.95	0.99	0.98	0.94
$\sigma_x^2 = 200$	1.06	0.99	1.00	1.03	1.04	1.04	0.96	1.01	1.01

3.b Ratios of means of normal-based variance estimators to variances of estimators based on the normal moment covariance matrix. $(E[\hat{\mathbf{V}}_1(\hat{\beta}_1)]/\mathbf{V}(\hat{\beta}_1))$

Parameter	Normal x_{ti}			Skewed x_{ti}			Skewed x_{ti}, u_{ti}, e_{ti}		
	n=100	n=500	n=1000	n=100	n=500	n=1000	n=100	n=500	n=1000
$\alpha = 1$	1.11	0.96	1.02	1.06	0.98	1.01	1.08	0.96	1.01
$\delta = 0$	1.00	1.01	1.00	1.06	0.96	0.99	1.01	0.98	0.99
$\sigma_u^2 = 60$	1.01	1.03	1.04	0.98	0.96	1.02	0.70	0.61	0.65
$\sigma_e^2 = 50$	1.01	1.00	0.98	1.03	1.01	0.95	0.49	0.47	0.44
$\sigma_x^2 = 200$	1.06	0.99	1.00	0.27	0.23	0.23	0.24	0.23	0.21

3.c Ratios of means of estimators of variances of estimators based on the jackknife covariance matrix to the variances of the estimators. $(E[\hat{\mathbf{V}}(\hat{\beta}_2)]/\mathbf{V}(\hat{\beta}_2))$

Parameter	Normal x_{ti}			Skewed x_{ti}			Skewed x_{ti}, u_{ti}, e_{ti}		
	n=100	n=500	n=1000	n=100	n=500	n=1000	n=100	n=500	n=1000
$\alpha = 1$	0.93	0.93	0.99	0.95	0.94	1.00	0.88	0.92	0.97
$\delta = 0$	0.88	0.98	0.99	0.98	0.94	0.99	0.89	0.96	0.98
$\sigma_u^2 = 60$	0.86	1.00	1.02	0.98	0.96	0.98	0.89	0.89	1.04
$\sigma_e^2 = 50$	0.92	0.97	0.96	0.89	0.97	0.93	0.90	0.93	0.90
$\sigma_x^2 = 200$	0.89	0.95	0.98	0.94	0.98	0.98	0.87	0.94	0.97