

# USING AN ESTIMATING FUNCTION BOOTSTRAP APPROACH FOR OBTAINING VARIANCE ESTIMATES WHEN MODELLING COMPLEX HEALTH SURVEY DATA

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## ABSTRACT

Whether survey data are being used for estimating descriptive statistics about the population from which the sample was drawn or in a design-based approach for more complex analyses, sufficient information about the design is required in order to produce adequate design-based variance estimates. For the Statistics Canada health surveys being used for analysis, such as the National Population Health Survey and the Canadian Community Health Survey, the design information is being provided in the form of a final weight variable and a set of bootstrap weight variables, each one corresponding to a bootstrap sample of psu's from the sampled psu's (see Rust and Rao, 1996, for approach). Much of the software available for using the design information in this form takes a "direct" approach to producing variance estimates for an estimated quantity – using the average of the squared differences between the bootstrap estimates and the final-weight estimate. While straightforward, this approach has been found to have drawbacks, particularly in the case of iterative model-fitting in a domain containing a small sample such as in the fitting of a logistic model to the sample from a specialized subpopulation. One option would be to use an estimating function bootstrap approach for such situations. Justification for the approach and some examples of its application will be discussed.

KEY WORDS: Estimating function bootstrap; Design-based methods; Logistic regression; Small-sample properties; Linearization

## RÉSUMÉ

Que ce soit pour faire l'estimation de statistiques décrivant la population à partir de laquelle l'échantillon a été tiré ou encore pour faire des analyses plus complexes fondées sur le plan de sondage, de l'information appropriée quant au plan de sondage est requise afin de produire des estimations de variance adéquates. Lorsque des enquêtes sur la santé, produites par Statistique Canada, sont utilisées à des fins analytiques, enquêtes telles que l'Enquête nationale sur la santé de la population (ENSP) et l'Enquête sur la santé dans les collectivités canadiennes (ESCC), l'information relative au plan de sondage est transmise sous la forme d'une variable contenant le poids final et un ensemble de variables de poids bootstrap, chacune d'elle correspondant à un échantillon bootstrap d'unités primaires d'échantillonnage (upé), prélevé parmi les upé échantillonnées (voir Rust et Rao, 1996, pour une discussion de cette approche). La plupart des logiciels utilisant l'information reliée au plan de sondage prennent une approche 'directe' pour produire les estimations de variance pour les quantités estimées – c'est-à-dire la moyenne des différences au carré entre les estimations bootstrap et l'estimation avec le poids final. Bien que directe, cette approche présente tout de même certains inconvénients, en particulier dans le cas d'une modélisation avec composante itérative pour un domaine contenant une faible taille d'échantillon, comme lors de l'utilisation d'un modèle de régression logistique construit à partir d'une sous-population spécialisée d'un échantillon. Une option consisterait à utiliser une approche bootstrap aux équations d'estimation dans ces situations. Une justification de l'approche et des exemples de son application seront présentés.

MOTS CLÉS: Bootstrap pour fonctions estimantes; méthodes basées sur le plan; régression logistique; petits échantillons; linéarisation

## 1. INTRODUCTION

The effective analysis of complex survey data through a design-based approach requires sufficient design information and adequate methods for producing variance estimates. For many of the Statistics Canada health surveys, this design

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information is provided in the form of bootstrap weight variables, each one corresponding to a bootstrap sample of primary sampling units. As well, recommendations for the use of these bootstrap weight variables have pointed towards a “direct” or “classical” approach to variance estimation. However, analysts have identified problems with implementing this approach, particularly when working with small samples. In order to respond to the need for a different bootstrapping approach, we examine the possibility of bootstrapping estimating functions rather than the estimates themselves.

In Section 2 we outline the two traditional approaches to design-based variance estimation - the analytical approach and the replication approach. Here, we describe the “classical” or “direct” bootstrapping approach and point out its problems. Then, in Section 3 we give a brief overview of the use of the estimating function bootstrap in the non-survey context and also of the use of estimating functions and replication variance estimation with survey data. Section 4 contains a description of the linearized estimating function bootstrap for survey data, which we are proposing as an alternative to the “classical” bootstrap. We also briefly outline an alternative estimating function approach proposed by Rao (2003). Section 5 consists of an empirical comparison of the linearized estimating function (LEF) bootstrap and the “classical” bootstrap when used with real data. Here, the favourable properties of the LEF bootstrap are illustrated in the case of logistic regression. In Section 6 we give some indications of future research.

## **2. TRADITIONAL APPROACHES TO DESIGN-BASED VARIANCE ESTIMATION FOR ANALYSIS**

When implementing a design-based method to analyse survey data, there are two commonly-used approaches for producing variance estimates of estimated quantities. The first of these, called the analytical approach - and frequently referred to as the Taylor-linearization approach - was the first to be implemented widely in analysis software. The second of these, called a replication approach, actually consists of a family of methods each of which involves subsampling from the sample and using the subsamples to estimate the variance. One of these replication methods could be called the “classical” survey bootstrap approach.

Section 2.1 contains a brief description of the analytical approach and explains why there has been a move away from this approach. Then Section 2.2 describes the “classical” bootstrap approach.

### **2.1 Analytical Approach to Design-based Variance Estimation**

Design-based variance estimation for a particular survey design generally begins with a standard formula for the variance estimation of an estimate of a total, where the estimated total has the form of a weighted sum and where the weights are the inverse of inclusion probabilities ( i.e.  $\hat{Y} = \sum_s w_i y_i = \sum_s y_i / \pi_i$ ). These standard formulae are then adapted, usually through a linearization method, when there are weight adjustments ( i.e.  $\hat{Y} = \sum_s w_i y_i = \sum_s a_i y_i / \pi_i$ ), such as adjustments for nonresponse or poststratification. Linearization is also used to extend to variance formulae for nonlinear statistics, such as variance formulae for ratios or for regression coefficients.

While the standard formula for the variance estimate of a simple total is straightforward for simple survey designs, it can be much more complicated for the more complex survey designs actually used in practice. Because of this complexity, a simplifying assumption about the survey design is generally made when an analytical variance estimation approach is taken: it is assumed that the design is stratified multistage, and that there is with- replacement sampling of primary sampling units (psu’s) at the first stage. Under this assumption, a variance estimation formula for a simple total has a form that is readily calculated.

Even though the simplifying assumption about the true survey design makes the implementation of an analytical approach much more tractable, in recent years there has still been a move away from this approach. A major reason for this is that the analytical approach requires development of a new formula for every estimator and for every weight adjustment - or requires further simplifying assumptions about negligible impact of ignoring some of the complexities of these adjustments. There has also been growing popularity of replication methods in other areas of statistics, which has led to increasing popularity of the application of replication methods to survey data. This has been due, in large part, to the greater computing power available to analysts.

## 2.2 “Classical” approach to bootstrapping for survey data

The “classical” or “direct” survey bootstrap approach is one of the replication methods that has gained popularity for use with survey data. It is, for example, the main variance estimation approach that is supported for several of the Statistics Canada social surveys. For this approach, the assumption is still made that the design of the survey is approximately stratified multistage, and that there is with- replacement sampling of primary sampling units (psu’s) at the first stage. Under this assumption, a bootstrapping approach has been developed that has good properties for estimating the variance of an estimated total (see, for example, Rust and Rao, 1996). This same approach is then used for estimating the variance of any estimate. The steps for obtaining the “classical” survey bootstrap variance estimate of the estimate  $\hat{\theta}$  of vector  $\theta$  are as follows:

- i) Use the full sample to get estimate  $\hat{\theta}$  of  $\theta$ .
- ii) Form the  $b$ -th replicate by sampling  $n_h - 1$  psu’s independently with replacement from the  $n_h$  sampled psu’s in each stratum.
- iii) Create the  $b$ -th replicate weight variable by adjusting the original weight variable on each unit, to account for the results of the replicate sampling, nonresponse, post-stratification, etc.
- iv) Calculate the estimate  $\hat{\theta}_b$  using the  $b$ -th replicate weight variable - in the same way as  $\hat{\theta}$  was calculated.
- vi) Repeat steps i) to iv) many times ( $B$  times).
- vii) Calculate the bootstrap estimate of the covariance matrix of  $\hat{\theta}$  as

$$\hat{V}_{BS} = \frac{B}{\sum_{b=1}^B} (\hat{\theta}_b - \hat{\theta})(\hat{\theta}_b - \hat{\theta})' / B.$$

While this “classical” survey bootstrap is making the same simplifying assumption about the design of the survey as is generally made in software implementing an analytical approach to variance estimation, it does overcome some of the problems encountered with the analytical approach. In particular, it can account for weight adjustments due to nonresponse and poststratification. As well, every estimate is treated in the same way, rather than having to develop a special procedure for estimating the variance of every different point estimate.

On the other hand, problems have been identified in the use of this approach. One problem - which is less of an issue with increased computer capacity - is the computational intensity of the approach, particularly if an iterative procedure is used in the calculation of the point estimates. A major difficulty occurs when the calculation of each  $\hat{\theta}_b$  involves the inversion of a matrix formed from the observations in the resample: it can happen that this matrix is ill conditioned for one or more of the resamples, even when the matrix for the full sample is not ill conditioned. This problem seems to be more prevalent when working with a small sample.

## 3. PREVIOUS WORK WITH ESTIMATING FUNCTIONS FOR VARIANCE ESTIMATION

### 3.1 Estimating Function Bootstrap in the Non-survey Context

Several researchers have done work on extending the concepts of the traditional bootstrapping approach in a non-survey context. They have gone from resampling the data to resampling residuals from the estimating function used to produce the parameter point estimates, and then have used these residuals in some way to obtain a variance estimate. Wu (1986), for example, considers one bootstrapping approach which implicitly makes use of the estimating equation, together with a selection of jackknifing approaches, for both linear and nonlinear parameters. Hu and Zidek (1995) propose a different estimating function bootstrap for the linear model, which appears to have desirable asymptotic properties; a simulation study described in the paper indicates that the small-sample properties of the variance estimator are also good. Hu and Kalbfleisch (2000) generalize this estimating function approach to a wider class of problems, but concentrate on the case of a univariate parameter for testing hypotheses and obtaining confidence intervals.

### 3.2 Estimating Functions and Replication Variance Estimation in Survey Context

Estimating functions are in common use and further applications are under research in the survey context. Many

finite population parameter estimates are obtained by solving sample estimating equations. The estimating function approach is also being used for making inference from complex survey data. In one of the earliest research papers on this topic, Binder (1983) combines the estimating equation approach with the Taylor linearization method for variance estimation, but does not explicitly study the implication of poststratification adjustments on the variance estimation. Rao, Yung and Hidiroglou (2002) examine the situation where the sample estimating equations involve design weights as well as adjustment factors based on poststratification information; for variance estimation, they study a Taylor linearization approach, a standard delete-one-cluster jackknife approach and a jackknife linearization approach, all of which account for the post-stratification adjustments. Then, Rao and Tausi (2004) apply the estimating function approach of Hu and Kalbfleisch (2000), together with jackknife resampling, to obtain variance estimators of generalized regression (GREG) estimators of totals and of parameters defined as solutions of census estimating equations. Rao and Tausi show that, for a total, the estimating function jackknife variance estimate is identical to the jackknife linearization variance estimator. They also point out the advantage of the estimating function jackknife variance estimate over the customary jackknife - there are no ill-conditioned matrices arising from the jackknife subsamples.

#### 4. ESTIMATING FUNCTION BOOTSTRAP APPROACHES TO VARIANCE ESTIMATION FOR SURVEY DATA

##### 4.1 Linearized Estimating Function (LEF) Bootstrap Approach

The linearized estimating equation bootstrap approach to variance estimation with survey data was motivated from the estimating function bootstrap of Hu and Kalbfleisch (2000). It can accommodate both univariate and multivariate inference. Our objective is to get an estimate  $\hat{\theta}$  of the finite population vector parameter  $\theta$ , and an estimate of the covariance matrix of  $\hat{\theta}$ . We proceed as follows:

We define the parameter  $\theta$  as the solution of the population estimating equation  $U(\theta) = \sum_U u_i(\theta) = 0$ , where the  $u_i(\theta)$  are suitably defined. For example, when  $\theta$  is the vector of coefficients of a linear regression model,  $u_i(\theta) = x_i(y_i - x_i'\theta)$ , while for the coefficients of a logistic regression model,  $u_i(\theta) = x_i[y_i - p_i(\theta)]$ , where  $p_i(\theta) = e^{x_i'\theta} / (1 + e^{x_i'\theta})$ . We can then produce the estimating function  $\hat{U}(\theta) = \sum_s w_i u_i(\theta)$ , which is a weighted sum over the sample of components  $u_i(\theta)$ .

Our next step is to define  $\hat{\theta}$  as the solution to the estimating equation  $\hat{U}(\hat{\theta}) = 0$ , i.e.  $\hat{U}(\hat{\theta}) = \sum_s w_i u_i(\hat{\theta}) = 0$ .

We then make a linear approximation to  $\hat{U}(\hat{\theta})$  around  $\hat{U}(\theta)$ :

$$0 = \hat{U}(\hat{\theta}) \approx \hat{U}(\theta) + E \left[ \frac{\partial \hat{U}(\theta)}{\partial \theta} \right] (\hat{\theta} - \theta).$$

Rearranging this equation, we can obtain an expression for  $\hat{\theta} - \theta$ ,

$$\hat{\theta} - \theta \approx - \left[ E \left( \frac{\partial \hat{U}(\theta)}{\partial \theta} \right) \right]^{-1} \hat{U}(\theta),$$

which then leads to a sandwich form expression to approximate the variance of  $\hat{\theta}$ :

$$V(\hat{\theta}) \approx \left[ E \left( \frac{\partial \hat{U}(\theta)}{\partial \theta} \right) \right]^{-1} V[\hat{U}(\theta)] \left[ E \left( \frac{\partial \hat{U}(\theta)}{\partial \theta} \right) \right]^{-1}.$$

It follows that the estimated variance of  $\hat{\theta}$  will also have the sandwich form:

$$\hat{V}(\hat{\theta}) = \left[ E \left( \frac{\partial \hat{U}(\theta)}{\partial \theta} \right) \right]^{-1} \hat{V}[\hat{U}(\theta)] \left[ E \left( \frac{\partial \hat{U}(\theta)}{\partial \theta} \right) \right]^{-1} \text{ evaluated at } \theta = \hat{\theta}.$$

Bootstrapping will then be used, as follows, to obtain an estimate of the “meat” of the sandwich. We take bootstrap samples from  $s$  and generate the bootstrap weight variables in the customary way. Then, for the  $b$ -th bootstrap sample, we calculate the value of the estimating function  $\hat{U}^{(b)}(\hat{\theta}) = \sum_s w_i^{(b)} u_i(\hat{\theta})$ , which makes use of the  $b$ -th bootstrap weight variable and the components  $u_i(\theta)$  evaluated at  $\hat{\theta}$ . Next, we will define the LEF bootstrap variance estimate of  $\hat{U}$  at  $\theta = \hat{\theta}$  to be

$$\hat{V}_{BS}[\hat{U}(\theta)]_{\theta=\hat{\theta}} = \frac{1}{B} \sum_{b=1}^B [\hat{U}^{(b)}(\hat{\theta}) - \hat{U}(\hat{\theta})][\hat{U}^{(b)}(\hat{\theta}) - \hat{U}(\hat{\theta})]', \text{ which finally leads to}$$

$$\hat{V}_{LEF}(\hat{\theta}) = \left[ \frac{\partial \hat{U}(\theta)}{\partial \theta} \Big|_{\theta=\hat{\theta}} \right]^{-1} \hat{V}_{BS}[\hat{U}(\theta)]_{\theta=\hat{\theta}} \left[ \frac{\partial \hat{U}(\theta)}{\partial \theta} \Big|_{\theta=\hat{\theta}} \right]^{-1}.$$

It should be noted that we did not actually obtain an estimate of  $\theta$  from each bootstrap sample. However, if such estimates are desired (such as for the production of diagnostic histograms as we do in a subsequent section), the following may be done.

Recall that 
$$\hat{\theta} - \theta \approx - \left[ E \left( \frac{\partial \hat{U}(\theta)}{\partial \theta} \right) \right]^{-1} \hat{U}(\theta).$$

It then follows that a reasonable definition for the  $b$ -th bootstrap estimate of  $\theta$  would be

$$\hat{\theta}^{(b)} = \hat{\theta} - \left[ \frac{\partial \hat{U}(\theta)}{\partial \theta} \Big|_{\theta=\hat{\theta}} \right]^{-1} \hat{U}^{(b)}(\hat{\theta}).$$

If we consider the particular case of  $\theta$  being the vector of coefficients of a logistic regression model, the values of the quantities given above are the following:

$$\begin{aligned} \hat{U}(\theta) &= \sum_s w_i x_i [y_i - p_i(\theta)] \text{ where } p_i(\theta) = e^{x_i' \theta} / (1 + e^{x_i' \theta}), \\ \hat{U}^{(b)}(\hat{\theta}) &= \sum_s w_i^{(b)} x_i [y_i - p_i(\hat{\theta})], \\ \frac{\partial \hat{U}(\theta)}{\partial \theta} &= \sum_s w_i x_i x_i' p_i(\theta) [1 - p_i(\theta)], \text{ and} \\ \hat{\theta}^{(b)} &= \hat{\theta} - \left[ \sum_s w_i x_i x_i' p_i(\hat{\theta}) [1 - p_i(\hat{\theta})] \right]^{-1} \left[ \sum_s w_i^{(b)} x_i [y_i - p_i(\hat{\theta})] \right]. \end{aligned}$$

When compared to the “classical” bootstrapping approach, there are advantages to the LEF bootstrap approach described above. For one, the estimating equations are solved only once, rather than  $B + 1$  times, which can be a considerable time advantage, particularly when iterative procedures are used in the solution. There is also no problem with ill-conditioned matrices, provided that an ill-conditioned matrix is not encountered when fitting the model with the full sample; this a particular advantage with small samples. It should also be noted that the bootstrap weights generated for use in the “classical bootstrap approach may be used for implementing the LEF bootstrap approach.

Advantages are gained, but at the cost of disadvantages. One great advantage of the “classical” bootstrap approach is that you simply “turn the crank” as you apply it to different point estimates; it is a completely repetitive process. However, with the LEF bootstrap, it is necessary to do the “linearization math” for each different model. (There is still an advantage over the analytical approach because linearizations since weight adjustments are not necessary.)

## 4.2 Alternative Estimating Function Approach due to Rao

There are other possibilities for making use of the estimating function idea with bootstrapping. In a private communication, Rao (2003) proposes the following.

Recall that  $\hat{U}(\theta)$  and  $\hat{U}^{(b)}(\hat{\theta})$  are defined respectively as  $\hat{U}(\theta) = \sum_s w_i u_i(\theta)$  and  $\hat{U}^{(b)}(\hat{\theta}) = \sum_s w_i^{(b)} u_i(\hat{\theta})$ . If we define the  $b$ -th bootstrap estimate of  $\theta$ , say  $\hat{\theta}^{*(b)}$ , to be the solution of  $\hat{U}(\theta^{*(b)}) = \hat{U}^{(b)}(\hat{\theta})$ , then an alternative estimating function bootstrap variance estimate of  $\hat{\theta}$  is

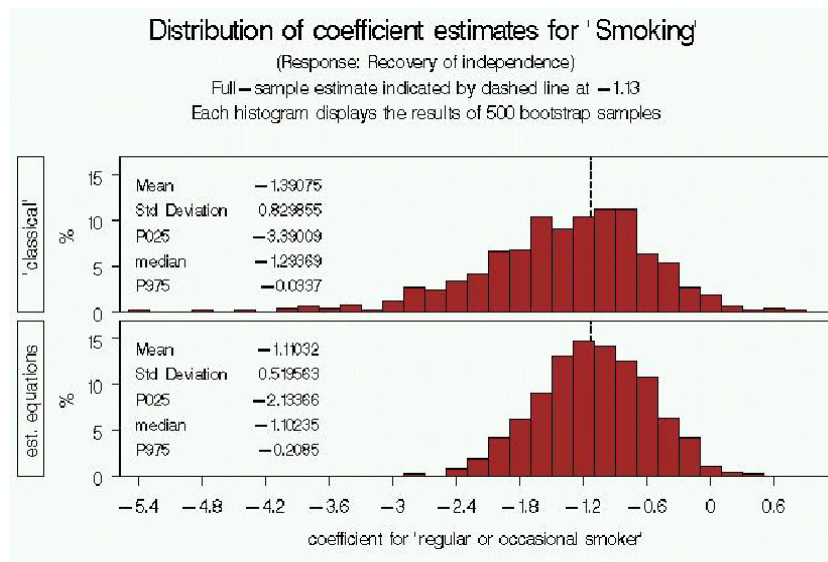
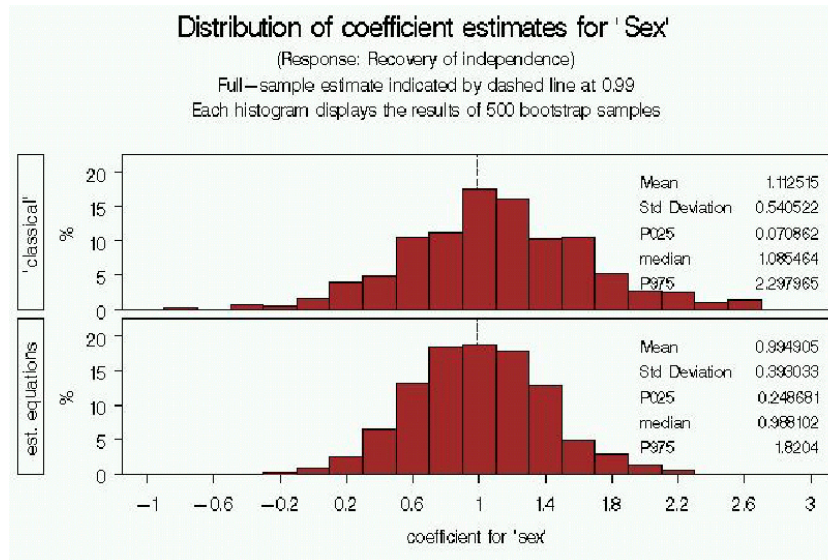
$$\hat{V}_{BS}^* = \frac{1}{B} \sum_{b=1}^B (\hat{\theta}^{*(b)} - \hat{\theta})(\hat{\theta}^{*(b)} - \hat{\theta})'$$

While this approach requires the solution of a system of equations for every bootstrap sample, there are no ill-conditioned matrices needing inversion.

## 5. EXAMPLE

In this section we give an empirical illustration of the difference in results between the use of the “classical” bootstrap approach and the LEF bootstrap approach for variance estimation in the case of logistic regression modelling. The data and logistic models examined are taken from Martel, Bélanger and Berthelot (2002). In this paper, the authors use the first two cycles of Statistics Canada’s National Population Health Survey (NPHS) to identify characteristics of dependent seniors that are related to their becoming independent. Their sample consisted of 399 individuals aged 65+ living in households at the time of the first cycle (1994/95) who met their criteria of being dependent, based on answers to questions about the need of help from other people for doing certain tasks. For the logistic model, the binary explanatory variable was the state of the individual at the time of the second NPHS cycle - independent or dependent (with a dependent person living either in a household or in a long-term care facility). The explanatory variables were a selection of demographic, chronic condition, behavioural, socio-economic and area-of-residence quantities, all binary variables measured at the time of the first cycle. We applied both the “classical” and the LEF bootstrap approaches for obtaining variance estimates of the regression coefficients, making use of the same set of 500 bootstrap weights for both, from 500 survey bootstrap samples. A program written in SAS implemented the two approaches. We employed PROC LOGISTIC to fit the logistic models, with the maximum number of iterations being set at 25; for the “classical” bootstrap approach, if the iterative procedure applied to a bootstrap sample had not converged in 25 iterations, the coefficient values on the 25<sup>th</sup> iteration were taken to be the coefficient estimates for that sample.

Shown below are the histograms of the 500 bootstrap estimates from the two different methods for the coefficients on a couple of the variables - the sex variable and the smoking variable. For both variables, the spread of the bootstrap estimates is much greater, there are more outliers, and there is less symmetry for the “classical” approach than for the LEF approach; as well, the mean of the “classical” bootstrap estimates is farther from the full-sample estimate. For the sex variable, the reported p-value of the Wald statistic is .07 under the “classical” approach and .01 under the LEF approach. By either approach, you are unlikely to drop the sex variable from your model. On the other hand, for the smoking variable, the reported p-values for the Wald statistic are .19 for the “classical” approach and .03 for the LEF approach. An examination of the output from the PROC logistic procedures for the “classical” approach revealed that for approximately 300 of the 500 replicates there were fitting problems, causing non-convergence of the iterative algorithm and possibly unacceptable coefficient estimates being used in the bootstrap variance calculations. All of these findings indicate that the LEF bootstrap could have more favourable properties for inference with survey data than the “classical” survey bootstrap.



For the example just discussed, the sample size is relatively small. The question then arises whether there would be such a difference in the results of the two approaches if a larger sample size were used. To study this, we took another data set and another logistic model from Martel, Bélanger and Berthelot (2002). In this case, the sample consisted of 1921 individuals aged 65+, living in households and independent at the time of the first cycle. The explanatory variable in the model was independence/dependence at the time of the second cycle and the explanatory variables were the same as for the first example. Again, both approaches were used to obtain variance estimates. There were fitting problems in 31 of the 500 replicates - a much smaller number than for the first example. A comparison of the histograms of bootstrap coefficient estimates revealed less of a difference in spread between the “classical” and LEF approaches and fewer outliers in the “classical” case, but differences still persisted. As well, variance estimates were always larger in the “classical” approach. These differences could have an impact on inferential results. As an example, the following table shows the difference in the number of coefficients with estimated p-value less than 0.05 for the Wald statistics testing the significance of individual coefficients.

## Number of coefficients with estimated p-value < 0.05 on Wald statistic

Bootstrap Method	Sample 1 Sample size: 399	Sample 2 Sample size: 1291
“Classical”	2	10
LEF	9	14

The empirical comparison of the implementation of the “classical” and LEF bootstrap approaches with real data indicates that the LEF method has many favourable properties, particularly when working with a small sample. These favourable properties continue to hold even with a larger sample.

## 6. CONCLUSION

From the empirical work done to date, it appears that the linearized estimating function bootstrap is a promising tool for obtaining variance estimates when analyzing complex survey data. When compared to the “classical” survey bootstrap approach, it overcomes the problem of ill-conditioned matrices which are frequently encountered with small sample sizes and is also more time-efficient.

But more extensive work still needs to be done. The LEF bootstrap needs to be examined under a variety of controlled conditions, both by studying its theoretical properties and by probing its small-sample properties through a simulation study. As well, alternative estimating function bootstraps need to be compared, including the one proposed by Rao and described in Section 4.2. Results of these studies will provide analysts of complex survey data with more effective analytical tools.

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