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ESTIMATING EQUATIONS AND THE BOOTSTRAP

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ABSTRACT

We consider interval estimation of a parameter θ when the estimation of θ is defined by a linear estimating equation based on independent observations. The proposed method involves bootstrap resampling of the estimating function that defines the equation with θ replaced by its estimated value. By this process, the distribution of the estimating function itself can be approximated, a confidence distribution for θ is induced and confidence regions can be simply defined. The procedure is termed the EF (Estimating Function) Bootstrap and, under fairly general conditions, can be shown to yield confidence intervals whose coefficients are accurate to first order. A simple studentized version is also defined and, in many instances, gives a second order approximation. In a number of examples, the method is shown to compare very well with classical bootstrap procedures. The intervals produced are more accurate, the method is more stable, and it has considerable computational advantage when compared to the classical approach. A number of comments and suggestions for future research are also given.

Key Words: Bootstrap, estimating functions, common means problem

1 Introduction

Over the past fifteen to twenty years, both estimating equations and the bootstrap have been very influential ideas in theoretical and applied statistics. In this article, we summarize some recent work that combines these two ideas to use bootstrap resampling as the basis of inference for estimating equations. There seems to have been relatively little work in this area. The articles by Lele (1991a,b) and Hu and Zidek (1995) are notable exceptions. A more complete discussion of the present work can be found in Hu and Kalbfleisch (1997a).

Estimating equations, the topic for this volume, provides a simple framework for the estimation of parameters. Godambe and Kale (1991) provide a nice recent review of the area. Although the theory leads to important results on optimality and substantial areas of application, methods of inference are primarily based on simple asymptotic approximations with little

available for inference in small samples nor for example, extensions to higher order asymptotics.

Since Efron's (1979) fundamental paper, the bootstrap has been the subject of much discussion and development. Like estimating equations, the idea is simple and straightforward yet it has powerful implications for applications and forms the basis of much theoretical work as well. Recent reviews can be found in the books by Efron and Tibshirani (1993) and Hall (1992). The most studied problem is that of constructing reliable and accurate confidence intervals for a parameter θ of interest. The general approach involves generating the bootstrap distribution for an estimator $\hat{\theta}$ and utilizing that distribution for interval estimation. DiCiccio and Romano (1988) give an excellent summary.

In this article, we use bootstrap procedures to construct confidence intervals for a parameter θ when the estimation of θ is based upon a linear estimating equation. The methods are simple to implement and, in a wide class of problems, lead to very accurate confidence intervals with coverage probabilities that are accurate to second order.

In section 2, we define a simple bootstrap method for the linear estimating equation and also give a studentized version. Our proposal involves resampling the components of the estimating function with the aim of estimating its distribution rather than the distribution of the estimator $\hat{\theta}$. This provides the basis to estimate a confidence distribution for θ and to develop approximate confidence regions. The ideas being used are similar to those of Hu and Zidek (1995) who develop related bootstrap methods for estimating equations in the linear model. The paper by Parzen, Wei and Ying (1994) is also closely related. They consider estimating functions whose distributions are very complex and use simulation methods to generate a confidence distribution for θ . Their approach, however, is not based on bootstrap resampling.

In Section 3, a few examples are given to compare the method with more classical procedures. Section 4 gives a series of comments and outlines some areas for further investigation.

2 Estimating Equations and Confidence Regions

Suppose that y_1, y_2, \dots, y_n are independent random variables, and our aim is to estimate an unknown parameter θ taking values in some space Ω . Further, we assume that

$$E_{\theta}(g_i(y_i, \theta)) = 0$$

for all i and $\theta \in \Omega$. The parameter θ is estimated by the root $\hat{\theta}$ of the unbiased linear estimating equation

$$S_y(\theta) = \sum_{i=1}^n g_i(y_i, \theta) = 0 \quad (2.1)$$

In what follows, we suppose that $S_y(\theta)$ is a one to one function of θ , and we focus on the construction of confidence intervals for θ . Note that the estimating function (2.1) is taken as given and is assumed to provide an appropriate method for estimation.

If the distribution of $S_y(\theta)$ is the same for all $\theta \in \Omega$ and C is a set that satisfies $P\{S_y(\theta) \in C\} \geq 1 - \alpha$, then $\{\theta \in \Omega : S_y(\theta) \in C\}$ is a confidence interval with coefficient at least $1 - \alpha$. Parzen, Wei and Ying (1994) consider this setup and develop methods for simulating the distribution of $S_y(\theta)$ in certain regression examples. More usually, however, the exact distribution of $S_y(\theta)$ depends on θ and its distribution is complex or not even specified by the assumed model. In such cases, it is customary to rely on asymptotic results.

Asymptotic Normal Approximations:

If θ is a scalar parameter, for example, and certain regularity conditions hold, asymptotic inferences could be based on a central limit theorem applied to $S_y(\theta)$ directly. Alternatively, a Taylor series approximation yields an asymptotic distribution for $\hat{\theta}$. Thus, in the former case we have

$$\frac{1}{\sqrt{n}} \sum g_i(y_i, \theta) \xrightarrow{\mathcal{D}} N(0, V_\theta) \quad (2.2)$$

and in the latter case

$$\sqrt{n}(\hat{\theta} - \theta) \xrightarrow{\mathcal{D}} N(0, V_\theta/W_\theta) \quad (2.3)$$

where $V_\theta = \lim_{n \rightarrow \infty} \frac{1}{n} \sum \text{var}(g_i(y_i, \theta))$ and $W_\theta = \lim_{n \rightarrow \infty} E(\frac{1}{n} \sum \frac{\partial}{\partial \theta} g_i(y_i, \theta))^2$. Using (2.2) or (2.3) with a consistent estimator of V_θ or V_θ/W_θ , approximate confidence intervals for θ can easily be obtained. Extensions to vector parameters are, of course, straightforward.

The result (2.3) is the most commonly used method, but it has several drawbacks:

- i) The approximation is first order only and convergence can be slow.
- ii) The method is not functionally invariant; estimation of $\lambda = h(\theta)$, where h is 1 : 1, can yield different results.
- iii) $S_y(\theta)$ must be smooth for the Taylor approximations; this means it cannot be used in some nonparametric problems of interest.

iv) There is no adaptation to small samples.

Use of (2.2) instead of (2.3) circumvents drawbacks ii) and iii). The EF Bootstrap discussed below is based on approximations to the distribution of $S_y(\theta)$ and also addresses ii), iii) and iv). In addition, a studentized version leads to higher order approximations.

The EF (Estimating Function) Bootstrap

The aim is to approximate the distribution of $S_y(\theta) = \sum g_i(y_i, \theta)$. For this purpose, let $z_i = g_i(y_i, \hat{\theta})$, $i = 1, \dots, n$ and proceed as follows:

EF1: Draw a bootstrap sample z_1^*, \dots, z_n^* from z_1, \dots, z_n .

EF2: Let $S_y^* = z_1^* + \dots + z_n^*$.

The empirical distribution of S_y^* is used, after many repetitions of EF1 and EF2, to approximate the distribution of $S_y(\theta)$. This procedure, termed the *EF Bootstrap*, typically gives a first order approximation to the distribution of $S_y(\theta)$.

A higher order approximation can typically be obtained by the following *Studentized EF Bootstrap* procedure. Instead of approximating the distribution of $S_y(\theta)$, we approximate that of

$$S_y^{(1)}(\theta) = \hat{v}^{-1/2} S_y(\theta) \quad (2.4)$$

where $\hat{v} = \sum z_i z_i'$. Thus, we use

$$S_y^{(1)*} = v_*^{-1/2} S_y^* \quad (2.5)$$

where $v_* = \sum (z_i^* - \bar{z}^*)(z_i^* - \bar{z}^*)'$ and $\bar{z}^* = \sum z_i^*/n$.

Details on the order of approximations are discussed in Hu and Kalbfleisch (1997a) and some further comments can be found in Section 4 of this article.

It should be clear that, once the distribution of $S_y(\theta)$ is estimated, approximate confidence intervals or regions can be readily obtained. For example, if θ is a scalar and $S_y(\theta)$ is monotone in θ , the quantiles of the empirical distribution of S_y^* (or $S_y^{(1)*}$) can be used to determine confidence intervals for θ . More generally, let θ^* (or $\theta^{(1)*}$) be the unique value of θ that satisfies $S_y(\theta) = S_y^*$ (or $S_y^{(1)}(\theta) = S_y^{(1)*}$). Then from the above EF bootstrap procedure, we obtain $\theta_1^*, \theta_2^*, \dots$ (or $\theta_1^{(1)*}, \theta_2^{(1)*}, \dots$) which generates a *joint bootstrap confidence distribution* for θ . An approximate $1 - \alpha$ confidence interval is given by a set A which is chosen so that $P^*(\theta^* \in A) = 1 - \alpha$ or $P^*(\theta^{(1)*} \in A) = 1 - \alpha$. Here P^* refers to the bootstrap probability. In the scalar case, A is most naturally determined as the interval defined by the $\alpha/2$ and $1 - \alpha/2$ quantiles in the bootstrap confidence distribution. This is the method used in Section 3 below.

The Classical Bootstrap:

An alternative approach, in the spirit of the classical bootstrap, proceeds as follows:

- C1: select $g_1^*(y_1^*, \theta), \dots, g_n^*(y_n^*, \theta)$ as a bootstrap sample from $g_1(y_1, \theta), \dots, g_n(y_n, \theta)$.
- C2: Find θ_c^* , the solution to $\sum g_i^*(y_i^*, \theta) = 0$

The sequence $\theta_{c_1}^*, \theta_{c_2}^*, \dots$ obtained by repeating this process can similarly be used to generate confidence regions for θ .

It should be noted that the classical procedure summarized in C1 and C2 is computationally demanding, much more so than the EF bootstrap. In essence, the classical procedure specifies a new estimating equation with each bootstrap sample. With the EF procedure, however, only the right side of the equation changes while the estimating function $S_y(\theta)$ remains unchanged. In the context of a regression model, for example, the classical method amounts to a new design matrix with each bootstrap sample. The EF procedure, however, maintains the same design matrix throughout.

3 Some Examples

The interested reader is referred to Hu and Kalbfleisch (1997a) for a more extensive and complete set of examples and discussion. In this article, we give only a brief treatment of two related examples.

Example 1:

Suppose that y_1, \dots, y_n are independent random variables and that $E(y_i) = \mu$, $\text{var}(y_i) = \sigma_i^2$, $i = 1, \dots, n$ where the σ_i^2 's are known. The minimum variance unbiased estimating equation is

$$S_y(\mu) = \sum_{i=1}^n \frac{y_i - \mu}{\sigma_i^2} = 0 \quad (3.1)$$

which yields the estimator $\hat{\mu} = (\sum y_i / \sigma_i^2) / \sum 1 / \sigma_i^2$. We make comparison of five approaches:

- The normal approximations to $S_y(\mu)$ or $\hat{\mu}$
- The classical bootstrap
- The studentized classical bootstrap
- The EF bootstrap
- The studentized EF bootstrap.

It is worth noting that, if all the σ_i 's are equal, this reduces to the standard benchmark problem of estimating a population mean based on an iid sample. The estimating equation (3.1) then defines the sample mean. Hu and Kalbfleisch (1997a) note that the EF Bootstrap and the classical bootstrap yield, in this case, identical results, and also have the same studentized

versions. In this case, and more generally, the Efron or classical bootstrap can be viewed as a special case of the EF Bootstrap.

In the simulations reported here, however, we consider the case $n = 40$, $\mu = 0$ and $\sigma_i = 2.2i$, $i = 1, \dots, 40$ with normal and uniform errors. There were 1000 simulations of 1000 bootstrap samples. Table 1 gives the coverage probabilities for each of the four methods for nominal coverage probabilities of .80, .90 and .95.

All five procedures do fairly well though in the case of normal errors the (exact) normal method and the studentized procedures have more accurate coverage probabilities. With uniform errors, the studentized bootstrap appears to do somewhat better than any of the others.

Table 1. Coverage Percentages and Average Confidence Intervals for Competing Methods

Normal Errors				
	80%	90%	95%	
Normal approx.	80 [-0.92, 0.95]	89 [-1.18, 1.21]	95 [-1.42, 1.44]	
Classical bootstrap	77 [-0.90, 0.92]	87 [-1.16, 1.19]	93 [-1.39, 1.42]	
Studentized classical	80 [-0.92, 0.95]	90 [-1.18, 1.22]	95 [-1.42, 1.44]	
EF bootstrap	77 [-0.88, 0.91]	87 [-1.14, 1.17]	93 [-1.36, 1.40]	
Studentized EF	80 [-0.92, 0.95]	90 [-1.18, 1.21]	95 [-1.41, 1.45]	
Uniform Errors				
Normal approx.	81 [-0.91, 0.96]	92 [-1.16, 1.23]	96 [-1.41, 1.46]	
Classical bootstrap	78 [-0.89, 0.95]	88 [-1.15, 1.23]	94 [-1.38, 1.44]	
Studentized Classical	81 [-0.92, 0.96]	90 [-1.14, 1.23]	95 [-1.41, 1.46]	
EF bootstrap	77 [-0.88, 0.94]	89 [-1.14, 1.19]	94 [-1.36, 1.43]	
Studentized EF	80 [-0.91, 0.96]	91 [-1.14, 1.23]	95 [-1.40, 1.46]	

Example 2:

A related example is the common means problem of Neyman and Scott (1948) which has received much attention in the literature (see, for example, Kalbfleisch and Sprott (1970), Bartlett (1936), Cox and Reid (1987) and Barndorff-Nielsen (1983)). Specifically, we have k independent strata and, in the i th stratum, $y_{ij} \sim N(\mu, \sigma_i^2)$, $j = 1, \dots, n_i$, independently where $i = 1, \dots, k$. The variables σ_i^2 are unknown and interest centres on the estimation of μ . Neyman and Scott show that the maximum likelihood estimate of μ can be asymptotically inefficient if the stratum sizes are at least 3. They propose the estimating equation

$$\sum_{i=1}^k \frac{n_i(n_i - 2)(\bar{y}_i - \mu)}{T_i(\mu)} = 0 \tag{3.2}$$

where $T_i(\mu) = \sum_{j=1}^{n_i} (y_{ij} - \mu)^2$ and $\bar{y}_i = \sum y_{ij}/n_i$. This same equation has been proposed by many other authors as well.

More generally, we could consider the case where the y_{ij} 's are independent as above, but relax the normality assumption. Thus, we assume only independence and $E(y_{ij}) = \mu$, $var(y_{ij}) = \sigma_i^2$, $i = 1, \dots, k$, $j = 1, \dots, n_i$ with $\sigma_1^2, \dots, \sigma_k^2$ unknown. In this more general framework, we could still utilize (3.2) for estimation of μ .

Hu and Kalbfleisch (1997a) consider various sampling schemes and aspects of this problem. Here, we look only at one approach. Specifically, we let $y_i = (y_{i1}, \dots, y_{in_i})$ and $g_i(y_i, \mu) = n_i(n_i - 2)(\bar{y}_i - \mu)/T_i(\mu)$. Thus, (3.2) can be rewritten as

$$\sum_{i=1}^k g_i(y_i, \mu) = 0, \tag{3.3}$$

exactly of the form (2.1). The EF or classical bootstrap can now be applied in a straightforward manner to (3.3). We compare them and some normal approximations in the following simulation.

In total, six methods are compared:

- *Normal 1*: An asymptotic normal approximation in which the asymptotic variance of $\hat{\mu}$ is approximated by

$$\hat{\sigma}(1)^2 = \left\{ \sum 1/\hat{\sigma}_i^2 \right\}^{-1}$$

where $\hat{\sigma}_i^2 = \frac{1}{n_i} \sum (y_{ij} - \hat{\mu})^2$.

- *Normal 2*: An asymptotic normal approximation based on (2.3) to the distribution of $\sqrt{n}(\hat{\mu} - \mu)$ with variance estimate

$$\hat{\sigma}(2)^2 = n \sum_{i=1}^k g_i^2(y_i, \hat{\mu}) / \left(\sum \frac{\partial}{\partial \mu} g_i(y_i, \hat{\mu}) \right)^2$$

- *Classical Bootstrap*: This is obtained by resampling $g_i^*(y_i^*, \mu)$ from $g_i(y_i, \mu)$; let $\hat{\mu}_c^*$ denote the bootstrap estimator.
- *The Studentized Classical Bootstrap*: use the variance estimator $\hat{\sigma}(2)^2$ along with the estimator $\hat{\mu}_c^*$.
- *The EF Bootstrap*

- *The Studentized EF Bootstrap*

For the simulation, we used $k = 40$, $\mu = 0$, $n_i = 5$ and $2\sigma_i = 1 + (i - 1)/10$, $i = 1, \dots, 40$. The errors were taken to be normal in one case and double exponential in the other (with p.d.f. $\exp(-|x - \mu|/2)/4$). Table 2 compares the methods for intervals of nominal 90% coverage.

Table 2. Coverage Percentage and Average Confidence Intervals for Competing Methods

	Normal 90%	Double Exponential 90%
Normal 1	69.8 [-0.10, 0.10]	69.5 [-0.06, 0.06]
Normal 2	84.4 [-0.15, 0.15]	80.9 [-0.09, 0.08]
Classical*	87.3 [-0.16, 0.18]	85.8 [-0.10, 0.10]
Studentized Classical**	87.5 [-0.20, 0.19]	85.2 [-0.11, 0.12]
EF	89.3 [-0.17, 0.16]	87.8 [-0.09, 0.09]
Studentized EF	89.5 [-0.17, 0.16]	88.5 [-0.10, 0.09]

*10% failures as noted in comment iii) below.

**15% failures

A few comments follow:

- i) The first normal approximation works very badly indeed and clearly should not be used. The difficulty here is that there is no consistent estimate of σ_i^2 with small n_i fixed and $k \rightarrow \infty$.
- ii) The second normal approximation is less accurate than any of the bootstrap methods. It does work considerably better than the first approximation since it involves, at least, a consistent estimate of the variance.
- iii) The classical bootstrap appears to work reasonably well. From the simulations, however, about 10% of the bootstrap samples do not converge, using Newton's method, to a finite estimate of μ from a starting value of 0. The coverage rates and average intervals are based on the subset of bootstrap samples that give estimates for μ .
- iv) The classical bootstrap involves, on each bootstrap iteration, the solving of the estimating equation

$$\sum_{i=1}^k g_i^*(y_i^*, \mu) = 0 .$$

The computations involved in its implementation greatly exceed those for EF or the studentized EF Bootstrap.

- v) The studentized classical bootstrap does not offer any improvement in this case from the unstudentized version. This could be because the variance estimator $\hat{\sigma}(2)^2$ is not very accurate or stable.
- vi) There is a clear indication that both the EF and the studentized EF bootstrap give more accurate results. In this example, they are also more stable and computationally much simpler than the classical approach.

Many other examples are in Hu and Kalbfleisch (1997a) including a discussion of the linear model. Although Hu and Zidek (1995) approach the problem from a somewhat different view, the bootstrap procedure they recommend is numerically equivalent to the EF Bootstrap. As they note, the method they propose has excellent robustness properties against heteroscedasticity and compares favourably, even in the homoscedastic case with classical proposals.

4 Discussion

In this article, we have attempted to give only a brief introduction to the EF Bootstrap. More detail, further examples and theoretical aspects can be found in Hu and Kalbfleisch (1997a).

We conclude this paper with a number of comments and note some areas where further work is needed.

- A. This paper, Hu and Kalbfleisch (1997a) and Hu and Zidek (1995) provide considerable empirical evidence that the EF Bootstrap, and especially the studentized version, has very good properties over a wide class of problems. The method gives accurate results, is numerically more stable than most competitors, and appears to have good robustness properties.
- B. The EF Bootstrap leads to a simple straightforward studentized version and avoids the many questions that arise about appropriate studentization of bootstrap samples of complex estimators. By concentrating on the linear estimating equation, the studentized version follows automatically and is easily implemented. It also gives very accurate results in many applications.
- C. There is substantial computational advantage, in many problems, to the EF Bootstrap versus the classical approach. In the EF Bootstrap,

the observed estimating function $S_y(\theta)$ is unaltered and so repeated numerical solution of a new equation with each bootstrap sample is avoided. This also has appeal from the viewpoint of conditionality of the inferential approach; in the context of linear regression, for example, the EF Bootstrap corresponds to maintaining a common design matrix in all bootstrap replications.

- D. Hu and Kalbfleisch (1997a) use Edgeworth expansions to investigate the accuracy of the approximations. Under fairly general conditions, they show that the EF Bootstrap provides a first order approximation to the true distribution of $S_y(\theta)$ and the studentized EF Bootstrap provides a 2nd order approximation to the distribution of $S_y^{(1)}(\theta)$. Thus, confidence intervals based on the Studentized EF Bootstrap are accurate to order n^{-1} . This theoretical asymptotic accuracy is also reflected in the simulations in finite samples.
- E. The role of conditionality in Bootstrap procedures is one that in general requires further thought and investigation. In the context of the EF Bootstrap, one can ask whether there are aspects of the data upon which one should condition in obtaining the distribution of $S_y(\theta)$ that is suitable for inference. Similar questions arise with the bootstrap. In the common means problem, for example, it seems natural to condition on the n_i 's in making inferences about the common mean μ . This would suggest defining bootstrap replications in which the n_i 's are held fixed. Hu and Kalbfleisch (1997a) explore various possibilities here. Classical bootstrap methods appear to have very poor properties when the n_i 's are at all small and the natural conditional approach is used; the EF Bootstrap has better properties for moderate n_i , but it too breaks down if the n_i 's are very small ($n_i = 1$ or 2). The estimating function itself may be a poor choice if the n_i 's are this small. In general, however, we need to balance considerations of conditionality against the need for a broad set of outcomes in the bootstrap sample so as to obtain good approximations.
- F. We have assumed in the above that $S_y(\theta)$ is $1 : 1$. In some cases, it may not be $1 : 1$ and there may in fact be multiple roots. If a consistent root can be identified, the EF Bootstrap could be applied. More generally, however, the difficulty with multiple roots is basic to methods based on the estimating function itself and not a particular difficulty with the EF Bootstrap.
- G. In this article, we have assumed that the y_i 's are independent. In many applications, however, it is important to relax this assumption.

Various correlation structures could be considered. Hu and Kalbfleisch (1997b) consider extensions to autoregressive processes.

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