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Computing empirical likelihood from the bootstrap

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Abstract

The close relationship between the bootstrap and empirical likelihood has been noted in the literature. The purpose of this paper is to show how to construct a bootstrap likelihood from a single bootstrap, without any nested bootstrapping nor any smoothing. For a wide class of M-estimators the likelihood agrees with the empirical likelihood up to order $O(n^{-1/2})$. The resulting likelihood may be used for display purpose, for computing likelihood-based confidence intervals or for future use in combining information. © 2000 Elsevier Science B.V. All rights reserved

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1. Introduction

Construction of nonparametric likelihood from the bootstrap is reviewed in Chapter 24 of Efron and Tibshirani (1993). In particular Davison et al. (1992,1995) showed that we can construct the likelihood for a general scalar parameter using a nested bootstrap procedure and some additional kernel smoothing or saddlepoint approximation, while the methods of Boos and Monahan (1986), Hall (1987) or Ogbonmwan and Wynn (1988) require a pivotal variate as well as some nonparametric smoothing. The purpose of this paper is to show that a bootstrap likelihood $L_B(\theta)$ can be constructed for a general scalar parameter θ without any nested bootstrapping nor any smoothing. For a wide class of M-estimators the resulting likelihood agrees with the empirical likelihood $L_E(\theta)$ up to order $O(n^{-1/2})$, which is the same result found by Davison et al. (1992).

The key step in the construction of the bootstrap likelihood is the use of the invariance property on the likelihood implied by the normal model (3) below; this is in contrast to Efron's (1993) implied likelihood, which starts with a set of confidence intervals. The same model (3) underpins the construction of bias-corrected–accelerated (BC_a) bootstrap confidence intervals (Efron, 1987), which means that the validity of the

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proposed likelihood is equivalent to that of the $\mathrm{BC_a}$ method. In particular Efron (1987) showed that, up to a second-order approximation, model (3) holds for any regular one-parameter problem.

We describe the method in Section 2 and prove that

$$\log L_{\mathrm{B}}(\psi) = \log L_{\mathrm{E}}(\psi) + \mathrm{O}(n^{-1}), \tag{1}$$

where $\psi = n^{1/2}(\theta - \hat{\theta})$. Some numerical examples and uses of the bootstrap-generated likelihood are given in Section 3, and some comparison using Monte Carlo simulations are shown in Section 4. For setting approximate confidence intervals the bootstrap-based empirical likelihood shares the main advantage of the $\mathrm{BC_a}$ method, which is the ability to capture the asymmetry of exact intervals. The advantages of the likelihood function are discussed in Section 5.

2. Methodology

2.1. Bootstrap likelihood construction

The $\mathrm{BC_a}$ method for setting the bootstrap confidence intervals is described clearly in Efron (1987) or Efron and Tibshirani (1993). We review it briefly here as a way of developing our notation. Let $y \equiv (x_1, \ldots, x_n)$ be a random sample from a continuous distribution F, $\theta \equiv t(F)$ is a real-valued parameter of interest, and $\hat{\theta}$ and $\hat{F}$ be the estimates of θ and F. Then

a. generate bootstrap data y^* by resampling from $\hat{F}$,
b. compute $\hat{\theta}^*$ based on y^*
c. repeat (a) and (b) B times. Denote by G the true distribution function of $\hat{\theta}^*$ and $\hat{G}$ its estimate based on $\hat{\theta}_i^*, \ldots, \hat{\theta}_{\mathrm{B}}^*$.
d. compute the bias correction term z_0 by

$$z_0 = \Phi^{-1}\{\hat{G}(\hat{\theta})\},$$

where $\Phi(z)$ is the standard normal distribution function, and the acceleration term a according to (4.4) in Efron (1987) or (14.15) in Efron and Tibshirani (1993).

e. compute the interval as

$$[\hat{G}^{-1}\{\Phi(z[\alpha])\}, \hat{G}^{-1}\{\Phi(z[1-\alpha])\}], \tag{2}$$

where $z[\alpha] \equiv z_0 + (z_0 + z^\alpha)/\{1 - a(z_0 + z^\alpha)\}$ and $z^\alpha \equiv \Phi^{-1}(\alpha)$.

For $B = \infty$ interval (2) is exact if there exists a normalizing transform $\phi = h(\theta)$ such that

$$\frac{\hat{\phi} - \phi}{\sigma_\phi} \sim \mathrm{N}(-z_0, 1), \tag{3}$$

where $\sigma_\phi = 1 + a\phi$, otherwise it is second-order correct for any regular one-parameter problem (Efron, 1987). The latter is true since intuitively (3) involves a higher-order normal approximation.

The idea in this paper can be summarized as follows: construct a likelihood function for ϕ assuming model (3), then use the fact that the likelihood is invariant under transformation to construct the likelihood for θ. Specifically, if $\{\phi, L(\phi)\}$ is the graph of ϕ-likelihood, where

$$\log L(\phi) = -\log \sigma_\phi - \frac{(\hat{\phi} - \phi + z_0\sigma_\phi)^2}{2\sigma_\phi^2},$$

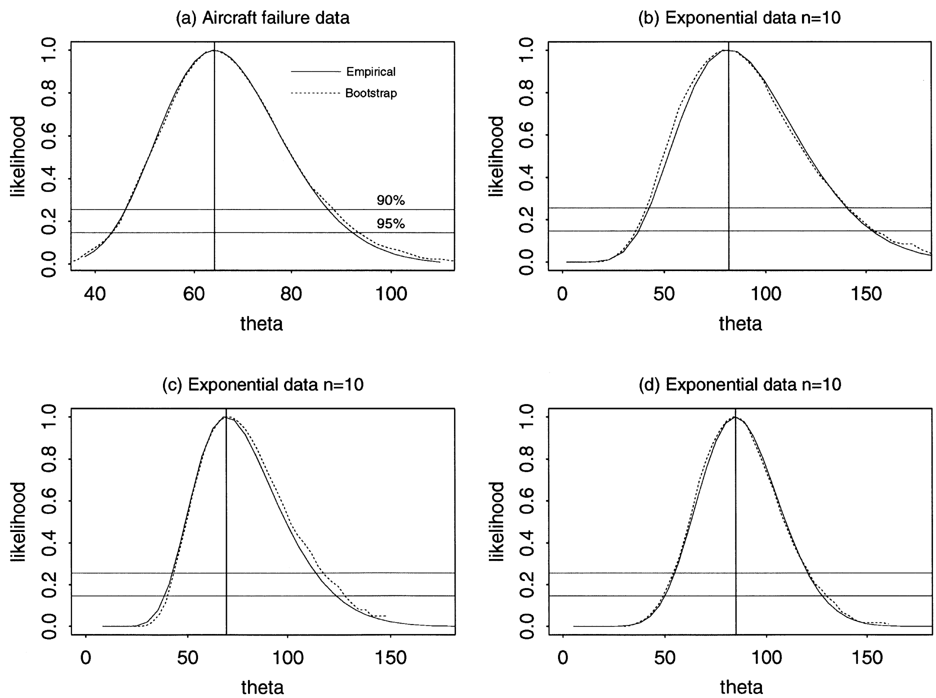

Fig. 1. (a) The bootstrap likelihood, in dotted line, and the empirical likelihood, in solid line, for the aircraft failure data; (b)–(d) same as in (a) for simulated exponential data with size $n=10$. The horizontal lines define the likelihood-based confidence interval limits based on χ_1^2 distribution. The vertical lines indicate the observed $\hat{\theta}$.

then $\{h^{-1}(\phi), L(\phi)\}$ is the graph of θ-likelihood. The proposed likelihood is defined as

$$L_{\mathrm{B}}(\theta) = L[\Phi^{-1}\{\hat{G}(\theta)\}], \tag{4}$$

where $\hat{\phi} = \Phi^{-1}\{\hat{G}(\hat{\theta})\}$ is used in computing $L(\phi)$. In effect this employs $h(\theta) = \Phi^{-1}\{\hat{G}(\theta)\}$ as the normalizing transform. This can be justified intuitively as follows: if $\hat{\theta}$ has distribution $G(\cdot)$, then $G(\hat{\theta})$ is standard uniform and $\Phi^{-1}\{G(\hat{\theta})\}$ is standard normal, so $\Phi^{-1}\{G(\cdot)\}$ is an exact normalizing transform for $\hat{\theta}$.

It is worth noting that no smoothing is needed in computing $L_{\mathrm{B}}(\theta)$, because for most practical purposes the bootstrap distribution G may be regarded as continuous (Hall, 1992, Appendix I); see also the examples in Figs. 1–3. In practice, we only need to ensure the bootstrap replication B is large enough for confidence interval computations; Efron (1987) indicated that $B = 1000$ is adequate. This is in contrast with Davison et al. (1992), where two levels of smoothing are needed, or Davison et al. (1995), where both smoothing and saddlepoint approximations are required. Following Davison and Hinkley (1988) Monte Carlo computation of the bootstrap distribution G may be replaced by a saddlepoint approximation.

2.2. Empirical likelihood

The empirical likelihood (Owen, 1988) is defined as the profile likelihood

$$L_{\mathrm{E}}(\theta) = \sup_{F_\theta} \prod_{i=1}^{n} p_i(\theta), \tag{5}$$

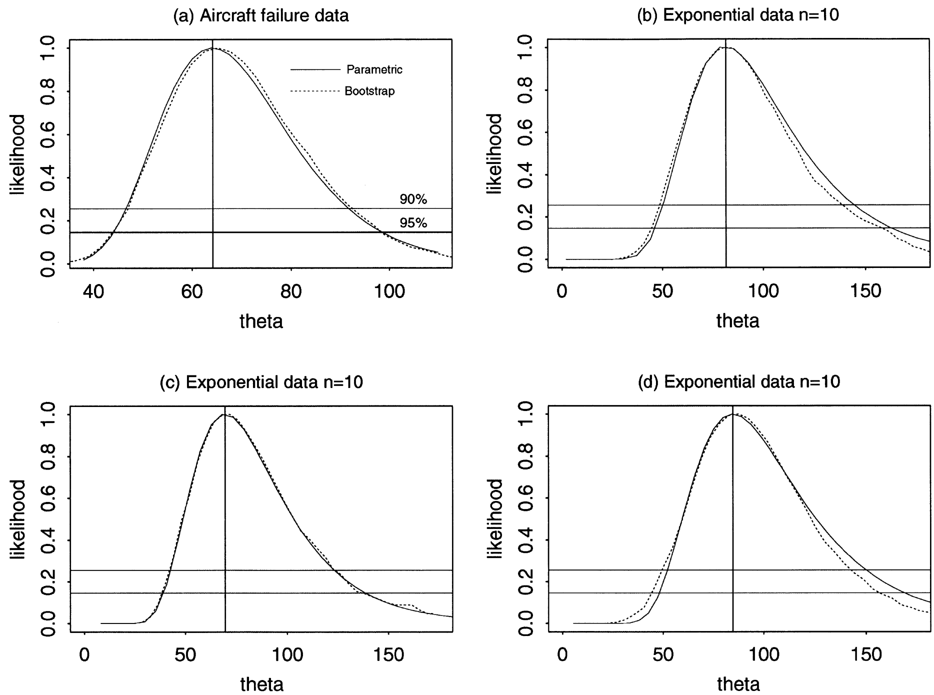

Fig. 2. (a)–(d) fully parametric likelihood, in solid lines, and the approximate bootstrap likelihood, in dotted lines, for the same data sets as in Fig. 1.

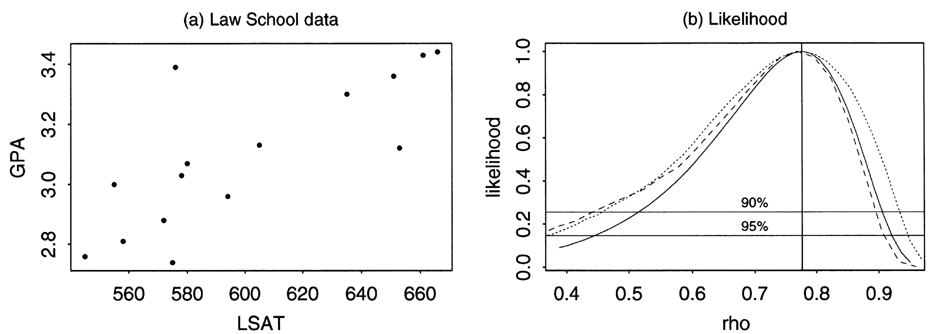

Fig. 3. (a) Law School data set from Table 4 of Efron (1987) showing the relationship between scholastic aptitude test and grade point average. (b) Parametric profile likelihood is in solid line, the nonparametric bootstrap likelihood in dotted line and the parametric bootstrap likelihood is dashed line.

where the supremum is taken over all possible distribution F_θ on $x_1,\dots,x_n$, which is characterized by $\{p_i(\theta),$ for $i=1,\dots,n\}$, such that functional $t(F_\theta)=\theta$.

Now suppose $\hat\theta$ is the solution of an estimating equation

$$\lambda(\theta)=n^{-1}\sum_{i=1}^{n}u(x_i,\theta)=0,$$

where $u(x;\theta)$ is monotone in θ for every x and smooth enough to allow up to second-order expansion around $\hat{\theta}$. Define the following quantity:

$$\kappa_{k,l,\dots} = n^{-1}\sum_{i=1}^{n} u^{(k)}(x_i,\hat{\theta})u^{(l)}(x_i,\hat{\theta})u^{(\dots)}(x_i,\hat{\theta}),$$

where $u^{(k)}(x_i,\hat{\theta})$ is the kth derivative of $u(x;\theta)$ with respect to θ evaluated at $\hat{\theta}$. For example

$$\kappa_{0,1} = n^{-1}\sum_{i=1}^{n} u(x_i,\hat{\theta})u'(x_i,\hat{\theta}).$$

Then Davison et al. (1992) showed that, for $\psi = n^{1/2}(\theta-\hat{\theta})$,

$$-\log L_{\mathrm{E}}(\psi) = \frac{1}{2}\psi^2\frac{\kappa_1^2}{\kappa_{0,0}} - \frac{n^{-1/2}}{6\kappa_{0,0}^3}\psi^3(6\kappa_{0,0}\kappa_{0,1}\kappa_1^2 - 2\kappa_{0,0,0}\kappa_1^3 - 3\kappa_{0,0}^2\kappa_1\kappa_2) + \mathrm{O}(n^{-1}).$$

2.3. Main result and its proof

We will now show that

$$\log L_{\mathrm{B}}(\psi) = \log L_{\mathrm{E}}(\psi) + \mathrm{O}(n^{-1}), \tag{6}$$

which means that the bootstrap likelihood agrees with the empirical likelihood up to order $\mathrm{O}(n^{-1/2})$.

We will assume that B is large enough, so that the error in estimating G is negligible (Efron, 1987, Section 9), and G will be treated as continuous with density g (Hall, 1992, Appendix I). First we show that $z_0 = a + \mathrm{O}(n^{-1})$, which extends Efron's (1987) Theorem 2 for maximum-likelihood estimation. Let $\lambda^*(t) = n^{-1}\sum_i u(x_i^*, t)$. For any t the event $(\hat{\theta}^* \leqslant t)$ is equivalent to $\{\lambda^*(t) \leqslant 0\}$ and, using the Edgeworth expansion (Hall, 1993, Chapter 3),

$$\begin{aligned} G(t) = P\{\lambda^*(t)\leqslant 0\} &= \Phi(z) - \varphi(z)n^{-1/2}\gamma_3(z^2-1)/6 + \mathrm{O}(n^{-1}) \\ &= \Phi(z) - \varphi(z)a(z^2-1) + \mathrm{O}(n^{-1}), \end{aligned} \tag{7}$$

where $\varphi(z)$ is the standard normal density,

$$z = -\frac{\sum_i u(x_i,t)}{\{\sum_i u^2(x_i,t)\}^{1/2}},$$

$\gamma_3 = \kappa_{0,0,0}/\kappa_{0,0}^{3/2}$ and $a = n^{-1/2}\gamma_3/6$.

At the observed value $t = \hat{\theta}$ we have $z = 0$, so

$$G(\hat{\theta}) = 0.5 + a\varphi(0) + \mathrm{O}(n^{-1})$$

and

$$\begin{aligned} z_0 = \Phi^{-1}\{G(\hat{\theta})\} &= \Phi^{-1}(0.5) + \frac{1}{\varphi\{\Phi^{-1}(0.5)\}}a\varphi(0) + \mathrm{O}(n^{-1}) \\ &= a + \mathrm{O}(n^{-1}). \end{aligned}$$

Third-order expansion of $-\log L(\phi)$ around $\hat{\phi}$, and using $z_0 = a + \mathrm{O}(n^{-1})$ and simplifying the terms of order $\mathrm{O}(n^{-1})$, yields

$$-\log L(\phi) = \tfrac{1}{2}(\phi-\hat{\phi})^2 - a(\phi-\hat{\phi})^3 + \mathrm{O}(n^{-1}).$$

Recalling that $\phi - \hat\phi = h(\theta) - h(\hat\theta)$, and making a second-order expansion on $h(\theta)$ around $\hat\theta$, we obtain

$$-\log L(\theta) = \tfrac{1}{2}h'(\hat\theta)^2(\theta-\hat\theta)^2 + \{\tfrac{1}{2}h'(\hat\theta)h''(\hat\theta) - ah'(\hat\theta)^3\}(\theta-\hat\theta)^3 + \mathrm{O}(n^{-1}).$$

Now use $h(\theta) = \Phi^{-1}\{G(\theta)\}$, so that $h'(\theta) = g(\theta)/\varphi\{h(\theta)\}$ and

$$h''(\theta) = g'(\theta)/\varphi\{h(\theta)\} + h'(\theta)h''(\theta)^2.$$

From (7) we get

$$g(\theta) = \varphi(z)z' - \varphi'(z)z'a(z^2-1) - 2\varphi(z)azz' \tag{8}$$

$$\begin{aligned} g'(\theta) = {} & \varphi'(z)(z')^2 + \varphi(z)z'' - \varphi''(z)(z')^2a(z^2-1) - \varphi'(z)z''a(z^2-1) \\ & -2\varphi'(z)z'azz' - 2\varphi'(z)z'azz' - 2\varphi(z)a\{(z')^2 + zz''\}, \end{aligned} \tag{9}$$

where we can show that $\varphi'(z) = -z\varphi(z)$ and $\varphi''(z) = -\varphi(z) - z\varphi'(z)$. Note that at the observed $\hat\theta$ we have $z = 0$ and, after much algebra,

$$z' = -n^{1/2}\kappa_1/\kappa_{0,0}^{1/2},$$

$$z'' = \frac{2n^{1/2}\kappa_1}{\kappa_{0,0}^{1/2}}\{\kappa_{0,1}/\kappa_{0,0} - \kappa_2/(2\kappa_1)\}.$$

Substituting all the appropriate terms in (8) and (9), evaluating $h'(\hat\theta)$ and $h''(\hat\theta)$, and using $a = n^{-1/2}\kappa_{0,0,0}/(6\kappa_{0,0}^{3/2})$ and $\psi = n^{1/2}(\theta - \hat\theta)$, we obtain

$$\begin{aligned} -\log L_{\mathrm{B}}(\psi) &= \frac{1}{2}\psi^2\frac{\kappa_1^2}{\kappa_{0,0}} - \frac{n^{-1/2}}{6\kappa_{0,0}^3}\psi^3(6\kappa_{0,0}\kappa_{0,1}\kappa_1^2 - 2\kappa_{0,0,0}\kappa_1^3 - 3\kappa_{0,0}^2\kappa_1\kappa_2) + \mathrm{O}(n^{-1}) \\ &= -\log L_{\mathrm{E}}(\psi) + \mathrm{O}(n^{-1}). \end{aligned}$$

3. Examples

Fig. 1 shows some examples of bootstrap likelihood $L_{\mathrm{B}}(\theta)$ based on the sample mean. In all cases the bootstrap likelihood, in dotted lines, are very close to the empirical likelihood, in solid lines, even for samples of size 10. The data for Fig. 1(a) are $n = 24$ intervals in hours between repairs and failures of an aircraft air-conditioning equipment: 50, 44, 102, 72, 22, 39, 3, 15, 197, 188, 79, 88, 46, 5, 5, 36, 22, 139, 210, 97, 30, 23, 13, 14. The same data set was analysed by Davison et al. (1992) using their nested bootstrap likelihood. Further examples in Fig. 1(b)–(d) are based on random samples of size 10 from the exponential distribution with mean θ. The true parameter $\theta_0 = 64.125$ is the mean of the aircraft data. In all cases the bootstrap replication $B = 2000$ is used.

The bootstrap method can be used to approximate a *parametric* likelihood, especially a profile likelihood for a scalar parameter. The computation is the same as before, but instead of using the empirical distribution, we generate bootstrap data according to a parametric model. As an illustration Fig. 2(a)–(d) compare the fully parametric exponential likelihood with the bootstrap approximation for exactly the same datasets as those for Fig. 1(a)–(d).

One may ask why we want to do this. The reason is that in multi-parameter problems a parametric profile likelihood is sometimes very tedious to compute, while the approximate bootstrap likelihood is still simple. For example, to compute the profile likelihood of the correlation coefficient ρ in a bivariate normal model, the full likelihood is a function of $(\mu_x, \sigma_x^2, \mu_y, \sigma_y^2, \rho)$. To get a profile likelihood for ρ we need to maximize over four-dimensional subspace of $(\mu_x, \sigma_x^2, \mu_y, \sigma_y^2)$ at each fixed value of ρ. There is no closed-form solution for this problem and a numerical solution may be too cumbersome for routine application.

In the single parameter case the parametric bootstrap likelihood would approximate the exact likelihood well if it is based on a sufficient statistic. The degree of approximation is determined by the normal model (3), which we know is correct up to the second order. When there are nuisance parameters, the profile likelihood of the parameter of interest θ is associated with the marginal distribution of $\hat{\theta}$; since in this case (3) is also a good approximation of the latter we expect the bootstrap likelihood to approximate the profile likelihood well. There is no formal proof for this, but for exponential family models Efron (1993) proved that the closely related implied likelihood agrees with the profile likelihood up to the second order.

Fig. 3(b) shows the nonparametric, exact and approximate parametric profile likelihood of the correlation coefficient for Law School data set as reported in Table 4 of Efron (1987). The data set, plotted in Fig. 3(a), shows the average scholastic aptitude tests and the grade point average from 15 Law schools in the United States. The discrepancy between the exact and approximate parametric likelihood is reduced if a is closer to zero. Further simulations with bivariate normal models indicate that some improvement is needed in the estimation of the acceleration constant a.

4. Simulation study

Here we describe a simulation study of the confidence intervals for the mean of the χ^2 distribution with one degree of freedom. Because of skewness this is comparable to estimation of the variance, which is known to be a hard nonparametric problem (Schenker, 1985; Owen, 1988). Specifically, $x_1, \ldots, x_n$ are an i.i.d. sample from $\theta\chi_1^2$, where we use a sample size $n = 20$ and the true $\theta = 1$. For each sample we compute the 90% confidence interval for the mean θ, using

(a) Exact method based on equi-tailed probability of the pivotal statistic $\sum_i x_i/\theta$:

$$\frac{\sum_i x_i}{\chi^2_{20,0.95}} \leqslant \theta \leqslant \frac{\sum_i x_i}{\chi^2_{20,0.05}}.$$

where $\chi^2_{20,0.95} = 31.41$ and $\chi^2_{20,0.05} = 10.85$.

(b) Exact likelihood method, based on the exact distribution of the likelihood ratio test (LRT). We can show that

$$\frac{L(\theta)}{L(\hat{\theta})} = \left(\sum_i x_i/\theta\right)^{n/2} \exp\left(-\sum_i x_i/\theta\right),$$

where $\hat{\theta} = \sum_i x_i/n$ is the MLE of θ. The exact likelihood interval is

$$\frac{\sum_i x_i}{c_1} \leqslant \theta \leqslant \frac{\sum_i x_i}{c_2},$$

where c_1 and c_2 satisfy

$$P\left(\sum_i X_i > c_1\right) + P\left(\sum_i X_i < c_2\right) = 0.1$$

and

$$c_1^{n/2} e^{-c_1/2} = c_2^{n/2} e^{-c_2/2}.$$

Table 1
Simulation results based on 1000 Monte Carlo replications of an i.i.d. sample of size 20 from the χ^2_1 distribution. The simulation standard error is around 0.01 for the 'lower average', 0.02 for the 'upper average', 0.7% for the 'left error' and the 'right error', and 1% for the 'total error'

Procedure	Lower average	Upper average	Left error	Right error	Total error
1. Parametric					
(a) Exact equi-tail	0.65	1.87	4.2	4.8	9.0
(b) Exact likelihood	0.63	1.80	3.3	5.9	9.2
(c) BC_a	0.65	1.87	4.4	4.9	9.3
(d) Bootstrap likelihood	0.63	1.79	3.3	6.0	9.3
2. Nonparametric					
(e) Percentile	0.56	1.50	2.9	13.9	16.8
(f) BC_a	0.62	1.64	4.9	9.7	14.6
(g) Bootstrap likelihood	0.61	1.60	4.5	10.5	15.0
(h) Empirical likelihood	0.63	1.57	4.7	11.5	16.2

Note that in this case the exact likelihood interval is also the confidence interval associated with the uniformly most powerful unbiased test for θ (Lehmann, 1986, p. 139). For $n=20$ we find $c_1=32.36987$ and $c_2=11.24881$, with $P(\sum_i X_i < c_2) = 0.06$ and $P(\sum_i X_i > c_1) = 0.04$.

(c) Parametric BC_a method: as described in Section 2 by bootstrapping from $\hat{\theta}\chi^2_1$.

(d) Parametric bootstrap likelihood: as described in Section 2 by bootstrapping from $\hat{\theta}\chi^2_1$.

(e) Nonparametric bootstrap using the percentile of the bootstrap distribution as confidence interval, i.e., $\hat{G}_{0.05} \leqslant \theta \leqslant \hat{G}_{0.95}$.

(f) Nonparametric BC_a as described in Section 2.

(g) Nonparametric bootstrap likelihood as described in Section 2, by defining the interval as the values of θ that satisfy

$$2 \log \frac{L_B(\theta)}{L_B(\hat{\theta})} \geqslant -\chi^2_{1,0.9} = -2.71.$$

(h) Empirical likelihood as described in Section 2, by defining the interval as in part (g) above.

In all bootstrap computations we use $B=2000$ bootstrap replications. The whole set of computations above is repeated 1000 times and the results are summarized in Table 1. The 'total error' column is the percent of times the confidence intervals do not cover the true; the standard error is around 1%, so for the parametric methods all observed errors are within one standard error of the true error (10%). The parametric bootstrap sampling works very well in this example, matching the performance of the corresponding exact methods and indicating the success of the approximating model (3). The failure of the nonparametric methods in this case is well known (e.g., Owen, 1988).

The 'lower average' and 'upper average' are the averages of the lower and upper limits of the confidence intervals. These averages show the asymmetry of the exact intervals, which is captured by the BC_a and the likelihood methods, but not by the percentile method. The 'left error' is the percent of times the left limit of the interval is greater than the true value, and the 'right error' is the percent of times the right limit of the interval is less than the true value. (The 'total error' is the sum of 'left' and 'right' errors.) For the parametric sampling the bootstrap methods achieve comparable one-sided errors with the exact methods. As shown under the 'right error' column, all nonparametric methods suffer from an under-coverage problem on the right, with the percentile method being the worst.

As expected theoretically, for nonparametric sampling the performance of the bootstrap likelihood is comparable to the empirical likelihood. While the total error characteristics are in good agreement, it is clear from the parametric sampling that the one-sided characteristics of the bootstrap likelihood intervals should not be directly compared with equi-tailed bootstrap intervals.

5. Discussion

In parametric problems we commonly plot the likelihood function to display the inferential information we have about a parameter θ. However, in nonparametric problems where we perform some bootstrapping, it is common practice to plot the bootstrap density or histogram, as if to represent the uncertainty about the parameter. This is a rather curious habit since, being a sampling density for a fixed parameter value, the bootstrap density does not carry a proper inferential information about θ. The latter is clear, for example, from the fact that the bootstrap density is a function of $\hat{\theta}$ rather than θ, and that the so-called percentile method, which is most closely connected to the bootstrap density, does not work well.

The 'density' that does carry such information is the likelihood function, but the current methods to compute a nonparametric likelihood function, such as nested bootstrapping, are still too computer intensive for routine use. Profiling the empirical likelihood for a single parameter in a multi-parameter case is also very computer intensive as it requires two-staged optimization; for example, to get a profile empirical likelihood of the correlation coefficient one needs a series of four-dimensional optimization routine running on top of a five-dimensional optimization (Owen, 1990).

In this paper we have shown that once bootstrapping step is finished one can compute the empirical likelihood immediately using formula (4). The likelihood function may be used for display purpose as in the parametric problems, and for computing and displaying likelihood-based confidence intervals. Other advantages were discussed in Davison et al. (1992). For example, the likelihood function is the natural quantity for combining information about a parameter as well as for incorporating prior information.

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