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ASYMPTOTIC ITERATED BOOTSTRAP CONFIDENCE INTERVALS

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An iterated bootstrap confidence interval requires an additive correction to be made to the nominal coverage level of an uncorrected interval. Such correction is usually performed using a computationally intensive Monte Carlo simulation involving two nested levels of bootstrap sampling. Asymptotic expansions of the required correction and the iterated interval endpoints are used to provide two new computationally efficient methods for constructing an approximation to the iterated bootstrap confidence interval. The first asymptotic interval replaces the need for a second level of bootstrap sampling with a series of preliminary analytic calculations, which are readily automated, and from which an approximation to the coverage correction is easily obtained. The second interval directly approximates the endpoints of the iterated interval and yields, for the first time, the possibility of constructing an approximation to an iterated bootstrap confidence interval which does not require any resampling. The theoretical properties of the two intervals are considered. The computation required for their construction is detailed and has been coded in a fully automatic user-friendly Fortran program which may be obtained by anonymous ftp. A simulation study which illustrates their effectiveness on three examples is presented.

1. Introduction. An iterated bootstrap confidence interval may be derived from the percentile method described by Efron [(1982), Section 10.4]. Beran (1987) proposed a prepivoting method to reduce coverage error, which is equivalent to making an additive correction to the nominal coverage level in the percentile method. Hall and Martin (1988) discuss this coverage correction approach within a general framework of bootstrap iteration. Our notion of an iterated bootstrap confidence interval refers to this approach. A precise definition is given in Section 2.

When constructing an iterated bootstrap confidence interval, the need to calculate a correction to the nominal coverage, or “calibrating coefficient,” is usually met by a double bootstrap procedure. In principle, we can iterate the procedure to reduce coverage error by a factor of $O(n^{-1})$ successively. Hall and Martin (1988) provide a unified account of the concept of iterated bootstrap. In practice we seldom go beyond the second level of bootstrap sampling, due to the increasing computational intensity rendered by successive levels of bootstrap sampling. In this paper we consider only an iterated bootstrap...
bootstrap confidence interval based on double bootstrapping, that is, with one level of nominal coverage correction.

The computational expense of the usual Monte Carlo construction, as considered by Booth and Hall (1994), has prompted a number of authors to develop computationally efficient procedures for approximation to the iterated bootstrap confidence interval. DiCiccio, Martin and Young (1992a, b) consider the use of analytic approximation methods to replace the inner of the two levels of resampling required by the double bootstrap procedure. An alternative approach described by Booth and Do (1993) uses the variance reduction method of balanced importance sampling at the first level of the iterated bootstrap to achieve computational savings over the standard Monte Carlo construction. Lee and Young (1993) describe an approach which performs the inner of the two levels of bootstrap sampling in a sequential manner. This approach, while still demanding, like the method of Booth and Do (1993), two levels of resampling, has the advantage of only requiring simple uniform resampling. In the current paper the goal is to develop approximations to the iterated bootstrap interval which eliminate the need for nested levels of resampling and which at the same time require only simple arithmetic computation.

Hall [(1992), Section 3.11.3] gives an account of the coverage properties of the iterated bootstrap confidence interval. Asymptotic expansions are also developed for the iterated interval endpoints, as well as for the calibrating coefficient, under his "smooth function model." Hall uses these expansions to explain theoretically why bootstrap iteration works. The complicated structure of the expansions might be felt to hold out little hope for their being of practical use. In this paper, however, we demonstrate how we may obtain explicit expressions, in terms of population moments, for the leading terms in the expansions of both the calibrating coefficient and interval endpoints. These asymptotic expressions are then used as the basis of two new computationally efficient and practically feasible procedures for constructing an approximation to the iterated bootstrap confidence interval.

The first asymptotic interval replaces the need for a second level of bootstrap sampling with a series of preliminary analytic calculations from which an approximation to the calibrating coefficient is easily obtained. The second interval directly approximates the endpoints of the iterated interval. This represents, for the first time, an approximation to the iterated bootstrap confidence interval which does not require any resampling.

The analytic computations required for construction of the asymptotic intervals are automated to provide practical procedures which are computationally extremely efficient when compared to the usual iterated bootstrap confidence interval construction which uses two nested levels of data resampling. The only input required from the user is a formula for the parameter of interest in terms of population moments, the maximum order of such moments and the dimension of the underlying distribution. In particular, techniques of exact numerical derivative evaluation are introduced to replace the need for any symbolic computation. The resulting procedures thus consist
only of simple numerical steps which can be efficiently implemented using a Fortran program. The computer time required is reduced by a factor of the order of thousands compared to a full-blown iterated bootstrap confidence interval based on 1000 outer level and 1000 inner level resamples.

Section 2 gives a formal definition of the iterated bootstrap confidence interval and presents briefly the forms of the asymptotic expansions to be used in our procedure of generating asymptotic iterated confidence intervals. Section 3 develops the theory about coverage properties of these asymptotic intervals. There they are also compared with the theoretical iterated bootstrap interval. A qualitative description of the practical procedures is presented in Section 4, with special attention paid to description of how they may be implemented by use of a general package consisting of two user-friendly Fortran programs. A simulation study has been carried out on the mean, the variance and the correlation coefficient examples, and their results are reported in Section 5, followed by a general discussion in Section 6. All the analytic computations necessary for construction of the asymptotic intervals are detailed in the Appendix.

2. Problem specification. Let $x = (X_1, X_2, \ldots, X_n)$ be a random sample drawn from a $d$-variate distribution function $F$. We wish to construct a two-sided, $\alpha$-level iterated bootstrap confidence interval, based on $x$, for a parameter $\theta$. Assume that $\theta = g(\mu)$ is a smooth function of the mean $\mu$ of $F$. The confidence interval is to be constructed from its sample estimate $\hat{\theta} = g(\bar{X})$, where $\bar{X} = n^{-1}\sum_{i=1}^{n}X_i$. Define $y_{\beta}$ to be the $\beta$-th quantile of the distribution of $\hat{\theta}$, so that

$$\mathbb{P}\left(\hat{\theta} \leq y_{\beta}\right) = \beta.$$ 

Let $x^* = (X_1^*, \ldots, X_n^*)$ denote a generic bootstrap resample drawn randomly from $x$ with replacement, and similarly let $x^{**}$ denote a generic resample from $x^*$. The conditional probability and expectation based on such uniform resampling from $x$ and $x^*$ are denoted by $\mathbb{P}(\cdot|x)$, $\mathbb{E}(\cdot|x)$, $\mathbb{P}(\cdot|x^*, x)$ and so on. Let $\hat{\theta}^*$ and $\hat{\theta}^{**}$ be the versions of the statistic $\hat{\theta}$ based on $x^*$ and $x^{**}$, respectively. Define the $\beta$-th quantile of the distribution of $\hat{\theta}^*$ conditional on $x$ to be

$$\hat{y}_{\beta} = \sup\{u: \mathbb{P}(\hat{\theta}^* \leq u|x) \leq \beta\},$$

for $0 \leq \beta \leq 1$. We will assume from now on that $\hat{y}_{\beta}$ is the exact solution to the equation

$$\mathbb{P}(\hat{\theta}^* \leq \hat{y}_{\beta}|x) = \beta,$$

since the error due to discreteness of the sampling distribution of $\hat{\theta}^*$ is negligible compared to other error terms to be met in this section [see Hall (1986)]. Put $\xi = \frac{1}{2}(1 + \alpha)$. Let $t$ be the solution to the equation

$$\mathbb{P}(\hat{y}_{\xi-t/2} \leq \theta \leq \hat{y}_{\xi+t/2}) = \alpha.$$

(1)
Similarly, the bootstrap version of \( t \) is given by \( \hat{t} \) which satisfies
\[
\Pr\left( \hat{y}^*_1 - \hat{t}/2 \leq \hat{\theta} \leq \hat{y}^*_1 + \hat{t}/2 | \mathcal{F} \right) = \alpha, \tag{2}
\]
where
\[
\Pr\left( \hat{\theta}^{**} \leq \hat{y}^*_\beta | \mathcal{F}^*, \mathcal{F} \right) = \beta,
\]
for \( 0 \leq \beta \leq 1 \). The two-sided iterated bootstrap confidence interval of nominal coverage level \( \alpha \) is then given by
\[
I_0 = \left[ \hat{y}^*_1 - \hat{t}/2, \hat{y}^*_1 + \hat{t}/2 \right].
\]
The sample-based quantity \( \hat{t} \) may be termed the calibrating coefficient of the nominal coverage level \( \alpha \), using the notion introduced by Loh (1987). In fact, the interval \( I_0 \) resembles a two-sided percentile method interval with its nominal coverage level \( \alpha \) calibrated to \( \alpha + \hat{t} \).

Note that \( \hat{t} \) can alternatively be obtained from the equation
\[
\Pr\left( |2U^* - 1| \leq \alpha + \hat{t} | \mathcal{F} \right) = \alpha, \tag{3}
\]
where
\[
U^* = \Pr\left( \hat{\theta}^{**} \leq \hat{\theta} | \mathcal{F}^*, \mathcal{F} \right).
\]
In practice, the sample-based interval \( I_0 \) may be approximated by double bootstrap resampling. An inner level of resampling is required to approximate \( U^* \) from the conditional distribution of \( \hat{\theta}^{**} \), while an outer level of resampling is used to approximate the distribution of \( U^* \) itself. Such a double bootstrap scheme is usually very time-consuming and computationally intensive.

Asymptotic formulae of \( \hat{t} \) and \( \hat{y}_\beta \) are, however, available under some mild conditions on \( g \) and \( F \). Suppose for the time being that both \( t \) and \( y_\beta \) admit Edgeworth expansions as follows:
\[
t = 2n^{-1}\pi_1(z_\xi)\phi(z_\xi) + 2n^{-2}\pi_2(z_\xi)\phi(z_\xi) + \cdots \tag{4}
\]
and
\[
y_\beta = \theta + n^{-1/2}\sigma\left\{ z_\beta + n^{-1/2}p_{11}(z_\beta) + n^{-1}p_{21}(z_\beta) + \cdots \right\}, \tag{5}
\]
for \( 0 < \beta < 1 \), where the \( \pi_j \)'s are odd polynomials, the \( p_{j1} \)'s are polynomials of degree at most \( j + 1 \) and are odd for even \( j \) and even for odd \( j \); \( \sigma^2 \) is the asymptotic variance of \( n^{1/2}(\hat{\theta} - \theta) \); \( \phi \) is the standard normal density function; and \( z_\beta = \Phi^{-1}(\beta) \) is the usual \( \beta \)th standard normal quantile. A detailed derivation of expansions (4) and (5) is given in Hall [(1992), Chapter 3]. Full explicit expressions for \( t \) and \( y_\beta \) are detailed in the Appendix. Since \( \sigma \) and the coefficients of the \( \pi_j \)'s and \( p_{j1} \)'s depend only on moments of \( F \) up to a certain order, we can easily write down the corresponding expansions for their bootstrap versions \( \hat{t} \) and \( \hat{y}_\beta \):
\[
\hat{t} = 2n^{-1}\hat{\pi}_1(z_\xi)\phi(z_\xi) + 2n^{-2}\hat{\pi}_2(z_\xi)\phi(z_\xi) + \cdots \tag{6}
\]
and
\[
\hat{y}_\beta = \hat{\theta} + n^{-1/2}\hat{\sigma}\left\{ z_\beta + n^{-1/2}\hat{p}_{11}(z_\beta) + n^{-1}\hat{p}_{21}(z_\beta) + \cdots \right\}, \tag{7}
\]
where $\hat{\pi}_j$, $\hat{p}_{j1}$ and $\hat{\sigma}$ are obtained by substituting sample moments for population moments in the definitions of $\pi_j$, $p_{j1}$ and $\sigma$, respectively. Define

$$\bar{t} = 2n^{-1}\hat{\pi}_1(z_\xi)\phi(z_\xi)$$

and

$$\bar{y}_\beta = \hat{\theta} + n^{-1/2}\hat{\sigma}\left\{z_\beta + n^{-1/2}\hat{p}_{11}(z_\beta) + n^{-1}\hat{p}_{21}(z_\beta)\right\}.$$  

Both expressions (8) and (9) can be evaluated exactly from sample moments, without simulation. By this means we arrive at two possible sample-based asymptotic confidence intervals, namely,

$$I_1 = \left[\hat{y}_{1-\xi-i/2}, \hat{y}_{\xi+i/2}\right] \text{ and } I_2 = \left[\hat{y}_{1-\xi-i/2}, \hat{y}_{\xi+i/2}\right].$$

Note that the interval $I_1$ still involves the sample quantity $\hat{y}_\beta$, which has to be approximated by one level of bootstrap resampling. However, the inner level of resampling is avoided by use of $\bar{t}$, which is computed directly without resampling. For the interval $I_2$, no resampling is required at all.

The next section investigates the asymptotic properties of all three intervals $I_0$, $I_1$ and $I_2$.

3. **Theory.** First we establish some notation. Define, for any vector $x \in \mathbb{R}^m$,

$$x^{(i)} = \text{the } i\text{th component of } x \text{ and } \|x\|^2 = \sum_{i=1}^{m} (x^{(i)})^2.$$  

We may sometimes for convenience write $x^{(i)}$ as $x_i$, provided no ambiguity is introduced in the context.

Throughout this section we shall make free use of Edgeworth expansions up to some order as deemed necessary in the context. Conditions for their validity are described in full detail in Hall ([1992], Chapter 5). Briefly, sufficient conditions for the results derived in this section to hold can be summarised as follows:

1. $g$ has eight bounded continuous derivatives in a neighbourhood around $\mu$;
2. for some sufficiently large $\nu > 0$, $\mathbb{E}[\|X\|^\nu] < \infty$;
3. $F$ satisfies Cramèr's condition, that is,

$$\limsup_{\|t\| \to \infty} \chi_F(t) < 1,$$

where $\chi_F(t) = \mathbb{E}[\exp(it^T X)]$ is the characteristic function of $F$.

In particular, Cramèr's condition holds if $F$ has a nondegenerate absolutely continuous component. In order to facilitate development of theoretical results about the asymptotic intervals we will assume conditions 1–3 from now on.

For convenience, append to the random vector $X$ products of the form

$$X^{(i_1)}X^{(i_2)}, X^{(i_1)}X^{(i_3)}X^{(i_2)}, \ldots, X^{(i_1)} \ldots X^{(i_p)},$$
up to a suitable order $p$, which must be at least the maximum order of moments of $F$ we come across in this section. For reasons explained in the Appendix, it suffices to take $p = 6$.

Suppose now that $X$ has this extended form, with dimension $d^\dagger$, say, and that $\mu = \mathbb{E}[X] \in \mathbb{R}^{d^\dagger}$. Noting that the original $X$ and $\mu$ are exactly the first $d$ components of their respective extended versions, we can redefine the function $g(x)$ on the more general domain $\mathbb{R}^{d^\dagger}$ in an obvious way so that $g$ depends on the first $d$ components of $x$ only. Define also

$$
\mu_{i_1 i_2 \ldots i_r} = \mathbb{E} \left[ (X - \mu)^{(i_1)} (X - \mu)^{(i_2)} \cdots (X - \mu)^{(i_r)} \right],
$$

where $i_j = 1, 2, \ldots, d^\dagger$.

The asymptotic variance of $n^{1/2} (\hat{\theta} - \theta)$ may then be obtained as

$$
\sigma^2 = \sum_{i, j = 1}^{d} \frac{\partial g}{\partial x_i} \bigg|_{x = \mu} \frac{\partial g}{\partial x_j} \bigg|_{x = \mu} \mu_{ij}.
$$

It is easy to see that $\sigma^2$ is a function of $\mu$ if the dimension $d^\dagger$ of $\mu$ is large enough. We can therefore define functions $h$ and $B$ on $\mathbb{R}^{d^\dagger}$ such that

$$
h(\mu) = \sigma \quad \text{and} \quad B(\mu) = \frac{g(x) - g(\mu)}{h(x)}.
$$

Then $n^{1/2} B(\bar{x}) = n^{1/2} (\hat{\theta} - \theta)/\hat{\sigma}$ represents a standardized version of $\hat{\theta}$, where $\hat{\sigma}$ is the sample version of $\sigma$.

Define also

$$
b_{i_1 i_2 \ldots i_r} = \frac{\partial^r B(\mu)}{\partial x_{i_1} \cdots \partial x_{i_r}} \bigg|_{x = \mu},
$$

for $i_j = 1, 2, \ldots, d^\dagger$. It is easily seen that

$$
\sum_{i, j = 1}^{d^\dagger} b_i b_j \mu_{ij} = 1. \quad (10)
$$

We now consider the coverage error of $I_0$. It may be shown using the general arguments of Hall and Martin (1988) that the coverage error of $I_0$ is of order $O(n^{-2})$. Martin (1990) provides an explicit expression for this leading $O(n^{-2})$ term, defined in terms of coefficients of an expansion of the joint density of

$$
\left[ n^{1/2} (\hat{\theta} - \theta)/\hat{\sigma}, \ n^{1/2} (\hat{\tau}_1(z) - \tau_1(z)) \right].
$$

We present here a different approach to obtaining an explicit leading term for the coverage error of $I_0$, which depends only on derivatives of the smooth function $g$. In fact, this approach may be used for any form of interval with endpoints expressible in terms of a known Edgeworth expansion, as will be appreciated later in this section. A detailed comparison can then be made between $I_0$ and its asymptotic competitors, $I_1$ and $I_2$, through explicit evaluation of the leading terms of their respective coverage errors.
The coverage error of a nominal \( \alpha \)-level confidence interval \( I \) for \( \theta \) is defined simply as \( \mathbb{P}(\theta \in I) - \alpha \). Set \( T_n = n^{1/2}(\hat{\theta} - \theta)/\hat{\sigma} \). Using (7) and noting that
\[
\hat{t} - t = 2n^{-1}(\hat{\pi}_1(z_\hat{\epsilon}) - \pi_1(z_\hat{\epsilon}))\phi(z_\hat{\epsilon}) + O_p(n^{-5/2}),
\]
we may write
\[
\mathbb{P}(\theta \leq \hat{\delta}_{\beta+\hat{t}/2}) = \mathbb{P}(S_n \geq -z_{\beta+t/2} - n^{-1/2}\hat{\rho}_{11}(z_{\beta+t/2}) - \cdots) + O(n^{-5/2}),
\]
where \( S_n = T_n + \delta_n \) and
\[
\delta_n = \phi(z_\beta)^{-1}\phi(z_\hat{\epsilon})\left\{n^{-1}(\hat{\pi}_1(z_\hat{\epsilon}) - \pi_1(z_\hat{\epsilon})) + n^{-3/2}p'_{11}(z_\beta)(\hat{\pi}_1(z_\hat{\epsilon}) - \pi_1(z_\hat{\epsilon}))\right\}.
\]
The order term \( O(n^{-5/2}) \) is deduced via the delta method [see Hall (1992), Section 2.7]. We first detail a few lemmas before we establish an Edgeworth expansion of the distribution of \( S_n \).

**Lemma 1.** For any statistic \( \Delta_n = O_p(n^{-3/2}) \) under distribution \( F \), define
\[
W_n = T_n + \Delta_n.
\]
Let \( \kappa_j \) and \( \kappa'_j \) be the \( j \)-th cumulants of \( T_n \) and \( W_n \), respectively. Then the difference \( (\kappa'_j - \kappa_j) \) is given, up to order \( O_p(n^{-5/2}) \), by the coefficient of \( (it)^{j-1}/j! \) in the power series expansion in \( (it) \) of the function
\[
Q_n(it) = \frac{\mathbb{E}[\Delta_n \exp(itT_n)]}{\mathbb{E}[\exp(itT_n)]}.
\]

**Proof.** Note that \( \kappa'_j \) and \( \kappa_j \) are given by coefficients of \( (it)^{j}/j! \) in the power series of \( \log \mathbb{E}[\exp(itW_n)] \) and \( \log \mathbb{E}[\exp(itT_n)] \), respectively. Consider
\[
\log \mathbb{E}[e^{itW_n}] = \log \left\{ \sum_{j=0}^{\infty} \frac{(it)^j}{j!} \sum_{k=0}^{j} \frac{j!}{k!} \mathbb{E}[T_n^{j-k}\Delta_n^k] \right\} = \log \mathbb{E}[e^{iT_n}] + itQ_n(it) + O(n^{-3}).
\]
The last equality holds because \( Q_n(it) \) is of order \( O(n^{-3/2}) \). Thus \( \kappa'_j \) and \( \kappa_j \) differ by the coefficient of \( (it)^{j-1}/j! \) in \( itQ_n(it) \) plus an error of order \( O(n^{-3}) \). \( \Box \)

**Corollary 1.** Define \( m_j = \mathbb{E}[T_n^j] \) for \( j = 1, 2, \ldots \). Then we have
\[
\kappa'_j - \kappa_j = \mathbb{E}[f_j(T_n)\Delta_n] + O(n^{-5/2}),
\]
where \( f_j(T_n) \) is a suitable function of \( T_n \).
where the \( f_j(T_n) \)'s are polynomials in \( T_n \). In particular, we have the following:

(i) \( f_1(T_n) = 1; \)
(ii) \( f_2(T_n) = 2(T_n - m_1); \)
(iii) \( f_3(T_n) = 3T_n^2 - 6T_n m_1 - 3m_2; \)
(iv) \( f_4(T_n) = 4T_n^3 - 12T_n^2 m_1 - 12T_n m_2 + 24m_1 m_2 - 4m_3; \)
(v) \( f_5(T_n) = 5T_n^4 - 20T_n^3 m_1 - 30T_n^2 m_2 + 120T_n m_1 m_2 + 30m_2^2 \\
- 20T_n m_3 - 5m_4; \)
(vi) \( f_6(T_n) = 6T_n^5 - 30T_n^4 m_1 - 60T_n^3 m_2 + 360T_n^2 m_1 m_2 + 180T_n m_2^2 \\
- 540m_1 m_2^2 - 60T_n^2 m_3 + 120m_2 m_3 - 30T_n m_4 \\
+ 60m_1 m_4 - 6m_5. \)

**Proof.** The proof is a tedious exercise of expanding \( Q_s(it) \) in a power series in \( it \) and using the fact that \( m_j \) has order \( O(n^{-1/2}) \) for odd \( j \) and \( O(1) \) for even \( j \). \( \Box \)

**Corollary 2.** The following hold for the polynomials \( f_j \):

(i) \( \mathbb{E}[f_1(T_n)] = 1; \)
(ii) \( \mathbb{E}[f_j(T_n)] = O(n^{-1}), \) for \( j = 2, 3, \ldots \).

**Proof.** For any statistic \( Y \) and nonrandom constant \( C \), the second- and higher-order cumulants of \( Y \) and \( Y + C \) coincide. The result follows by letting \( \Delta_n = n^{-3/2}C \) in Corollary 1. \( \Box \)

**Lemma 2.** Let \( \omega(x) \) be a smooth function on \( \mathbb{R}^{d_1} \). Suppose \( \omega \) has three bounded continuous derivatives in a neighbourhood of \( \mu \). Set

\[
\Gamma_n = n^{1/2}(\omega(\bar{X}) - \omega(\mu)) \quad \text{and} \quad \omega_{i_1 \cdots i_d} = \frac{\partial^d \omega(x)}{\partial x_{i_1} \cdots \partial x_{i_d}} \bigg|_{x = \mu},
\]

for \( i_j = 1, 2, \ldots, d \). Then

(i) \( \mathbb{E}[f_1(T_n)\Gamma_n] = n^{-1/2} \sum_{i,j=1}^{d} \omega_{ij} \mu_{ij} + O(n^{-3/2}); \)
(ii) \( \mathbb{E}[f_2(T_n)\Gamma_n] = 2 \sum_{i,j=1}^{d} b_{ij} \omega_{ij} \mu_{ij} + O(n^{-1}); \)
(iii) \[ E[f_j(T_n)\Gamma_n] = \frac{n^{-1/2}}{3} \left\{ \sum_{i,j,k=1}^{d^\dagger} b_i b_j \omega_k \mu_{ijk} \right. \\
\left. + \sum_{i,j,k,l=1}^{d^\dagger} (2b_i b_{jk} \omega_l \mu_{ij} \mu_{kl} + b_i b_j b_{kl} \mu_{ik} \mu_{jl}) \right\} + O(n^{-3/2}); \]
(iv) \[ E[f_j(T_n)\Gamma_n] = O(n^{-1}) \quad \text{for } j = 4, 5, 6. \]

**Proof.** Again, the results are obtained by expanding \( f_j(T_n) \) and \( \Gamma_n \) in Taylor series with terms \( (\bar{X} - \mu)^{i_1}(\bar{X} - \mu)^{i_2} \cdots (\bar{X} - \mu)^{i_d} \), using Corollary 1 and identity (10), and taking expectations. \( \square \)

Now recall that \( \pi_1(z) \) is a polynomial in \( z \) with coefficients depending only on \( \mu \). Therefore, \( \pi_1(z) \) can be generalized to a function \( \pi_1(z; \mathbf{x}) \) on \( \mathbb{R} \times \mathbb{R}^{d^\dagger} \), with \( \pi_1(z; \mu) = \pi_1(z) \). Define

\[ \eta_{i_1 \cdots i_d}(z) = \frac{\partial^\dagger \pi_1(z; \mathbf{x})}{\partial x_{i_1} \cdots \partial x_{i_d}} \bigg|_{\mathbf{x} = \mu} \]

for \( i_j = 1, 2, \ldots, d^\dagger \). For convenience, we write \( \eta_{i_1 \cdots i_d}(z_\xi) \). Letting \( \Delta_n = \delta_n \) in Corollary 1, and setting

\[ \omega(x) = n^{-3/2} \pi_1(z_\xi; \mathbf{x}) \phi(z_\beta)^{-1} \phi(z_\xi) \]

and

\[ \omega(x) = n^{-2} p_1'(z_\beta) \pi_1(z_\xi; \mathbf{x}) \phi(z_\beta)^{-1} \phi(z_\xi) \]

successively in Lemma 2, we deduce

\[ \kappa_1' - \kappa_1 = n^{-2} \frac{3}{2} \tau_1 \phi(z_\beta)^{-1} \phi(z_\xi) + O(n^{-5/2}), \]

\[ \kappa_2' - \kappa_2 = 2(n^{-3/2} + n^{-2} p_1'(z_\beta)) \tau_2 \phi(z_\beta)^{-1} \phi(z_\xi) + O(n^{-5/2}), \]

\[ \kappa_3' - \kappa_3 = n^{-2} 3 \tau_3 \phi(z_\beta)^{-1} \phi(z_\xi) + O(n^{-5/2}), \]

\[ \kappa_j' - \kappa_j = O(n^{-5/2}) \quad \text{for } j = 4, 5, 6, \]

where \( \kappa_j \) and \( \kappa'_j \) denote the \( j \)th cumulants of \( T_n \) and \( S_n \), respectively, and

\[ \tau_1 = \sum_{i,j=1}^{d^\dagger} \eta_{ij} \mu_{ij}, \]

\[ \tau_2 = \sum_{i,j=1}^{d^\dagger} b_i \eta_{ij} \mu_{ij} \text{ and} \]

\[ \tau_3 = \sum_{i,j,k=1}^{d^\dagger} b_i b_j \eta_{ik} \mu_{ijk} + \sum_{i,j,k,l=1}^{d^\dagger} (2b_i b_{jk} \eta_{il} \mu_{ij} \mu_{kl} + b_i b_j \eta_{kl} \mu_{ik} \mu_{jl}). \]
Note that $\mathbb{P}(T_n \leq x)$ admits an Edgeworth expansion

\[
\mathbb{P}(T_n \leq x) = \Phi(x) + n^{-1/2}q_1(x)\phi(x) + n^{-1}q_2(x)\phi(x) + n^{-3/2}q_3(x)\phi(x) + n^{-2}q_4(x)\phi(x) + O(n^{-5/2}),
\]

where each $q_j$ is a polynomial with coefficients depending on cumulants of $F$, and $q_j$ is odd for even $j$ and even for odd $j$. In particular, we can show that

\[
q_1(x) = -\left\{ k_{12} + \frac{k_{31}(x^2 - 1)}{6} \right\},
\]

\[
q_2(x) = -x\left\{ \frac{k_{12}^2 + k_{22}}{2} + \frac{(4k_{12}k_{31} + k_{41})(x^2 - 3)}{24} + \frac{k_{31}(x^4 - 10x^2 + 15)}{72} \right\},
\]

\[
q_3(x) = -\left\{ k_{13} + \frac{3k_{12}k_{22} + k_{32}}{6}(x^2 - 1) + \frac{k_{22}k_{31}(x^4 - 6x^2 + 3)}{12} \right\} + r_3(x, k_{12}, k_{31}, k_{41}, k_{51}),
\]

\[
q_4(x) = -x\left\{ \frac{(2k_{12}k_{13} + k_{23})}{2} + \frac{(6k_{12}k_{22} + 3k_{22}^2 + 4k_{13}k_{31} + 4k_{12}k_{32})(x^2 - 3)}{24} + \frac{(12k_{12}k_{22}k_{31} + 4k_{31}k_{32} + 3k_{22}k_{41})(x^4 - 10x^2 + 15)}{144} + \frac{k_{22}k_{31}^2(x^6 - 21x^4 + 105x^2 - 105)}{144} \right\} + r_4(x, k_{12}, k_{31}, k_{41}, k_{42}, k_{51}, k_{61}),
\]

where the $k_{ij}$ are constants depending on $F$ such that

\[
k_j = n^{-(j - 2)/2}(k_{j1} + n^{-1}k_{j2} + n^{-2}k_{j3} + \ldots)
\]

for $j = 1, 2, 3, \ldots$, with $k_{11} = 0$ and $k_{21} = 1$. The remainders $r_j(x; k_{12}, \ldots)$ are polynomials with coefficients depending only on those $k_{ij}$ included in their brackets. In fact, the coefficients of each $r_i$ are unaffected by changes (12) up to an error of order $O(n^{-5/2})$ and so need not be considered in the distribution of $S_n$ on the right-hand side of (11). Hall [(1992), Theorem 2.1] verifies (16) by an elaborate proof. Knowing expressions (15) and (16), we can
therefore incorporate the cumulant differences as given by (12) into expansion (14) and obtain a corresponding Edgeworth expansion for \( S_n \): 

\[
\mathbb{P}(S_n \leq x) = \mathbb{P}(T_n \leq x) - n^{-3/2} \tau_2 \phi(z_\beta)^{-1} \phi(z_\xi) x \phi(x) \\
- n^{-2} \left( \frac{3}{2} \tau_1 + (k_{12} \tau_2 + \frac{1}{2} \tau_3)(x^2 - 1) \right) \\
+ \frac{1}{6} k_{31} \tau_2 (x^4 - 6x^2 + 3) + p'_{11}(z_\beta) \tau_2 x \\
\times \phi(z_\beta)^{-1} \phi(z_\xi) \phi(x) + O(n^{-5/2}).
\]

(17)

Now set 

\[
\delta_n = n^{-1/2} \hat{p}_{11}(z_{\beta + t/2}) + n^{-1} \hat{p}_{21}(z_{\beta + t/2}) + \ldots, \\
S_n' = S_n + \delta_n \text{ and } T_n' = T_n + \delta_n.
\]

Using similar arguments as in Lemma 1, we have 

\[
\log \mathbb{E}[\exp(itS_n')] = \log \mathbb{E}[\exp(itT_n')] + itQ_n + O(n^{-5/2}),
\]

where \( Q_n = \mathbb{E}[\delta_n \exp(itT_n')]/\mathbb{E}[\exp(itT_n')] \). Thus, by similar arguments as those leading to (12), we know that cumulants of \( S_n' \) differ from those of \( T_n' \) by the same differences as given by (12), up to errors of order \( O(n^{-5/2}) \). Therefore the distributions of \( S_n' \) and \( T_n' \) are related in a similar way as that between \( S_n \) and \( T_n \) as given by (17), with \( k_{12} \) and \( k_{31} \) replaced by the corresponding \( k_{12}' \) and \( k_{31}' \) for \( T_n' \).

Since 

\[
\mathbb{E}[T_n'] = \kappa_1 + n^{-1/2} p_{11}(z_\beta) + O(n^{-1}),
\]

we can adjust \( k_{12} \) to be 

\[
k_{12}' = k_{12} + p_{11}(z_\beta) + O(n^{-1/2}).
\]

(19)

Similarly, by considering the third cumulant of \( T_n' \), we have 

\[
k_{31}' = k_{31} + O(n^{-1/2}).
\]

(20)

Substituting (19) and (20) for \( k_{12} \) and \( k_{31} \) in (17), we obtain 

\[
\mathbb{P}(S_n' \leq x) = \mathbb{P}(T_n' \leq x) - n^{-3/2} \tau_2 \phi(z_\beta)^{-1} \phi(z_\xi) x \phi(x) \\
- n^{-2} \left( \frac{3}{2} \tau_1 + \left( k_{12}' \tau_2 + p_{11}(z_\beta) \tau_2 + \frac{1}{2} \tau_3 \right)(x^2 - 1) \right) \\
+ \frac{1}{6} k_{31}' \tau_2 (x^4 - 6x^2 + 3) + p'_{11}(z_\beta) \tau_2 x \\
\times \phi(z_\beta)^{-1} \phi(z_\xi) \phi(x) + O(n^{-5/2}).
\]

(21)

Setting \( x = -z_{\beta + t/2} \) and using (11), we deduce 

\[
\mathbb{P}(\theta \leq \tilde{\gamma}_{\beta+t/2}) = \mathbb{P}(T_n' \geq -z_{\beta + t/2}) - n^{-3/2} z_\beta \tau_2 \phi(z_\xi) \\
+ n^{-2} \lambda(\beta) \phi(z_\xi) + O(n^{-5/2}),
\]

(22)
where
\[
\lambda(\beta) = \frac{1}{2} \tau_1 + (k_{12} \tau_2 + p_{11}(z_\beta) \tau_2 + \frac{1}{2} \tau_3)(z_\beta^2 - 1) \\
+ \frac{1}{6} k_{31} \tau_2 (z_\beta^4 - 6z_\beta^2 + 3) \\
- z_\beta p'_{11}(z_\beta) \tau_2.
\]
(23)

Changing the signs of \( t \) and \( \hat{t} \) throughout, we obtain
\[
\mathbb{P}(\theta \leq \hat{y}_{\beta-t/2}) = \mathbb{P}(T'_n \geq -z_{\beta-t/2}) + n^{-3/2}z_\beta \tau_2 \phi(z_\xi) - n^{-2} \lambda(\beta) \phi(z_\xi) + O(n^{-5/2}).
\]
(24)

Finally, setting \( \beta = \xi \) in (22) and \( \beta = 1 - \xi \) in (24) and then subtracting, we have
\[
\mathbb{P}(\theta \in I_0) = \mathbb{P}(\theta \leq \hat{y}_{\xi-t/2}) - \mathbb{P}(\theta \leq \hat{y}_{1-\xi-t/2}) \\
= \mathbb{P}(\theta \in \left[ \hat{y}_{1-\xi-t/2}, \hat{y}_{\xi+t/2} \right]) + n^{-2} 2 \lambda(\xi) \phi(z_\xi) + O(n^{-5/2}),
\]
(25)

using the facts that \( z_{1-\xi} = -z_\xi \) and \( \lambda(\xi) = \lambda(1-\xi) \). Noting that \( \left[ \hat{y}_{1-\xi-t/2}, \hat{y}_{\xi+t/2} \right] \) is the correct \( \alpha \)-level interval, we have proved the following proposition.

**Proposition 1.** *The coverage error of \( I_0 \) is given by*
\[
\mathbb{P}(\theta \in I_0) - \alpha = n^{-2} 2 \lambda(\xi) \phi(z_\xi) + O(n^{-5/2}),
\]
*where \( \xi = (1 + \alpha)/2 \) and \( \lambda(\xi) \) is defined as in (23).*

By modifying the definition of \( \delta_n \) slightly, we may obtain the coverage errors of \( I_1 \) and \( I_2 \) as given by the following propositions.

**Proposition 2.** *The coverage error of \( I_1 \) is given by*
\[
\mathbb{P}(\theta \in I_1) - \alpha = n^{-2} 2 \{ \lambda(\xi) - \pi_2(z_\xi) \} \phi(z_\xi) + O(n^{-5/2}),
\]
*where \( \xi = (1 + \alpha)/2 \), and \( \lambda(\xi) \) and \( \pi_2(z_\xi) \) are defined as in (23) and (4), respectively.*

**Proof.** Take
\[
\delta_n = \phi(z_\beta)^{-1} \phi(z_\xi) \{ n^{-1}(\hat{\pi}_1(z_\xi) - \pi_1(z_\xi)) \\
+ n^{-3/2} p'_{11}(z_\beta)(\hat{\pi}_1(z_\xi) - \pi_1(z_\xi)) - n^{-2} \pi_2(z_\xi) \}.
\]
Clearly, from Corollary 2, we have here the same situation as in the case of \( I_0 \), except that now
\[
\kappa'_1 - \kappa_1 = n^{-2}(\frac{1}{2} \tau_1 - \pi_2(z_\xi)) \phi(z_\beta)^{-1} \phi(z_\xi) + O(n^{-5/2})
\]
in (12). The result follows immediately. □
Define
\begin{equation}
\xi(z) = \sum_{i,j=1}^{d_i} b_{ij} \mu_{ij} \left. \frac{\partial p_{31}(z; \mathbf{x})}{\partial x_j} \right|_{x=\mu}
\end{equation}
and
\begin{equation}
\lambda_0(\beta) = \left(k_{12} + p_{11}(z_\beta) + \frac{1}{6}k_{31}(z_\beta^2 - 3)\right)z_\beta p_{31}(z_\beta) + z_\beta \xi(z_\beta) - p_{41}(z_\beta),
\end{equation}
where \(p_{31}(z; \mathbf{x})\) is obtained by generalising \(p_{31}(z)\) as in the case of \(\pi_1(z; \mathbf{x})\), and \(p_{41}(z_\beta)\) is obtained from (5).

**Proposition 3.** The coverage error of \(I_2\) is given by
\[
\mathbb{P}(\theta \leq I_2) - \alpha = n^{-2} \mathbb{P}(\lambda(\xi) - \pi_2(\xi) + \lambda_0(\xi)) \phi(\xi) + O(n^{-5/2}),
\]
where \(\xi = \frac{1}{2}(1 + \alpha)\), and the functions \(\lambda(\xi), \pi_2(\xi)\) and \(\lambda_0(\xi)\) are given by formulae (23), (4) and (27), respectively.

**Proof.** Take
\[
\delta_n = \phi(z_\beta)^{-1} \phi(\xi) \left\{ n^{-1}(\hat{\pi}_1(z_\xi) - \pi_1(z_\xi)) + n^{-3/2} p_{11}(\hat{\pi}_1(z_\xi) - \pi_1(z_\xi)) - n^{-2} \pi_2(z_\xi) \right\}
\]
\[
- n^{-3/2} \hat{\pi}_{31}(z_\beta) - n^{-2} p_{41}(z_\beta).
\]
The changes in (12) then become
\[
\kappa'_1 - \kappa_1 = -n^{-3/2} p_{31}(z_\beta) + n^{-2} \left( \frac{1}{2} \tau_1 - \pi_2(z_\xi) \right) \phi(z_\beta)^{-1} \phi(z_\xi)
\]
\[
- n^{-2} p_{41}(z_\beta) + O(n^{-5/2}),
\]
and
\[
\kappa'_2 - \kappa_2 = 2 \left( n^{-3/2} + n^{-2} p_{11}(z_\beta) \right) \tau_2 \phi(z_\beta)^{-1} \phi(z_\xi)
\]
\[
- 2 n^{-2} \xi(z_\beta) + O(n^{-5/2}).
\]
It follows from (22) that
\[
\mathbb{P}(\theta \leq \tilde{\xi}_{\beta + \xi/2})
\]
\[
= \mathbb{P}(T_n \geq -z_{\beta + \xi/2}) - n^{-3/2} z_\beta \tau_2 \phi(z_\xi) - n^{-3/2} p_{31}(z_\beta) \phi(z_\beta)
\]
\[
+ n^{-2} \left( \lambda(\beta) - \pi_2(z_\xi) \right) \phi(z_\xi) + n^{-2} \lambda_0(\beta) \phi(z_\beta) + O(n^{-5/2}).
\]
Similarly, we may obtain an expression for \(\mathbb{P}(\theta \leq \tilde{\xi}_{\beta - \xi/2})\). The result follows by setting \(\beta = \xi\) in the first expression and \(1 - \xi\) in the second and then subtracting, using the facts that \(\lambda_0(1 - \xi) = -\lambda_0(\xi), p_{31}\) is an even function and \(p_{41}\) is odd. □

All three intervals \(I_0, I_1\) and \(I_2\) enjoy a coverage error of \(O(n^{-2})\). Among them, \(I_2\) is the most efficient to evaluate, since it requires no resampling but
simply substitution of sample moments into formulae (8) and (9). The next section and the Appendix describe how these formulae can be calculated in practice through an automatic procedure requiring no preliminary analytic calculation from the user.

It should be noted that the last term in (9) is essential for a coverage error of \( O(n^{-2}) \), as it corrects for kurtosis. Scrapping this term from \( I_2 \) results in an extra coverage error of \(-2n^{-1}p_{3d}(z_\xi)\phi(z_\xi)\), as can be deduced using arguments similar to those given earlier.

A potential drawback in the use of \( I_2 \) is the possibility of its giving an empty interval when \( \hat{\gamma}_{1-\xi-t/2} \geq \hat{\gamma}_{t+t/2} \). This problem is most significant if the theoretical iterated bootstrap interval \( I_0 \) has a poor coverage in the first place. Therefore, the interval \( I_2 \) may have potential use for diagnostic purposes in validating the bootstrap method itself.

On the other hand, the interval \( I_1 \) requires, in general, a single outer level of resampling and is approximated by

\[
\left[ \hat{\theta}_0^{*}(B_{(1-\xi-t/2)}+1) \right]^{\ast},
\]

where \([\cdot]\) denotes the integer-part function, possibly with some adjustment to ensure well-ordering of the end points. The details of such adjustment are given at the end of the Appendix. The need for one level of resampling makes \( I_1 \) less efficient to calculate than \( I_2 \). Also, the Monte Carlo construction introduces a simulation error of size \( O(n^{-1/2}B^{-1/2}) \) to its endpoints [see Booth and Hall (1994)]. This is inherited by the coverage error as a term of \( O(B^{-1/2}) \), according to a delta method calculation. The analytic approximation method suggested by DiCiccio, Martin and Young (1992a, b), which estimates \( t \) by analytic means, provides an alternative to the interval \( I_1 \).

The leading coverage error terms of all three of the intervals considered in this section consist mainly of leading terms from \( \mathbb{E}[T^j_n(\hat{\ell} - t)] \) for \( j = 0, 1, 2 \), as well as those from the mean and skewness of \( T_n \). The half-asymptotic, half-resampled interval \( I_1 \) brings in an extra error term \(-n^{-2}2\pi_3(z_\xi)\phi(z_\xi)\), owing to approximation of \( \hat{\ell} \) by the leading term in its asymptotic expansion. The coverage error of the completely asymptotic interval \( I_2 \) includes other terms involving higher-order cumulants of \( T_n \). There is no straight clear message from these coverage error expressions about the relative performance of these intervals. Since \( \delta_n = O(n^{-3/2}) \) in all three cases, we have

\[
\hat{\gamma}_{t+t/2} - \hat{\gamma}_{\hat{\ell}+t/2} = \hat{\gamma}_{t+t/2} - \hat{\gamma}_{\hat{\ell}+t/2} = \hat{\gamma}_{t+t/2} - \hat{\gamma}_{\hat{\ell}+t/2} = O(n^{-2}),
\]

which implies that all the intervals are third-order correct compared with the true nominal \( \alpha \)-level interval \([\hat{\gamma}_{1-\xi-t/2}, \hat{\gamma}_{\hat{\ell}+t/2}]\), using terminology given in Hall [(1992), Section 3.4].

To conclude this section, we remark that the \( O(n^{-2}) \) coverage errors of the asymptotic intervals, as given by Propositions 2 and 3, can be reduced further by explicit Edgeworth correction. Hall (1983) gives an account of this approach. However, complexity of the functions \( \lambda \) and \( \lambda_0 \) makes Edgeworth correction a formidable task. Moreover, the gain from such correction is very
much asymptotic and dubious for small samples. Also, we know from Hall
[(1992), Section 3.8] that a two-sided normal approximation interval corrected
for skewness also has coverage error of order $O(n^{-2})$. It is interesting to
compare such an Edgeworth corrected interval with our asymptotic iterated
intervals. Heuristically, the Edgeworth corrected interval tries to correct an
already poor interval, such as one obtained from normal approximation,
whereas our asymptotic iterated intervals approximate the correct $\alpha$-level
interval $[\hat{\gamma}_{1-i/2}^\xi, \hat{\gamma}_{i/2}^\xi]$ and should therefore result in more accurate
coverages. We shall return to this point in the simulation study of Section 5.

4. Practical evaluation of asymptotic iterated intervals. In this
section we give a user-oriented qualitative description of an automatic
procedure, which we have programmed in Fortran and which takes care of all the
lengthy algebra and calculations necessary for obtaining the endpoints of $I_1$
and $I_2$ for a general parameter. Special attention is paid to a built-in
automatic derivative evaluation routine for computing the exact numerical
values of any required derivatives, and by use of which the need for execution
of symbolic operations is avoided. No separate software such as Mathematica
is needed. To set the program running, the user needs only to enter a few
trivial parameter values and the formula of the function $g(\mu)$ in a compre-
hensible coded form. The detailed calculations involved in the automatic
procedure are described in the Appendix. The Fortran programs, which also
simulate coverage probabilities under any predetermined underlying dis-
tributions, are available by anonymous ftp. Details of how to obtain the pro-
grams are given at the end of this section.

We first set up some notation. Suppose $G$ is an $r$-variate distribution and
$Y = (Y_1, Y_2, \ldots, Y_r)^T$ is a random vector from $G$. The parameter of interest
$\theta = g(\mu)$ is assumed to depend only on moments of $G$ up to order $s$. For any
positive integer $m$, we can, by means of a recursive algorithm, list all the
distinct $r$-sequences

$$(i_1, i_2, \ldots, i_r)$$

such that $\sum_{j=1}^r i_j = m$, with the $i_j$ being nonnegative integers. For instance, if
$m = 2$ and $r = 3$, then we have a list

$$\{(2, 0, 0), (1, 1, 0), (1, 0, 1), (0, 2, 0), (0, 1, 1), (0, 0, 2)\}.$$  

Define $d(r, m)$ to be the number of such $r$-sequences corresponding to order
$m$, and define $\rho_i(r, m)$ to be the $i$th sequence in this list, for $i = 1, 2, \ldots, d(r, m)$. Define also $Y^{(i_1, i_2, \ldots, i_r)}$ to be the product $Y_1^{i_1}Y_2^{i_2} \cdots Y_r^{i_r}$. We can then extend the random vector $Y$ to some $X$, say, so that

$$X = (Y_{\rho_1(r, 1)}, Y_{\rho_2(r, 1)}, \ldots, Y_{\rho_{d(r, 1)}(r, 1)}, Y_{\rho_1(r, 2)}, \ldots, Y_{\rho_{d(r, 2)}(r, 2)}, \ldots, Y_{\rho_{d(r, 6s)}(r, 6s)}, \ldots, Y_{\rho_{d(r, 6s)}(r, 6s)})^T,$$
that is, \( \mathbf{X} \) is a sequence of products \( Y_{i_1}^{j_1} \cdots Y_{i_r}^{j_r} \) up to order 6s. Let \( F \) be the distribution of \( \mathbf{X} \) under \( G \). Define
\[
d = \sum_{m=1}^{2s} d(r, m), \quad d' = \sum_{m=1}^{2s} d(r, m), \quad d'' = \sum_{m=1}^{3s} d(r, m)
\]
and
\[
d''' = \sum_{m=1}^{6s} d(r, m).
\]
Also, set \( \mu = \mathbb{E}[\mathbf{X}] \) and extend the domain of \( g \) to \( \mathbb{R}^{d''} \) so that \( g(\mu) = \theta \). In fact, \( g \) depends on \( \mu \) only through its first \( d \) elements.

The preliminary Fortran program \texttt{prelim.f} computes automatically the values of \( d, d', d'' \), and \( d''' \), which are stored, respectively, in the variables \( \text{ND0}, \text{ND1}, \text{ND2} \) and \( \text{ND3} \). The extended vector \( \mathbf{X} \) is also printed in terms of the defining \( \mathbf{Y} \) products. This is particularly useful for later reference when we feed into the main program the formula of \( g(\mu) \) in terms of the \( \mathbf{X} \) components. The only input required by \texttt{prelim.f} from the user are
\[
\text{NVAR} = r, \quad \text{NORD} = s \quad \text{and} \quad \text{NORD6} = 6s,
\]
defined via the \texttt{PARAMETER} command line.

The generality of this setup lies in the fact that the parameter of interest \( g(\mu) \) in a smooth function model usually has a closed-form algebraic expression in terms of moments of \( G \) up to a certain order. The program \texttt{prelim.f} orders the moments systematically to form the vector \( \mathbf{X} \) and so eliminates any ambiguity in the definition of \( g(\mu) \) via moments. The trivial input \texttt{NVAR}, \texttt{NORD} and \texttt{NORD6} also makes \texttt{prelim.f} extremely straightforward to implement.

Next follows the execution of the main program \texttt{asymp.f}. Its basic input includes the variables mentioned above, namely,
\[
\text{NVAR}, \text{NORD}, \text{NORD6}, \text{ND0}, \text{ND1}, \text{ND2}, \text{ND3},
\]
as well as the formula of \( g(\mu) \), the parameter of interest, which is entered through the command
\[
\text{CALL EVAL}( g(\text{IX}(1), \text{IX}(2), \ldots, \text{IX}(\text{NDO})), \text{VECTOR} ).
\]
Here the function \( g(\text{IX}(1), \ldots, \text{IX}(\text{NDO})) \) stands for a Fortran coded form of \( g(\mu) \), where \( \text{IX} \) is a Fortran integer array to be identified with the first \( d \) components of \( \mathbf{X} \). To specify \( g(\cdot) \), we first break up its definition into a sequence of basic algebraic operations such as addition, subtraction, multiplication, division, logarithm and so on. To each basic operation corresponds a Fortran user-defined function: for example, the addition operation goes with the function \( \text{TADD}(\cdot, \cdot) \), multiplication goes with \( \text{TMUL}(\cdot, \cdot) \), logarithm goes with \( \text{ILOG}(\cdot) \) and so on. These user-defined functions constitute a kind of routine library which enables us to define most common parameters with algebraic formulae. A fairly comprehensive library of algebraic operations is already attached to the program \texttt{asymp.f}. See the comments in the program.
for more details about this library. Here we illustrate its use with the variance case in which \( g(x_1, x_2) = x_2 - x_1^2 \) so that \( g(\mathbb{E}Y, \mathbb{E}Y^2) \) is the variance of the random variable \( Y \). The corresponding Fortran instruction (30) is

\[
\text{CALL EVAL(IX(2), IMUL(IX(1), IX(1))), VECTOR).}
\]

The subroutine EVAL evaluates the exact numerical values of \( g(x) \) and its partial derivatives up to the third order, all evaluated at the sample moments, and stores the output in a Fortran real array VECTOR. The details of this automatic derivative evaluation procedure are discussed in Kagiwada, Kalaba, Rasakhoo and Spingarn [1986], Chapters 1 and 2] and follow the approach described by Wexler (1988). We have generalised the procedure to deal with any user-input dimension of the domain of \( g \) and any partial derivatives up to the third order. The automatic differentiation done by EVAL makes any preliminary symbolic calculation unnecessary. The output, which is stored in VECTOR, is used in subsequent straightforward algebraic calculations in asymp.f to produce the endpoints of the asymptotic iterated intervals. The Appendix details step by step the calculations carried out by the program.

The program asymp.f is applicable to a variety of smooth function models and no problem-specific recoding is necessary. The programs prelim.f and asymp.f may be obtained by anonymous ftp from ftp.statslab.cam.ac.uk. Give anonymous as your user name and your full e-mail address as your password. Then type cd pub/CI; the two programs are fetched by typing mget prelim.f asymp.f.

5. Simulation study. A simulation study was conducted to investigate coverage properties of the asymptotic intervals \( I_1 \) and \( I_2 \). Three examples of smooth function models were studied: mean, variance and correlation coefficient. In all examples, \( I_1 \) and \( I_2 \) were compared with the percentile method confidence interval \( I_p \). Because of the extremely intensive computation involved in its construction, the “full-blown” standard iterated confidence interval \( I_p \) was only included for comparison in the mean example and for small sample sizes in the variance example. A variety of other asymptotic confidence intervals were also studied alongside \( I_1 \) and \( I_2 \) in the three examples. These include the Edgeworth-inversion-based confidence interval \( I_W \) of Withers (1983), the two-sided Edgeworth corrected confidence interval \( I_{EC} \), the approximate bootstrap confidence (ABC) interval \( I_{ABC} \) and the asymptotic “short” confidence interval \( I_{SH} \). See Hall [(1992), Section 3.8] and DiCiccio and Efron (1992) for details of \( I_{EC} \) and \( I_{ABC} \), respectively. The interval \( I_{SH} \) was taken to be the asymptotic version of the “short” interval proposed by Hall (1988), namely,

\[
I_{SH} = \left[ \hat{\theta} - n^{-1/2} \hat{\sigma} \left( z_{\hat{\sigma}} + n^{-1/2} \hat{\sigma} \right), \hat{\theta} - n^{-1/2} \hat{\sigma} \left( -z_{\hat{\sigma}} + n^{-1/2} \hat{\sigma} \right) \right],
\]

where \( \hat{\sigma} \) is the estimated standard deviation.
where the endpoints are obtained by asymptotically expanding the theoretical “short” interval endpoints up to order \(O(n^{-3/2})\). Finally, the accelerated bias-corrected confidence interval \(I_{BC^a}\), which requires one level of bootstrap resampling, was also included together with \(I_{ABC}\) for interest. See Efron (1987) for details of its construction.

It should be remarked that all the confidence intervals thus far mentioned were constructed in such a way that they have coverage error of order \(O(n^{-2})\), except for \(I_p\) and \(I_{SH^*}\), which have coverage error of order \(O(n^{-1})\).

Perhaps we should emphasize here that it is our main interest to demonstrate in the simulation study the practical feasibility and advantages of approximating the standard iterated bootstrap confidence interval by asymptotic expansions, while maintaining its desirable accuracy. We do not attempt in this paper to provide a thorough comparison involving all the existing competing confidence intervals of the asymptotic kind. However, our simulation results are encouraging in that they show the asymptotic intervals \(I_1\) and \(I_2\) to outperform many existing asymptotic forms of confidence interval.

We now describe in detail the setting of our simulation study. In all examples the coverage probabilities of the various confidence intervals were approximated from 1600 random samples, so that each figure has a standard error of approximately 0.01. Intervals \(I_1\), \(I_p\) and \(I_{BC^a}\) were constructed using \(B = 1000\) bootstrap resamples. The full-blown iterated interval \(I_F\) was constructed using \(C = 1000\) inner level bootstrap resamples. The asymptotic intervals \(I_2\), \(I_w\), \(I_{EC}\), \(I_{ABC}\) and \(I_{SH^*}\) generally require no resampling. However, in cases of erratic asymptotic endpoints where, for example, the lower limit exceeds the upper limit, certain kinds of bootstrap intervals were substituted for those erratic asymptotic intervals. To be specific, we replaced any erratic \(I_2\) by \(I_1\), any erratic \(I_w\) by \(I_p\), and any erratic \(I_{ABC}\) by \(I_{BC^a}\). For any erratic \(I_{EC}\) or \(I_{SH^*}\), \(B = 1000\) bootstrap resamples were drawn and the interval rectified to \([\hat{\theta}_1^*, \hat{\theta}_B^*]\). This adjustment is largely pragmatic, as the theoretical bootstrap interval is likely to undercover in this situation and the widest interval possible is given by the extreme pair of bootstrap quantities \(\hat{\theta}_1^*\) and \(\hat{\theta}_B^*\). Throughout the whole study, the nominal level \(\alpha\) was taken to be 0.9.

**Example 1 (Mean).** In the mean example, the parameter of interest \(\theta\) and its estimate \(\hat{\theta}\) were taken to be the population and sample means, respectively. For input to the automatic procedure described in Section 4 we have \(NVAR = NORD = 1\). Our asymptotic iterated intervals \(I_1\) and \(I_2\) were compared with \(I_p, I_F, I_w, I_{ABC}\) and \(I_{BC^a}\). Four different underlying distributions, normal, folded normal, negative exponential and lognormal, were studied using sample sizes \(n = 15\) and 30. The results are tabulated and shown in Table 1. In the cases of \(I_2, I_w\) and \(I_{ABC}\), the proportions of adjustments by bootstrap resampling required out of the 1600 simulations are given in parentheses following the corresponding estimated coverage probabilities.

It is found that the full-blown standard iterated interval \(I_F\) gives the most accurate coverage probabilities in all cases. The asymptotic intervals \(I_1\) and
## Table 1

<table>
<thead>
<tr>
<th>Interval</th>
<th>( I_1 )</th>
<th>( I_2 )</th>
<th>( I_P )</th>
<th>( I_F )</th>
<th>( I_W )</th>
<th>( I_{ABC} )</th>
<th>( I_{BC^*} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n = 15 )</td>
<td>0.891</td>
<td>0.894</td>
<td>0.860</td>
<td>0.897</td>
<td>0.875</td>
<td>0.862</td>
<td>0.859</td>
</tr>
<tr>
<td>( n = 30 )</td>
<td>0.901</td>
<td>0.903</td>
<td>0.892</td>
<td>0.902</td>
<td>0.899</td>
<td>0.893</td>
<td>0.889</td>
</tr>
<tr>
<td>( n = 15 )</td>
<td>0.876</td>
<td>0.873</td>
<td>0.839</td>
<td>0.833</td>
<td>0.866</td>
<td>0.861</td>
<td>0.855</td>
</tr>
<tr>
<td>( n = 30 )</td>
<td>0.885</td>
<td>0.881</td>
<td>0.869</td>
<td>0.898</td>
<td>0.879</td>
<td>0.875</td>
<td>0.882</td>
</tr>
<tr>
<td>( n = 15 )</td>
<td>0.862</td>
<td>0.867</td>
<td>0.819</td>
<td>0.874</td>
<td>0.834</td>
<td>0.826</td>
<td>0.824</td>
</tr>
<tr>
<td>( n = 30 )</td>
<td>0.896</td>
<td>0.898</td>
<td>0.876</td>
<td>0.901</td>
<td>0.881</td>
<td>0.875</td>
<td>0.876</td>
</tr>
<tr>
<td>( n = 15 )</td>
<td>0.813</td>
<td>0.811</td>
<td>0.765</td>
<td>0.829</td>
<td>0.780</td>
<td>0.788</td>
<td>0.783</td>
</tr>
<tr>
<td>( n = 30 )</td>
<td>0.847</td>
<td>0.846</td>
<td>0.815</td>
<td>0.853</td>
<td>0.827</td>
<td>0.819</td>
<td>0.826</td>
</tr>
</tbody>
</table>

\( I_2 \) are excellent approximations to \( I_F \). They are more accurate than \( I_P, I_{BC^*} \) and the other asymptotic intervals by a considerable margin. Also, their coverages are consistently smaller than those of \( I_F \), although by a very small magnitude. No adjustments by bootstrap resampling due to erratic endpoints were recorded, with the exception of a few cases related to \( I_2 \).

**Example 2 (Variance).** We consider next the variance example studied by Schenker (1985) and DiCiccio, Martin and Young (1992a). The parameter of interest \( \theta \) is the population variance, and the estimate \( \hat{\theta} \) is the (biased) sample variance. Here we set \( \text{NVAR} = 1 \) and \( \text{NORD} = 2 \) in our automatic procedure. Intervals chosen for study in parallel with \( I_1 \) and \( I_2 \) included \( I_P, I_F, I_W, I_{BC} \) and \( I_{SH} \). Four different underlying distributions with various degrees of skewness and kurtosis were used: the standard normal \( \mathcal{N}(0,1) \), with no skewness and no kurtosis; the folded normal \( \mathcal{N}(0,1) \), with high skewness and low kurtosis; the double exponential of unit rate with no skewness and high kurtosis; and, finally, the lognormal, \( \exp(\mathcal{N}(0,1)) \), which has high skewness and high kurtosis. The variances are, respectively, 1, \( 1 - 2/\pi \), 2 and \( e(e - 1) \). Three different sample sizes were taken: \( n = 20, 35, \) and 100, respectively. The full-blown iterated interval \( I_F \) was not constructed for \( n = 100 \) due to its immense computational demands in this case.

The simulation results are reported in Table 2. Again, for those asymptotic intervals which might need bootstrap adjustments, the proportions of such adjustments are given in parentheses. We observe that the full-blown inter-
Table 2

Example 2—estimated coverage probabilities for variance, based on 1600 random samples of sizes $n = 20, 35$ and 100 drawn from each of four different distributions: intervals $I_1$ and $I_p$ are based on 1000 outer level bootstrap resamples; for the other asymptotic intervals, outer level resampling is carried out only if the asymptotic endpoints turn out to be faulty; the frequency of such failures is given in parentheses following the estimated coverage; the full-blown iterated interval $I_p$ is based on 1000 outer and 1000 inner level bootstrap resamples.

<table>
<thead>
<tr>
<th>Interval</th>
<th>Coverage, $n = 20$</th>
<th>Coverage, $n = 35$</th>
<th>Coverage, $n = 100$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Normal data $N(0, 1)$ (no skew, no kurtosis)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_1$</td>
<td>0.833</td>
<td>0.854</td>
<td>0.883</td>
</tr>
<tr>
<td>$I_2$</td>
<td>0.832 (0.161)</td>
<td>0.853 (0.014)</td>
<td>0.884 (0.000)</td>
</tr>
<tr>
<td>$I_p$</td>
<td>0.727</td>
<td>0.793</td>
<td>0.857</td>
</tr>
<tr>
<td>$I_e$</td>
<td>0.848</td>
<td>0.859</td>
<td></td>
</tr>
<tr>
<td>$I_w$</td>
<td>0.804 (0.000)</td>
<td>0.843 (0.000)</td>
<td>0.883 (0.000)</td>
</tr>
<tr>
<td>$I_{EC}$</td>
<td>0.802 (0.000)</td>
<td>0.841 (0.000)</td>
<td>0.883 (0.000)</td>
</tr>
<tr>
<td>$I_{SH}$</td>
<td>0.821 (0.000)</td>
<td>0.850 (0.000)</td>
<td>0.887 (0.000)</td>
</tr>
<tr>
<td></td>
<td>Folded normal data $</td>
<td>N(0, 1)</td>
<td>$ (high skew, low kurtosis)</td>
</tr>
<tr>
<td>$I_1$</td>
<td>0.803</td>
<td>0.821</td>
<td>0.874</td>
</tr>
<tr>
<td>$I_2$</td>
<td>0.800 (0.285)</td>
<td>0.819 (0.101)</td>
<td>0.880 (0.003)</td>
</tr>
<tr>
<td>$I_p$</td>
<td>0.686</td>
<td>0.753</td>
<td>0.843</td>
</tr>
<tr>
<td>$I_e$</td>
<td>0.815</td>
<td>0.834</td>
<td></td>
</tr>
<tr>
<td>$I_w$</td>
<td>0.759 (0.000)</td>
<td>0.800 (0.000)</td>
<td>0.868 (0.000)</td>
</tr>
<tr>
<td>$I_{EC}$</td>
<td>0.779 (0.000)</td>
<td>0.810 (0.000)</td>
<td>0.874 (0.000)</td>
</tr>
<tr>
<td>$I_{SH}$</td>
<td>0.799 (0.000)</td>
<td>0.824 (0.000)</td>
<td>0.881 (0.000)</td>
</tr>
<tr>
<td></td>
<td>Double exponential data $\frac{1}{2} \exp(-</td>
<td>x</td>
<td>)$ (no skew, high kurtosis)</td>
</tr>
<tr>
<td>$I_1$</td>
<td>0.811</td>
<td>0.846</td>
<td>0.869</td>
</tr>
<tr>
<td>$I_2$</td>
<td>0.809 (0.304)</td>
<td>0.848 (0.118)</td>
<td>0.872 (0.013)</td>
</tr>
<tr>
<td>$I_p$</td>
<td>0.698</td>
<td>0.776</td>
<td>0.834</td>
</tr>
<tr>
<td>$I_e$</td>
<td>0.826</td>
<td>0.854</td>
<td></td>
</tr>
<tr>
<td>$I_w$</td>
<td>0.746 (0.000)</td>
<td>0.806 (0.000)</td>
<td>0.855 (0.000)</td>
</tr>
<tr>
<td>$I_{EC}$</td>
<td>0.771 (0.000)</td>
<td>0.832 (0.000)</td>
<td>0.868 (0.000)</td>
</tr>
<tr>
<td>$I_{SH}$</td>
<td>0.787 (0.000)</td>
<td>0.844 (0.000)</td>
<td>0.879 (0.000)</td>
</tr>
<tr>
<td></td>
<td>Lognormal data $\exp(N(0, 1))$ (high skew, high kurtosis)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_1$</td>
<td>0.526</td>
<td>0.602</td>
<td>0.696</td>
</tr>
<tr>
<td>$I_2$</td>
<td>0.526 (0.533)</td>
<td>0.602 (0.393)</td>
<td>0.686 (0.216)</td>
</tr>
<tr>
<td>$I_p$</td>
<td>0.416</td>
<td>0.504</td>
<td>0.608</td>
</tr>
<tr>
<td>$I_e$</td>
<td>0.544</td>
<td>0.630</td>
<td></td>
</tr>
<tr>
<td>$I_w$</td>
<td>0.430 (0.000)</td>
<td>0.523 (0.000)</td>
<td>0.662 (0.000)</td>
</tr>
<tr>
<td>$I_{EC}$</td>
<td>0.485 (0.000)</td>
<td>0.559 (0.000)</td>
<td>0.659 (0.000)</td>
</tr>
<tr>
<td>$I_{SH}$</td>
<td>0.510 (0.000)</td>
<td>0.576 (0.000)</td>
<td>0.681 (0.000)</td>
</tr>
</tbody>
</table>

Val $I_p$ gives the most accurate coverage and is consistently undercovering. Our asymptotic intervals $I_1$ and $I_2$ offer close approximations to $I_p$. They have virtually the same coverage and generally outperform the other asymptotic intervals $I_w$, $I_{EC}$ and $I_{SH}$, especially when $n$ is small or the underlying distribution is of the lognormal type with high skewness and high kurtosis. The percentile method interval $I_p$ is noticeably poor in coverage. It should be
noted that the coverage of $I_{SH}$ is quite similar to that of $I_1$ or $I_2$ for large sample sizes, despite its having a coverage error of greater order asymptotically. This observation, of course, demonstrates the inadequacy of using asymptotic theory alone in an assessment of different confidence interval construction procedures. With the lognormal distribution, all seven confidence intervals display very poor coverage properties. However, it is in this case where the most pronounced difference between performances of the intervals can be observed: here the asymptotic iterated intervals $I_1$ and $I_2$ clearly approximate the full-blown $I_P$ best.

Another point should be made about the proportions of adjustments by bootstrap resampling required by the intervals $I_2$, $I_W$, $I_{BE}$ and $I_{SH}$. Asymptotic endpoint failures are reported only in the case of $I_2$ where the failure (or adjustment) proportions reflect remarkably the general coverage error of the bootstrap confidence intervals. A poor coverage generally results in a higher chance of getting a faulty pair of endpoints for $I_2$ and having to adjust by resampling, as pointed out in our discussion at the end of Section 3.

To appreciate the huge impact on coverage error made by different underlying distributions, we computed the theoretical leading terms of the expansions of the calibrating coefficient $t$ and coverage error, for the theoretical iterated bootstrap confidence interval $I_0$. These are, respectively, $2 \pi_2(\xi) \phi(\xi)n^{-1}$ for $t$, as given by (4), and $2 \lambda(\xi) \phi(\xi)n^{-2}$ for the coverage error, as given by Proposition 1. The results are listed in Table 3. We can easily understand why the lognormal distribution yields relatively huge coverage error and why the asymptotics are hardly revealing in this case.

EXAMPLE 3 (Correlation coefficient). We repeated the simulation study conducted by DiCiccio, Martin and Young (1992b) concerning the construction of confidence intervals for a correlation coefficient. Our parameter of interest $\theta$ and its corresponding estimate $\hat{\theta}$ were taken to be the population and sample correlation coefficients, respectively. The input parameters for the automatic procedure were therefore $NVAR = NORD = 2$. Intervals $I_1$, $I_2$, $I_P$, $I_{BE}$ and $I_{SH}$ were constructed in this example. The much more computationally intensive full-blown interval $I_P$ was not examined here. Nevertheless,

<table>
<thead>
<tr>
<th>True distribution</th>
<th>Calibrating coefficient $t$</th>
<th>Coverage error $P(\theta \in I_0) - \alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard normal, $N(0, 1)$</td>
<td>$3.109 n^{-1}$</td>
<td>$-1.499 \times 10^2 n^{-2}$</td>
</tr>
<tr>
<td>Folded normal, $</td>
<td>N(0, 1)</td>
<td>$</td>
</tr>
<tr>
<td>Double exponential, $\exp(-</td>
<td>x</td>
<td>)/2$</td>
</tr>
<tr>
<td>Lognormal, $\exp(N(0, 1))$</td>
<td>$1.411 \times 10^6 n^{-1}$</td>
<td>$-2.488 \times 10^{20} n^{-2}$</td>
</tr>
</tbody>
</table>
our conclusions are not compromised very much by such omission, as we observe coverage results for $I_1$ and $I_2$ which, compared to the other examples, are relatively accurate, and the full-blown figures might therefore reasonably be expected to be close to those of the asymptotic intervals in this example. Six different underlying distributions were combined with four sample sizes $n = 15, 20, 30$ and $50$ in the complete simulation study.

Let $W_1$, $W_2$ and $W_3$ be independent standard normal variates. The underlying distributions were taken to be, respectively, as follows:

1. $Y = |W_1|$ and $Z = |W_2|$ so that $(Y, Z)$ are independent folded normal variates;
2. $Y = |W_1| + |W_3|$ and $Z = |W_2| + |W_3|$ so that $(Y, Z)$ are correlated folded normal variates with $\rho = 0.5$;
3. $Y = W_1$ and $Z = W_2$ so that $(Y, Z)$ are independent normal variates;
4. $Y = (W_1 + \sqrt{3} W_2)/2$ and $Z = (-W_1 + \sqrt{3} W_2)/2$ so that $(Y, Z)$ are correlated normal variates with $\rho = 0.5$;
5. $Y = \exp(W_1)$ and $Z = \exp(W_2)$ so that $(Y, Z)$ are independent lognormal variates;
6. $Y = \exp((W_1 + W_3)/\sqrt{2})$ and $Z = \exp((W_2 + W_3)/\sqrt{2})$ so that $(Y, Z)$ are correlated lognormal variates with $\rho = (e^{3/2} - e)/(e^2 - e)$.

Table 4 reports the complete simulation results, with proportions of adjustments by bootstrap resampling given in parentheses. It is clear that our asymptotic iterated intervals $I_1$ and $I_2$ outperform the other three methods by a considerable margin. The coverage of $I_1$ slightly dominates that of $I_2$ in all but a few rare cases. Also, our asymptotic iterated intervals result in coverage rather stable against the various sample sizes considered in the study. The percentile interval $I_p$ performs moderately well, quite unlike the poor coverage revealed in the variance example. Its dependence on sample size is only token. The Edgeworth corrected interval $I_{EC}$ and asymptotic short interval $I_{SH}$ turn out to be the poorest in terms of coverage error, especially for lognormal data or for small to moderate sample sizes such as $n = 15$ or $20$. Their coverage depends more strongly on sample size and thus enables them to regain some advantage over $I_p$ in a few cases when $n = 30$ and $50$. Again, the asymptotically more accurate interval $I_{EC}$ is, contrary to expectation, always outperformed by the interval $I_{SH}$, which is asymptotically much inferior.

As in the variance example, the failure proportions of intervals $I_2$, $I_{EC}$ and $I_{SH}$ have an apparent diagnostic quality concerning coverage accuracy.

6. Comments. The simulation study reported above suggests that, in terms of coverage accuracy, the asymptotic iterated intervals $I_1$ and $I_2$ approximate the standard iterated bootstrap confidence interval excellently and are more effective than the percentile method and many other existing asymptotic methods.

We note also that the improvement in coverage accuracy made by $I_1$ and $I_2$ over the percentile method is similar to that which results from the analytic
<table>
<thead>
<tr>
<th>Interval</th>
<th>$n = 15$</th>
<th>$n = 20$</th>
<th>$n = 30$</th>
<th>$n = 50$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_1$</td>
<td>0.889</td>
<td>0.882</td>
<td>0.892</td>
<td>0.893</td>
</tr>
<tr>
<td>$I_2$</td>
<td>0.877 (0.0000)</td>
<td>0.879 (0.0000)</td>
<td>0.893 (0.0000)</td>
<td>0.893 (0.0000)</td>
</tr>
<tr>
<td>$I_P$</td>
<td>0.866</td>
<td>0.857</td>
<td>0.872</td>
<td>0.877</td>
</tr>
<tr>
<td>$I_{EC}$</td>
<td>0.841 (0.0006)</td>
<td>0.844 (0.0000)</td>
<td>0.866 (0.0000)</td>
<td>0.878 (0.0000)</td>
</tr>
<tr>
<td>$I_{SH}$</td>
<td>0.850 (0.0006)</td>
<td>0.855 (0.0000)</td>
<td>0.874 (0.0000)</td>
<td>0.883 (0.0000)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_1$</td>
<td>0.901</td>
<td>0.895</td>
<td>0.901</td>
<td>0.896</td>
</tr>
<tr>
<td>$I_2$</td>
<td>0.892 (0.0000)</td>
<td>0.893 (0.0000)</td>
<td>0.897 (0.0000)</td>
<td>0.893 (0.0000)</td>
</tr>
<tr>
<td>$I_P$</td>
<td>0.873</td>
<td>0.873</td>
<td>0.875</td>
<td>0.874</td>
</tr>
<tr>
<td>$I_{EC}$</td>
<td>0.849 (0.0000)</td>
<td>0.856 (0.0000)</td>
<td>0.878 (0.0000)</td>
<td>0.889 (0.0000)</td>
</tr>
<tr>
<td>$I_{SH}$</td>
<td>0.863 (0.0000)</td>
<td>0.871 (0.0000)</td>
<td>0.888 (0.0000)</td>
<td>0.894 (0.0000)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_1$</td>
<td>0.884</td>
<td>0.889</td>
<td>0.904</td>
<td>0.898</td>
</tr>
<tr>
<td>$I_2$</td>
<td>0.871 (0.0006)</td>
<td>0.887 (0.0000)</td>
<td>0.899 (0.0000)</td>
<td>0.894 (0.0000)</td>
</tr>
<tr>
<td>$I_P$</td>
<td>0.853</td>
<td>0.869</td>
<td>0.883</td>
<td>0.887</td>
</tr>
<tr>
<td>$I_{EC}$</td>
<td>0.824 (0.0000)</td>
<td>0.858 (0.0000)</td>
<td>0.876 (0.0000)</td>
<td>0.887 (0.0000)</td>
</tr>
<tr>
<td>$I_{SH}$</td>
<td>0.839 (0.0000)</td>
<td>0.865 (0.0000)</td>
<td>0.895 (0.0000)</td>
<td>0.893 (0.0000)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_1$</td>
<td>0.873</td>
<td>0.863</td>
<td>0.862</td>
<td>0.859</td>
</tr>
<tr>
<td>$I_2$</td>
<td>0.836 (0.0031)</td>
<td>0.835 (0.0019)</td>
<td>0.846 (0.0025)</td>
<td>0.849 (0.0006)</td>
</tr>
<tr>
<td>$I_P$</td>
<td>0.851</td>
<td>0.839</td>
<td>0.841</td>
<td>0.845</td>
</tr>
<tr>
<td>$I_{EC}$</td>
<td>0.705 (0.0013)</td>
<td>0.723 (0.0006)</td>
<td>0.750 (0.0006)</td>
<td>0.786 (0.0000)</td>
</tr>
<tr>
<td>$I_{SH}$</td>
<td>0.706 (0.0019)</td>
<td>0.728 (0.0006)</td>
<td>0.760 (0.0006)</td>
<td>0.789 (0.0000)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$I_1$</td>
<td>0.863</td>
<td>0.849</td>
<td>0.852</td>
<td>0.857</td>
</tr>
<tr>
<td>$I_2$</td>
<td>0.834 (0.0081)</td>
<td>0.821 (0.0069)</td>
<td>0.843 (0.0069)</td>
<td>0.856 (0.0044)</td>
</tr>
<tr>
<td>$I_P$</td>
<td>0.815</td>
<td>0.806</td>
<td>0.812</td>
<td>0.819</td>
</tr>
<tr>
<td>$I_{EC}$</td>
<td>0.689 (0.0050)</td>
<td>0.718 (0.0050)</td>
<td>0.748 (0.0019)</td>
<td>0.779 (0.0019)</td>
</tr>
<tr>
<td>$I_{SH}$</td>
<td>0.697 (0.0050)</td>
<td>0.723 (0.0056)</td>
<td>0.753 (0.0025)</td>
<td>0.791 (0.0025)</td>
</tr>
</tbody>
</table>

**Table 4**

Example 3—estimated coverage probabilities for correlation coefficient $\rho$, based on 1600 random samples of sizes $n = 15, 20, 30$ and $50$ drawn from each of six different distributions: intervals $I_1$ and $I_P$ are based on 1000 outer level bootstrap resamples; for the asymptotic intervals, outer level resampling is used only in case the endpoints turn out to be faulty; the proportion of using outer level resampling is given in parentheses following the estimated coverage probability in this case.
approximations proposed by DiCiccio, Martin and Young (1992a, b). Moreover, the problem of overcovering by analytic approximations in the correlation coefficient example reported by DiCiccio, Martin and Young (1992b) does not exist for our asymptotic iterated methods.

The relative performances of \( I_1 \) and \( I_2 \) depend on the particular parameter of interest. Since it is the computationally more efficient method, the interval \( I_2 \) is very attractive when both \( I_1 \) and \( I_2 \) have similar coverage error. The need for bootstrap resampling typically renders construction of \( I_1 \) slower than that of \( I_2 \) by a factor of around 100 on an HP9000 workstation, depending on the number of bootstrap samples drawn. Nevertheless, both intervals \( I_1 \) and \( I_2 \) are far quicker to compute than the standard full-blown iterated bootstrap confidence interval, which requires two levels of bootstrap resampling. For example, in the case of constructing a confidence interval for the mean based on a sample of size \( n = 15 \), an HP9000 workstation took about 0.0012 second to compute \( I_2 \) using the automatic package described in Section 4, and about 155 seconds to compute \( I_F \), the full-blown iterated confidence interval based on 1000 outer and 1000 inner level bootstrap resamples. Here the automatic package outruns the double bootstrap procedure by a factor of almost 130,000. Of course, the above comparison might have exaggerated the general computational savings offered by the automatic procedure, given that the population mean is a particularly simple parameter of interest. Nevertheless, the computational savings may still be expected in most problems to be as dramatic as a factor of thousands. Moreover, the automatic procedure has been packaged by means of a single Fortran program which takes care of all analytic calculations. The simple input requirements of the program makes construction of the asymptotic intervals practically feasible for general use.

It should also be remarked that the built-in exact derivative evaluation routine utilised in our automatic procedure for construction of asymptotic iterated percentile bootstrap confidence intervals can in fact be incorporated into any asymptotic confidence interval construction procedure, especially those based on the smooth function model. Its numerical yet exact nature makes any symbolic calculation or numerical approximations unnecessary. It thus opens up the possibility of packaging many existing confidence interval construction methods for general application, in a way that demands no analytic calculation from the user.

Finally, as observed from our simulation results, the interval \( I_2 \) is more likely to be erratic (and to require adjustment by the method described above) if the coverage of common bootstrap intervals fails to approximate the nominal level accurately. In this case, the real fault is not due to the asymptotic nature of \( I_2 \), but rather to the general failure of bootstrap intervals. Therefore, the use of bootstrap resampling to substitute for the asymptotic endpoints does little to rectify the coverage error. Nevertheless, such need for resampling adjustment may be seen as a sign of bootstrap inadequacy and is therefore of some diagnostic value. Further research in
this direction may be beneficial to our general understanding of bootstrap methods as applied to confidence interval construction.

APPENDIX

Detailed calculations for constructing $I_1$ and $I_2$. We now give a complete account of calculations coded in the program asymp.f. The notation follows that introduced in Section 4.

Consider first the infinite list $\mathcal{L}$ of sequences of the $\rho_i(r, j)$,

$\mathcal{L} = \{ \rho_1(r, 1), \rho_2(r, 1), \ldots, \rho_{d(r, 1)}(r, 1), \rho_1(r, 2), \ldots, \rho_{d(r, 2)}(r, 2), \ldots, \rho_1(r, m), \ldots, \rho_{d(r, m)}(r, m), \ldots \}.$

Let $\rho_i(r)$ denote the $i$th sequence in $\mathcal{L}$. Define an operation $\otimes$ on $\mathbb{N} \times \mathbb{N}$ such that, for any $i, j \in \mathbb{N}$, we have

$i \otimes j = k$ if $\rho_i(r) + \rho_j(r)$ is the $k$th sequence in $\mathcal{L}$.

Therefore, we have

$X^{(i)}X^{(j)} = X^{(i \otimes j)}$,

provided $i \otimes j$ does not exceed the dimension of $X$. To perform this operation we set up an initial list

$\mathcal{L}_0 = \{ \rho_1(r, 1), \rho_2(r, 1), \ldots, \rho_{d(r, 1)}(r, 1), \rho_1(r, 2), \ldots, \rho_{d(r, 2)}(r, 2), \ldots, \rho_1(r, 6s), \ldots, \rho_{d(r, 6s)}(r, 6s) \}$

as the basis underlying the operation. An order of $6s$ is adequate for the entire range of moments likely to be encountered.

Suppose now we observe a random sample $Y_1, \ldots, Y_n$ from $G$. Let $X_i$ denote the extended vector $X$ corresponding to $Y_i$. Our automatic procedure operates as follows:

1. Calculate

$\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$.

2. Partially differentiate $g(x)$ up to the third order. Define

$g_i(x) = \frac{\partial g(x)}{\partial x_i}, \quad g_{ij}(x) = \frac{\partial^2 g(x)}{\partial x_i \partial x_j} \quad \text{and} \quad g_{ijk}(x) = \frac{\partial^3 g(x)}{\partial x_i \partial x_j \partial x_k},$

for $i, j, k = 1, 2, \ldots, d'$.

3. Evaluate the sample values of $g(\bar{X}), g_i(\bar{X}), g_{ij}(\bar{X})$ and $g_{ijk}(\bar{X})$.

4. For $x \in \mathbb{R}^{d''}$, define the following functions:

$\mu_{ij}(x) = x_{i \otimes j} - x_i x_j,$
for $i = 1, 2, \ldots, d'$ and $j = 1, 2, \ldots, d''$;

$$
\mu_{ijk}(\mathbf{x}) = x_{i \otimes j \otimes k} - x_{i \otimes j} x_k - x_{j \otimes k} x_i - x_{k \otimes i} x_j + 2 x_i x_j x_k,
$$

for $i, j, k = 1, 2, \ldots, d'$; and

$$
\mu_{ijkl}(\mathbf{x}) = x_{i \otimes j \otimes k \otimes l} - x_{i \otimes j \otimes k} x_l - x_{j \otimes k \otimes l} x_i - x_{k \otimes l \otimes i} x_j - x_{l \otimes i \otimes j} x_k + x_{i \otimes j} x_k x_l + x_{i \otimes k} x_l x_j + x_{j \otimes k} x_l x_i + x_{j \otimes l} x_i x_k + x_{k \otimes l} x_i x_j - 3 x_i x_j x_k x_l,
$$

for $i, j, k, l = 1, 2, \ldots, d$.

5. Partially differentiate $\mu_{ij}$ and $\mu_{ijk}$ to get the following:

$$
\frac{\partial}{\partial t} \mu_{ij}(\mathbf{x}) = \frac{\partial \mu_{ij}(\mathbf{x})}{\partial x_l},
$$

for $i, j = 1, 2, \ldots, d$ and $l = 1, 2, \ldots, d'$; and

$$
\frac{\partial}{\partial t} \mu_{ijk}(\mathbf{x}) = \frac{\partial \mu_{ijk}(\mathbf{x})}{\partial x_l},
$$

for $i, j, k = 1, 2, \ldots, d$ and $l = 1, 2, \ldots, d''$.

6. Evaluate the sample values of all the functions defined in steps 4 and 5, that is, $\mu_{ij}(\mathbf{X}), \ldots$ and so on.

To simplify notation, we now drop the bracketed arguments of the sample values of functions so far evaluated, by setting, for example, $g = g(\mathbf{X})$, $g_i = g_i(\mathbf{X}), \ldots$.

7. Evaluate

$$
h = \left( \sum_{i, j=1}^{d} g_i g_j \mu_{ij} \right)^{1/2}.
$$

8. Evaluate

$$
\alpha_i = \frac{g_i}{h}, \quad \alpha_{ij} = \frac{g_{ij}}{h} \quad \text{and} \quad \alpha_{ijk} = \frac{g_{ijk}}{h},
$$

for $i, j, k = 1, 2, \ldots, d''$.

9. Evaluate

$$
h_k = (2h)^{-1} \sum_{i, j=1}^{d} \left( 2g_{ik} g_{j} \mu_{ij} + g_{i} g_{j} \partial_k \mu_{ij} \right)
$$

and

$$
h_{kl} = h^{-1} \sum_{i, j=1}^{d} \left[ g_{ikl} g_{j} \mu_{ij} + g_{ik} g_{jl} \mu_{ij} + g_{ik} g_{j} \partial_l \mu_{ij} + g_{il} g_{j} \partial_k \mu_{ij} \right] - h^{-1} \{ h_k h_l + g_{kl} g_i \},
$$

for $k, l = 1, 2, \ldots, d'$.
10. Evaluate
\[ b_i = h^{-1} g_i, \]
for \( i = 1, 2, \ldots, d, \)
\[ b_{ij} = h^{-1} g_{ij} - h^{-2} (g_i h_j + g_j h_i), \]
and
\[ b_{ijk} = h^{-1} g_{ijk} - h^{-2} (g_{i}h_{k} + g_{k}h_{i} + g_{j}h_{i} + g_{i}h_{j} + g_{j}h_{k} + g_{k}h_{j}) + 2h^{-3} (g_{i} h_{j} h_{k} + g_{j} h_{k} h_{i} + g_{k} h_{i} h_{j}), \]
for \( i, j, k = 1, 2, \ldots, d'. \)

11. Evaluate
\[ l_{12} = \frac{1}{2} \sum_{i,j=1}^{d} a_{ij} \mu_{ij}, \]
\[ l_{31} = \sum_{i,j,k=1}^{d} a_{ij} a_{k} \mu_{ijk} + 3 \sum_{i,j,k,l=1}^{d} a_{ij} a_{kl} \mu_{ijkl}, \]
\[ l_{22} = \sum_{i,j,k,l=1}^{d} \left\{ \frac{1}{2} a_{ij} a_{kl} \mu_{ijkl} + a_{ij} a_{k} \mu_{ijkl} \right\} + \sum_{i,j,k=1}^{d} a_{ij} a_{jk} \mu_{ijk} \]
and
\[ l_{41} = \sum_{i,j,k,l=1}^{d} a_{ij} a_{k} a_{l} \mu_{ijkl} + 12 \sum_{i,j,k,l,m=1}^{d} a_{ij} a_{k} a_{lm} \mu_{ijl} \mu_{km} \]
\[ + \sum_{i,j,k,l,m,n=1}^{d} \left\{ 4 a_{ij} a_{k} a_{lmn} \mu_{ijkl} \mu_{jmn} \mu_{kn} + 12 a_{ij} a_{k} a_{lmn} \mu_{ijkl} \mu_{jmn} \mu_{kn} \right\} - 3. \]

12. Similarly, evaluate
\[ k_{12} = \frac{1}{2} \sum_{i,j=1}^{d'} b_{ij} \mu_{ij}, \]
\[ k_{31} = \sum_{i,j,k=1}^{d} b_{i} b_{j} b_{k} \mu_{ijk} + 3 \sum_{i,j=1}^{d} \sum_{k,l=1}^{d'} b_{i} b_{j} b_{kl} \mu_{ijkl}, \]
\[ k_{22} = \frac{1}{2} \sum_{i,j,k,l=1}^{d'} b_{ij} b_{kl} \mu_{ijkl} \]
\[ + \sum_{i=1}^{d} \sum_{j,k,l=1}^{d'} b_{i} b_{jkl} \mu_{ijkl} + \sum_{i=1}^{d} \sum_{j=1}^{d'} b_{i} b_{jk} \mu_{ijk}, \]
and
\[ k_{41} = \sum_{i,j,k,l=1}^{d} b_i b_j b_k b_l \mu_{ijkl} + 12 \sum_{i,j,k=1}^{d} \sum_{l,m=1}^{d'} b_i b_j b_k b_{lm} \mu_{ijl} \mu_{km} \]
\[ + 4 \sum_{i,j,k=1}^{d} \sum_{l,m,n=1}^{d'} b_i b_j b_k b_{lmn} \mu_{ijl} \mu_{jkm} \mu_{kn} \]
\[ + 12 \sum_{i,j,k=1}^{d} \sum_{l,m,n=1}^{d'} b_i b_j b_{kl} b_{mn} \mu_{ik} \mu_{jlm} \mu_{ln} - 3. \]

13. Evaluate
\[ \partial_m l_{12} = \frac{1}{2} \sum_{i,j=1}^{d} \left( a_{ijm} \mu_{ij} + a_{imj} \partial_m \mu_{ij} \right) - \frac{l_{12} h_m}{h}, \]
for \( m = 1, 2, \ldots, d' \), and
\[ \partial_m l_{31} = \sum_{i,j,k,l=1}^{d} \left\{ 6a_{im} a_j a_{kl} \mu_{ik} \mu_{jl} + 3a_i a_j a_{klm} \mu_{ik} \mu_{jl} + 6a_i a_j a_{kl} \mu_{jlm} \partial_m \mu_{ik} \right\} \]
\[ + \sum_{i,j,k=1}^{d} \left\{ 3a_{im} a_j a_k \mu_{ijk} + a_i a_j a_k \partial_m \mu_{ijk} \right\} - \frac{3l_{31} h_m}{h}, \]
for \( m = 1, 2, \ldots, d'' \).

14. Set \( \xi = \frac{1}{3}(1 + \alpha) \). Evaluate \( z_\xi = \Phi^{-1}(\xi) \).

15. Evaluate
\[ a_\xi = \sum_{i=1}^{d} \sum_{j=1}^{d'} \mu_{ij} b_i \partial_j l_{12} + \frac{1}{6} \left( z_\xi^2 - 1 \right) \sum_{i=1}^{d} \sum_{j=1}^{d'} \mu_{ij} b_i \partial_j l_{31}. \]

16. Evaluate
\[ p_1(z_\xi) = -\left( l_{12} + \frac{l_{31}(z_\xi^2 - 1)}{6} \right), \]
\[ p_2(z_\xi) = -z_\xi \left\{ \frac{l_{12}^2 + l_{22}}{2} + \frac{(4l_{12} l_{31} + l_{41})(z_\xi^2 - 3)}{24} \right. \]
\[ + \frac{l_{31}^2(z_\xi^4 - 10z_\xi^2 + 15)}{72} \],
\[ p_1'(z_\xi) = - \frac{l_{31} z_\xi}{3} \]
and
\[ p_2'(z_\xi) = -\left\{ \frac{l_{12}^2 + l_{22}}{2} + \frac{(4l_{12} l_{31} + l_{41})(3z_\xi^2 - 3)}{24} \right. \]
\[ + \frac{l_{31}^2(5z_\xi^4 - 30z_\xi^2 + 15)}{72} \].
ASYMPTOTIC CONFIDENCE INTERVALS

Evaluate also \( q_1(z_\xi), q_2(z_\xi), q'_1(z_\xi) \) and \( q'_2(z_\xi) \) by replacing \( l_{ij} \) with \( k_{ij} \) in the above formulae for the \( p_i \) and \( p'_i \).

17. Evaluate

\[
\pi_1(z_\xi) = p_2(z_\xi) - q_2(z_\xi) - p_1(z_\xi)\{p'_1(z_\xi) - z_\xi p_1(z_\xi) + q'_1(z_\xi) - z_\xi q_1(z_\xi)\} + a_\xi z_\xi
\]

and

\[
\tilde{t} = n^{-1/2} \pi_1(z_\xi) \phi(z_\xi).
\]

If \( 0 < \xi + \tilde{t}/2 < 1 \), then evaluate

\[
\tilde{y}_\beta = g + n^{-1/2} h \left\{ z_\beta - n^{-1/2} p_1(z_\beta) + n^{-1} \left( p_1(z_\beta) p'_1(z_\beta) - p_2(z_\beta) - z_\beta p'_2(z_\beta) \right) \right\}
\]

for \( \beta = \xi + \tilde{t}/2 \) and \( 1 - \xi - \tilde{t}/2 \), respectively, where the functions \( p_1, p_2 \) and \( p'_1 \) are recalculated using formulae in the last step.

Note that the notation used in the above description follows that given in Section 3, except that now all quantities represent sample versions. Only steps 2 and 5 require anything other than arithmetic operations: these can be most conveniently handled by an exact derivative evaluation routine, as described in Section 4 above and Kagiwada, Kalaba, Rasakhoo and Spingarn [(1986), Chapters 1 and 2]. This routine evaluates derivatives exactly and numerically, thus saving a great deal of analytic effort and/or computer time spent on symbolic operations. Note that the term \( \mu_{d'd'd}(\mathbf{x}) \), defined in step 4 and evaluated subsequently in step 6, depends on a moment of order \( 6s \), the highest throughout the whole procedure. This observation explains our choice of the maximum dimension \( d'' \).

As pointed out in step 17, it may happen that \( \xi + \tilde{t}/2 \not\in (0,1) \) so that \( z_{\xi+\tilde{t}/2} \) is infinite and the formula for \( \tilde{y}_{\xi+\tilde{t}/2} \) is not defined. Also, if \( \tilde{y}_{1-\xi-\tilde{t}/2} \geq \tilde{y}_{\xi+\tilde{t}/2} \), the interval \( I_2 \) would be empty and meaningless. In these situations, we suggest obtaining an approximation to \( I_1 \) by means of bootstrap resampling. The calibrated coverage level \( \alpha + \tilde{t} \) should also be forced to its nearest point within the interval \([0,1] \). To be more specific, we draw \( B \) random resamples \( \chi_1^*, \ldots, \chi_B^* \) from \( \chi \), calculate the version of \( \hat{\theta}, \hat{\theta}_b^* \) say, based on each \( \chi_b^* \), order these quantities as \( \hat{\theta}_{(1)}^* \leq \cdots \leq \hat{\theta}_{(B)}^* \), and then approximate \( I_1 \) by

\[
[\hat{\theta}_{(m_1)}, \hat{\theta}_{(m_2)}],
\]

where \( m_1 = \max\{1, [(B + 1)(1 - \xi')]\} \), \( m_2 = \min\{B, [(B + 1)\xi']\} \), \( \lfloor \cdot \rfloor \) denotes the integer part, and \( \xi' = \max\{1/2, \xi + \tilde{t}/2\} \). Such choices of \( m_1, m_2 \) and \( \xi' \) ensure that \( 1 \leq m_1 \leq m_2 \leq B \).
REFERENCES


