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# ON THE NUMBER OF BOOTSTRAP REPETITIONS FOR BOOTSTRAP STANDARD ERRORS, CONFIDENCE INTERVALS, AND TESTS

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November 1996 Revised August 1997

# On the Number of Bootstrap Repetitions for Bootstrap Standard Errors, Confidence Intervals, and Tests

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#### Abstract

This paper considers the problem of choosing the number of bootstrap repetitions B for bootstrap standard errors, confidence intervals, and tests. For each of these problems, the paper provides a threestep method for choosing B to achieve a desired level of accuracy. Accuracy is measured by the percentage deviation of the bootstrap standard error estimate, confidence interval endpoint(s), test's critical value, or test's *p*-value based on B bootstrap simulations from the corresponding ideal bootstrap quantities for which  $B = \infty$ . Monte Carlo simulations show that the proposed methods work quite well.

The results apply quite generally to parametric, semiparametric, and nonparametric models with independent and dependent data. The results apply to the standard nonparametric iid bootstrap, moving block bootstraps for time series data, parametric and semiparametric bootstraps, and bootstraps for regression models based on bootstrapping residuals.

*Keywords:* Bootstrap, bootstrap repetitions, coefficient of excess kurtosis, confidence interval, density estimation, hypothesis test, *p*-value, quantile, simulation, standard error estimate.

JEL Classification: C12, C13, C14, C15.

# 1. Introduction

Bootstrap methods have gained a great deal of popularity in empirical research. Although the methods are easy to apply, determining the number of bootstrap repetitions, B, to employ is a common problem in the existing literature. Typically, this number is determined in a somewhat ad hoc manner. This is problematic, because one can obtain a "different answer" from the same data merely by using different simulation draws if B is chosen to be too small. On the other hand, it is expensive to compute the bootstrap statistics of interest, if B is chosen to be extremely large. Thus, it is desirable to be able to determine a value of B that obtains a suitable level of accuracy for a given problem at hand. This paper addresses this issue in the context of the three main branches of statistical inference, viz., point estimation, interval estimation, and hypothesis testing.

We provide methods for determining B to attain specified levels of accuracy for bootstrap standard error estimates, confidence intervals, and hypothesis tests.<sup>2</sup> A three-step method for choosing B is proposed for each case. Three steps are required because one needs to determine the relevant features of the problem in the initial two steps before one can determine a suitable choice of B in the third step.

The measure of accuracy differs somewhat across the cases considered. For standard error estimates, we measure accuracy in terms of the percentage deviation of the bootstrap standard error estimate for a given value of B, from the ideal bootstrap estimate, for which  $B = \infty$ . For confidence intervals, we measure accuracy in terms of the percentage deviation of the bootstrap endpoint(s) of the confidence interval for a given value of B, from the ideal bootstrap endpoint(s). For symmetric two-sided confidence intervals, this measure of accuracy is equivalent to a measure based on the percentage deviation of the length of the confidence interval for a given value of B, from the ideal bootstrap length.

For tests with a specified significance level  $\alpha$ , we measure accuracy in terms of the percentage deviation of the bootstrap critical value of the test for a given value of B, from the ideal bootstrap critical value. For tests in which one wants to report a p-value, we measure accuracy in terms of the percentage deviation of the bootstrap pvalue for a given value of B, from the ideal bootstrap p-value. (We note that reporting a bootstrap p-value exploits the potential higher-order improvements of the bootstrap that are available for tests; see Section 4 below.) For each type of statistical inference, the measure of accuracy is directly related to the issue of whether one could obtain a "different answer" from the same data merely by using different simulation draws.

The accuracy obtained by a given choice of B is stochastic, because the bootstrap simulations are random. To determine a suitable value of B, we specify a bound on the relevant percentage deviation, denoted pdb, and we require that the actual percentage deviation is less than this bound with a specified probability,  $1-\tau$ , close to one. The three-step method takes pdb and  $\tau$  as given and specifies a data-dependent method of determining a value of B, denoted  $B^*$ , such that the desired level of accuracy is obtained. For example, one might take  $(pdb, \tau) = (10, .05)$ . Then, the three-step method yields a value  $B^*$  such that the relevant percentage deviation is less than 10% with approximate probability .95. The three-step methods are applicable in parametric, semiparametric, and nonparametric models with independent and identically distributed (iid) data, independent and non-identically distributed (inid) data, and time series data. The methods are applicable when the bootstrap employed is the standard nonparametric iid bootstrap, a moving block bootstrap for time series, a parametric or semiparametric bootstrap, or a bootstrap for regression models that is based on bootstrapping residuals. The methods are applicable to statistics that have normal and non-normal asymptotic distributions. Essentially, the results are applicable whenever the bootstrap samples are simulated to be iid across different bootstrap samples. We do not require that the simulations are iid within each bootstrap sample—in fact, they are not for most time series applications.

The results for confidence intervals apply to symmetric, equal-tailed, and onesided percentile t confidence intervals, as defined in Hall (1992). Efron's (1987)  $AB_c$ confidence intervals are not considered. They will be considered elsewhere. The results for tests apply to a wide variety of tests of parametric restrictions and model specification based on t statistics, Wald statistics, Lagrange multiplier statistics, likelihood ratio statistics, etc.

For bootstrap standard error estimates, the three-step method depends on an estimate of the *coefficient of excess kurtosis*,  $\gamma_2$ , of the bootstrap distribution of the parameter estimator. We consider the usual estimator of  $\gamma_2$  as well as a bias-corrected estimator of it. We compare these two methods via simulation. Because the computational cost of carrying out the bias correction is small and the gains are significant in some cases, we recommend use of the bias-corrected estimator of  $\gamma_2$ .

For confidence intervals and critical values of tests, the three-step method depends on estimates of the "density" evaluated at specific quantiles of the bootstrap distribution of the statistic that is used to construct the confidence interval or test. For this purpose, we use an estimator of Siddiqui (1960) with an optimal data-dependent smoothing parameter, which is a variant of that proposed by Hall and Sheather (1988).

The three-step methods are justified by asymptotic results. The small sample accuracy of the asymptotic results is evaluated via simulation experiments. We assess the performance of the three-step methods for standard error estimates and symmetric percentile t confidence intervals. In short, the simulations show that the methods work very well in the cases considered.

The closest results in the literature to the standard error results given here are those of Efron and Tibshirani (1986, Sec. 9). Efron and Tibshirani provide a simple formula that relates the coefficient of variation of the bootstrap standard error estimator, as an estimate of the true standard error, to the coefficient of variation of the ideal bootstrap standard error estimator, as an estimate of the true standard error. Their formula depends on some unknowns that are not estimable. Hence, Efron and Tibshirani only use their formula to suggest a range of plausible values of B. An advantage of our approach over that of Efron and Tibshirani is that the unknowns in our approach can be estimated quite easily. This allows us to specify an explicit method of choosing B to obtain a desired degree of accuracy of the bootstrap standard error estimator as an estimate of the ideal bootstrap standard error estimator.

The closest results in the literature to the confidence interval results given here are those of Hall (1986). His paper has two parts. The part that deals with coverage probabilities considers *unconditional* coverage probabilities, i.e., coverage probabilities with respect to the randomness in the data and the bootstrap simulations. In constrast, we consider *conditional* coverage probabilities, i.e., coverage probabilities with respect to the randomness in the data conditional on the bootstrap simulations. We do so because the bootstrap simulation randomness is *ancillary* and, hence, should be conditioned on when making inference according to the principle of ancillarity or conditionality; see Kiefer (1982). We do not want to be able to obtain "different answers" from the same data due to the use of different simulation draws.

The second part of Hall's (1986) paper (see Section 3) considers the asymptotic distribution of the difference between a bootstrap percentile t confidence interval endpoint based on B bootstrap repetitions and the ideal bootstrap endpoint. He considers the case where the bootstrap employed is the nonparametric iid bootstrap and the t statistic is a normalized sample mean of iid random variables.

While our three-step methods rely on similar results, we use a proof that differs from that of Hall in that it does not rely on smoothing the bootstrap distribution of the statistic. Furthermore, our results apply to a much wider array of statistics, types of bootstraps, and assumptions regarding the iid, inid, or dependent nature of the original sample than do Hall's, although it may be possible to generalize Hall's results along these lines. In addition, our results allow B to be data-dependent, as is necessary for the three-step methods.

In any event, the focus of Hall's results is quite different from that of this paper. Hall uses his results to demonstrate the near continuity of the discrete nonparametric iid bootstrap distribution of the t statistic. In contrast, we address the question of choosing a desired number,  $B^*$ , of bootstrap repetitions.

The closest results in the literature to the test results given here are those of Davidson and MacKinnon (1997). Davidson and MacKinnon consider the effect of the number of bootstrap repetitions on the unconditional power of a bootstrap test, i.e., the power with respect to the randomness in the data and the bootstrap simulations. They propose a pretesting method of choosing B that aims to achieve good unconditional power for a given significance level  $\alpha$ . In contrast, the method that we consider aims to achieve a bootstrap test that has good conditional significance level given the simulation randomness. We do so for the same reason as given above for confidence intervals, viz., the bootstrap simulation randomness is ancillary and, hence, should be conditioned on when making inference according to the principle of ancillarity or conditionality.

The remainder of this paper is organized as follows. Sections 2, 3, and 4 provide the results for standard error estimates, confidence intervals, and tests respectively. Section 2.1 introduces notation and definitions for the standard error results. The notation follows that of Efron and Tibshirani (1993). Section 2.2 presents a formula for the accuracy of the bootstrap standard error estimator for finite B as an estimator of the ideal bootstrap standard error estimator. Section 2.3 introduces the threestep method for determining B for bootstrap standard error estimates. Section 2.4 presents Monte Carlo simulation results for the three-step method of determining B. Section 2.5 introduces a bias-corrected three-step method of determining B for bootstrap standard error estimates. Section 2.6 assesses its performance via Monte Carlo simulation.

Section 3.1 introduces notation and definitions for symmetric percentile t confidence intervals. The notation follows that of Hall (1992). Section 3.2 provides the three-step method for these confidence intervals. Section 3.3 provides the asymptotic justification of the three-step method for these confidence intervals. Section 3.4 presents Monte Carlo simulation results for the three-step method of determining Bfor symmetric confidence intervals. Section 3.5 extends the results of Sections 3.1–3.3 to equal-tailed and one-sided percentile t confidence intervals.

Section 4.1 provides the three-step method and its justification for tests with a specified significance level. Section 4.2 provides the three-step method and its justification for tests when a p-value is to be reported.

An Appendix of Proofs provides proofs of the results given in Sections 2–4.

#### 2. Standard Error Results

In this section, we present the results for bootstrap standard error estimates.

#### **2.1.** Notation and Definitions

The observed data are a sample of size n:  $\mathbf{X} = (X_1, ..., X_n)'$ . Let  $\hat{\theta} = \hat{\theta}(\mathbf{X})$  be an estimator of a scalar parameter  $\theta_0$  based on the sample  $\mathbf{X}$ . We are interested in estimation of the standard error, se, of  $\hat{\theta}$ . By definition,

(2.1) 
$$se = \left(E(\widehat{\theta}(\mathbf{X}) - E\widehat{\theta}(\mathbf{X}))^2\right)^{1/2},$$

where E denotes expectation with respect to the randomness in X. Of course, se depends on n, but we take n to be fixed in this section except where stated otherwise.

Let  $\mathbf{X}^* = (X_1^*, ..., X_n^*)'$  be a bootstrap sample of size n based on the original sample  $\mathbf{X}$ . When the original sample  $\mathbf{X}$  is comprised of iid or inid random variables, the bootstrap sample  $\mathbf{X}^*$  often is an iid sample of size n drawn from some distribution  $\widehat{F}$ . For example, for the nonparametric bootstrap,  $\widehat{F}$  is the empirical distribution function based on  $\mathbf{X}$ . That is,  $\widehat{F}(x) = \frac{1}{n} \sum_{i=1}^{n} 1(X_i \leq x)$ , where  $1(X_i \leq x)$  denotes the indicator function of  $X_i \leq x$ . For parametric and semiparametric bootstraps,  $\widehat{F}$  typically depends on estimators of  $\theta_0$  and other parameters. When the original sample  $\mathbf{X}$  is comprised of dependent data, the bootstrap sample often is taken to be a moving block bootstrap or some variation of this; see Carlstein (1986), Kunsch (1989), Hall and Horowitz (1996), and Li and Maddala (1996). When the model is a regression model with independent or dependent data, the bootstrap sample is sometimes generated by bootstrapping the residuals; see Freedman (1981), Li and Maddala (1996), and the references therein. All of these bootstrap methods are covered by our results. The "ideal" bootstrap standard error estimator of se is

(2.2) 
$$\widehat{se}_{\infty} = \left( E^* (\widehat{\theta}(\mathbf{X}^*) - E^* \widehat{\theta}(\mathbf{X}^*))^2 \right)^{1/2},$$

where  $E^*$  denotes expectation with respect to the randomness in the bootstrap sample  $X^*$  conditional on the observed data X.

Analytic calculation of the ideal bootstrap standard error is usually intractable. Instead one usually approximates it using bootstrap simulations. Consider B iid bootstrap samples  $\{\mathbf{X}_b^* : b = 1, ..., B\}$  each with the same distribution as  $\mathbf{X}^*$ . The quantity B is referred to as the number of bootstrap repetitions. The corresponding B bootstrap estimates of  $\theta_0$  are denoted by  $\hat{\theta}_b^* = \hat{\theta}(\mathbf{X}_b^*)$  for b = 1, ..., B. The bootstrap standard error estimator for B bootstrap repetitions is

(2.3) 
$$\widehat{se}_B = \left(\frac{1}{B-1}\sum_{b=1}^B \left(\widehat{\theta}_b^* - \frac{1}{B}\sum_{c=1}^B \widehat{\theta}_c^*\right)^2\right)^{1/2}.$$

Note that

(2.4) 
$$\lim_{B \to \infty} \widehat{se}_B = \widehat{se}_{\infty}$$

in probability and almost surely by the law of large numbers provided  $E^*(\hat{\theta}(\mathbf{X}^*))^2 < \infty$ . The latter holds automatically for the nonparametric bootstrap due to its finite support.

Here and below (except as stated otherwise), all probability statements and the probability and expectation operators  $P^*$  and  $E^*$ , respectively, refer to the randomness in the iid bootstrap samples  $\{\mathbf{X}_b^* : b = 1, ..., B\}$  conditional on the observed data **X**. We note that our results are applicable in any bootstrap context in which the simulated bootstrap samples  $\{\mathbf{X}_b^* : b = 1, ..., B\}$  are iid over the index b.

Let  $\mu$  and  $\gamma_2$  denote the mean and the coefficient of excess kurtosis of the bootstrap estimator  $\hat{\theta}_b^*$ . By definition,

(2.5) 
$$\mu = E^* \hat{\theta}(\mathbf{X}^*) \text{ and} \gamma_2 = \frac{E^* (\hat{\theta}(\mathbf{X}^*) - \mu)^4}{(E^* (\hat{\theta}(\mathbf{X}^*) - \mu)^2)^2} - 3 = \frac{E^* (\hat{\theta}(\mathbf{X}^*) - \mu)^4}{\widehat{se}_{\infty}^4} - 3.$$

(From above, the standard error of  $\hat{\theta}_b^*$  is  $\hat{se}_{\infty}$ .) Note that  $\gamma_2 = 0$  if  $\hat{\theta}_b^*$  has a normal distribution,  $\gamma_2 > 0$  if  $\hat{\theta}_b^*$  has kurtosis greater than that of a normal distribution, and  $\gamma_2 < 0$  otherwise. For example, for a t distribution with df degrees of freedom, the coefficient of excess kurtosis is 6/(df-4). Thus, for df = 10,  $\gamma_2 = 1$ ; for df = 7,  $\gamma_2 = 2$ ; and for df = 5,  $\gamma_2 = 6$ . The range of possible values of  $\gamma_2$  across all distributions is  $[-2,\infty)$ . (The normal and t distributions are mentioned here for illustrative purposes only. For the nonparametric bootstrap, it is not possible for  $\hat{\theta}(\mathbf{X}^*)$  to have a normal or t distribution, because the distribution of  $\hat{\theta}(\mathbf{X}^*)$  is discrete. Nevertheless,  $\hat{\theta}(\mathbf{X}^*)$  may have a discrete distribution that is closely approximated by a normal or t distribution.)

Often  $\{d_n(\hat{\theta}_b^* - \theta_0) : n \ge 1\}$  converges to a normal distribution as  $n \to \infty$  and is uniformly integrable to the fourth power, where  $\{d_n : n \ge 1\}$  is a divergent sequence of positive constants, such as  $n^{1/2}$  or  $n^{2/5}$ . In such cases,  $\gamma_2 \to_p 0$  as  $n \to \infty$ . In many applications, however,  $\gamma_2$  is greater than zero in finite samples.

Estimates of  $\mu$  and  $\gamma_2$  are given by

(2.6) 
$$\widehat{\mu}_B = \frac{1}{B} \Sigma^B_{b=1} \widehat{\theta}^*_b \text{ and}$$
$$\widehat{\gamma}_{2B} = \frac{\frac{1}{B-1} \Sigma^B_{b=1} (\widehat{\theta}^*_b - \widehat{\mu}_B)^4}{\widehat{se}^4_B} - 3.$$

These estimators are consistent by the law of large numbers and Slutsky's Theorem:

(2.7) 
$$\lim_{B \to \infty} \hat{\mu}_B = \mu \text{ and } \lim_{B \to \infty} \hat{\gamma}_{2B} = \gamma_2$$

in probability and almost surely, provided  $\widehat{se}_{\infty} \neq 0$ .

Let  $\chi^2_{1-\tau}$  denote the  $(1-\tau)$ -th quantile of a chi-squared distribution with one degree of freedom for  $\tau \in (0,1)$ . That is,  $P(Y \leq \chi^2_{1-\tau}) = 1-\tau$ , where Y has  $\chi^2$  distribution with one degree of freedom.

# 2.2. A Formula for the Accuracy of $\widehat{se}_B$ as an Approximation for $\widehat{se}_{\infty}$

In this section, we give a simple formula which provides a probabilistic statement of how close  $\widehat{se}_B$  is to  $\widehat{se}_\infty$  as a function of the number of bootstrap repetitions B. The results are justified by asymptotics as  $B \to \infty$  and are established by a simple application of the delta method.

The percentage deviation of  $\widehat{se}_B$  as an estimate of  $\widehat{se}_{\infty}$  is

(2.8) 
$$100 \frac{|\widehat{se}_B - \widehat{se}_{\infty}|}{\widehat{se}_{\infty}}$$

Let  $1 - \tau$  denote a probability close to one, such as .95. Let pdb be a bound on the percentage deviation of  $\widehat{se}_B$  from  $\widehat{se}_\infty$ . We want to determine  $B = B(pdb, \tau)$  such that

(2.9) 
$$P^*\left(100\frac{|\widehat{se}_B - \widehat{se}_{\infty}|}{\widehat{se}_{\infty}} \le pdb\right) = 1 - \tau.$$

Alternatively, for given B and  $\tau$ , we want to determine  $pdb = pdb(B,\tau)$  such that (2.9) holds.

The relationship between B, pdb, and  $\tau$  that is determined by (2.9) satisfies the following approximate formula:

(2.10) 
$$pdb \doteq 50(\chi_{1-\tau}^{2}(2+\gamma_{2})/B)^{1/2} \text{ or equivalently} \\ B \doteq 2,500\chi_{1-\tau}^{2}(2+\gamma_{2})/pdb^{2}.$$

This formula is accurate in the sense that

(2.11) 
$$\lim_{B \to \infty} P^* \left( 100 \frac{|\widehat{se}_B - \widehat{se}_\infty|}{\widehat{se}_\infty} \le 50 \left( \chi_{1-\tau}^2 (2+\gamma_2)/B \right)^{1/2} \right) = 1 - \tau.$$

The proof of this result and others below are given in the Appendix of Proofs.

Formula (2.10) is not operational because it depends on the unknown parameter  $\gamma_2$ . One can substitute the consistent estimator  $\hat{\gamma}_{2B}$  of (2.6) for  $\gamma_2$  to obtain

(2.12) 
$$pdb \doteq 50 \left( \chi_{1-\tau}^2 (2+\hat{\gamma}_{2B})/B \right)^{1/2} \text{ or equivalently} \\ B \doteq 2,500 \chi_{1-\tau}^2 (2+\hat{\gamma}_{2B})/pdb^2.$$

Equations (2.7) and (2.11) combine to give

(2.13) 
$$\lim_{B \to \infty} P^* \left( 100 \frac{|\widehat{se}_B - \widehat{se}_\infty|}{\widehat{se}_\infty} \le 50 \left( \chi_{1-\tau}^2 (2+\widehat{\gamma}_{2B})/B \right)^{1/2} \right) = 1 - \tau,$$

which justifies (2.12).

We now show how the formula of (2.12) can be utilized. Suppose *B* has been specified, perhaps by the author of some research paper of interest. We are interested in whether this choice of *B* is sufficiently large to yield  $\widehat{se}_B$  close to  $\widehat{se}_{\infty}$ . Take  $1-\tau$  close to one, say .95. Then,  $\chi^2_{1-\tau} = 3.84$  and

(2.14) 
$$pdb \doteq 98 \left( (2 + \hat{\gamma}_{2B})/B \right)^{1/2}.$$

Table 1 provides the values of pdb that correspond to an array of values of  $\hat{\gamma}_{2B}$  and B when  $1 - \tau = .95$ . For example, if  $\hat{\gamma}_{2B} = 0$  (which corresponds to the kurtosis of the normal distribution) and B = 50, then  $pdb \doteq 20$ . That is, with probability approximately .95,  $\hat{se}_B$  is within  $\pm 20\%$  of  $\hat{se}_\infty$ . Or, with probability approximately .95,  $\hat{se}_\infty$  is within  $\pm 20\%$  of  $\hat{se}_B$ . (The latter interpretation is valid because (2.13) holds with  $\hat{se}_\infty$  in the denominator replaced by  $\hat{se}_B$ .)

Table 1 shows that to obtain very accurate estimates of  $\widehat{se}_{\infty}$ , say pdb = 5, one needs quite large values of B, e.g., B = 750 when  $\widehat{\gamma}_{2B} = 0$  and B = 2,000 when  $\widehat{\gamma}_{2B} = 3$ . Much smaller values of B are required to obtain moderate accuracy, say pdb = 20, e.g., B = 50 when  $\widehat{\gamma}_{2B} = 0$  and B = 100 when  $\widehat{\gamma}_{2B} = 2$ .

# 2.3. A Three-step Method for Determining the Number of Bootstrap Repetitions

We now specify a three-step method for determining B to achieve a desired accuracy of  $\widehat{se}_B$  for estimating  $\widehat{se}_{\infty}$ . The desired accuracy is specified by a  $(pdb, \tau)$  combination, such as (10, .05). The method involves the following steps:

**Step 1.** Suppose  $\gamma_2 = 0$  and use (2.10) to specify a preliminary value of *B*, denoted  $B_0$ . By definition,

(2.15) 
$$B_0 = \operatorname{int}(5,000\chi_{1-\tau}^2/pdb^2),$$

where int(a) denotes the smallest integer greater than or equal to a.

**Step 2.** Simulate  $B_0$  bootstrap estimates  $\{\hat{\theta}_b^* : b = 1, ..., B_0\}$  and compute  $\hat{\gamma}_{2B_0}$  as defined in (2.6) with B replaced by  $B_0$ .

**Step 3.** Take the desired number of bootstrap repetitions,  $B^*$ , to equal  $B^* = \max\{B_1, B_0\}$ , where

(2.16) 
$$B_1 = \operatorname{int}(2, 500\chi_{1-\tau}^2 (2 + \hat{\gamma}_{2B_0})/pdb^2).$$

If  $\hat{\gamma}_{2B_0} \leq 0$ , then  $B^* = B_0$  and one computes  $\widehat{se}_{B^*}$  using the  $B_0$  bootstrap estimates  $\{\hat{\theta}_b^* : b = 1, ..., B_0\}$  calculated in Step 2. If  $\hat{\gamma}_{2B_0} > 0$ , one has to compute  $B_1 - B_0$  additional bootstrap estimates  $\{\hat{\theta}_b^* : b = B_0 + 1, ..., B_1\}$  before computing  $\widehat{se}_{B^*}$ .

Using the three-step method above, as  $pdb \to 0$  or  $\tau \to 0$ , we have  $B_0 \to \infty$ ,  $\hat{\gamma}_{2B_0} \to \gamma_2$  in probability and almost surely,  $B_1 \to \infty$  provided  $\gamma_2 > -2$ , and  $B_0 \leq B^* \to \infty$ . The justification of the above method is that as  $pdb \to 0$ , we have  $B_1 \to \infty$  and

(2.17) 
$$P^*\left(100\frac{|\widehat{se}_{B_1} - \widehat{se}_{\infty}|}{\widehat{se}_{\infty}} \le pdb\right) \to 1 - \tau$$

provided  $\gamma_2 > -2$ . We stress that  $B_1$  depends on pdb in (2.17) via (2.16). Equation (2.17) implies that the three-step method attains precisely the specified accuracy asymptotically using "small pdb" asymptotics when  $\gamma_2 \ge 0$ . Of course, if  $\gamma_2 < 0$ , then  $B^* = B_0 > B_1$  with probability that goes to one as  $pdb \to 0$  and the accuracy of  $\widehat{se}_{B^*}$  for approximating  $\widehat{se}_{\infty}$  exceeds that of  $(pdb, \tau)$ . (This is a consequence of the fact that it would be silly to throw away the extra  $B_0 - B_1$  bootstrap estimates that have already been calculated in Step 2.) Because one normally specifies a small value of pdb, the asymptotic result (2.17) should be indicative of the relevant non-zero pdbbehavior of the three-step method. The simulation results of Sections 2.4 and 2.6 are designed to examine this. We note that the asymptotics used here are completely analogous to large sample size asymptotics with pdb driving  $B_1$  to infinity as  $pdb \to 0$ and  $B_1$  playing the role of the sample size.

When  $\tau = .05$ , equations (2.15) and (2.16) become

(2.18) 
$$B_0 = \operatorname{int}(19, 200/pdb^2)$$
 and  $B_1 = \operatorname{int}(9, 600(2 + \hat{\gamma}_{2B_0})/pdb^2)$ .

For illustrative purposes, Table 2 provides values  $B_1$  that correspond to several values of  $\hat{\gamma}_{2B_0}$  and pdb, with  $\tau = .05$ . The values of pdb considered are 20 (moderately accurate), 10 (accurate), and 5 (very accurate). Table 2 indicates that the necessary  $B_1$  values increase very quickly as the desired level of accuracy increases.

The three-step method discussed above is based on a scalar parameter  $\theta_0$ . In most applications, however, one has a vector of unknown parameters. In this case, one can apply the three-step method to several parameters of interest, or all the parameters in the model, to obtain  $B_1^*, ..., B_{\omega}^*$ , say, when considering  $\omega$  parameters, and then take  $B^*$  to equal the maximum of these values. Then,  $B^*$  is the number of bootstrap repetitions needed to obtain the desired accuracy for all of the  $\omega$  bootstrap standard error estimates (where accuracy is defined as above parameter by parameter).

#### 2.4. Monte Carlo Simulations

In this section we evaluate the performance of the three-step method introduced in Section 2.3. The proposed method is justified by the limit result of (2.17). We wish to see whether this limit result is indicative of finite sample behavior for a range of values of pdb and  $\tau$  in a standard econometric model. More specifically, given several  $(pdb, \tau)$  combinations, we want to see how close  $P^*(100|\widehat{se}_{B_1} - \widehat{se}_{\infty}|/\widehat{se}_{\infty} \leq pdb)$  is to  $1 - \tau$ .

Note that we focus initially on  $B_1$  rather than  $B^*$  because, for  $B_1$ , equation (2.17) implies that  $P^*(100|\widehat{se}_{B_1} - \widehat{se}_{\infty}|/\widehat{se}_{\infty} \leq pdb)$  should be approximately equal to  $1 - \tau$ , whereas for  $B^*$  equation (2.17) only implies the less precise result that  $P^*(100|\widehat{se}_{B^*} - \widehat{se}_{\infty}|/\widehat{se}_{\infty} \leq pdb)$  should be approximately greater than or equal to  $1 - \tau$ . Of course, our interest ultimately is in the performance of  $B^*$ .

The model we consider is the linear regression model

(2.19) 
$$y_i = x'_i \beta + u_i \text{ for } i = 1, ..., n,$$

where n = 25,  $X_i = (y_i, x'_i)'$  are iid over i = 1, ..., n,  $x_i = (1, x_{1i}, ..., x_{5i})' \in \mathbb{R}^6$ ,  $(x_{1i}, ..., x_{5i})$  are mutually independent normal random variables,  $x_i$  is independent of  $u_i$ , and  $Eu_i = 0$ . The simulation results are invariant with respect to the means and variances of  $(x_{1i}, ..., x_{5i})$ , the variance of  $u_i$ , and the value of the regression parameter  $\beta$ , so we need not be specific as to their values. For reasons discussed below, we consider three error distributions: standard normal (denoted N(0, 1)), t with five degrees of freedom (denoted  $t_5$ ), and chi-squared with five degrees of freedom shifted to have mean zero (denoted  $\chi_5^2$ ).

We estimate  $\beta$  by least squares (LS). We focus attention on bootstrap standard error estimates for the LS estimator of the first slope coefficient. Thus, the parameter  $\theta$  of Sections 2.1–2.3 is  $\beta_2$ , the second element of  $\beta$ .

The LS estimator of  $\theta$  is a linear combination of the errors  $\{u_i : i \leq n\}$ . Thus, for normal errors, the coefficient of excess kurtosis of the LS estimator of  $\theta$  is zero. The crucial parameter  $\gamma_2$ , however, is the coefficient of excess kurtosis of the (discrete) *bootstrap* distribution of the LS estimator of  $\theta$ . In general, the parameter  $\gamma_2$  depends on the sample and need not equal zero. Nevertheless, the value of  $\gamma_2$  will tend to be close to zero for normal errors for most samples, because the bootstrap distribution mimics the true distribution of the LS estimator. Correspondingly, for fat-tailed error distributions, the value of  $\gamma_2$  will tend to be large for most samples.

To obtain samples for which  $\gamma_2$  is close to zero, we consider normal errors. To obtain samples with larger values of  $\gamma_2$ , we consider the fat-tailed error distributions  $t_5$  and  $\chi_5^2$ . The  $t_5$  and  $\chi_5^2$  distributions have similar tail behavior and generate samples with similar values of  $\gamma_2$ . The  $t_5$  and normal distributions are symmetric, whereas the  $\chi_5^2$  distribution is highly skewed. The results for the  $\chi_5^2$  error distribution are used to determine whether skewness of the error distribution has an impact in finite samples on the performance of our three-step procedure for determining *B*. The results of Section 2.2 establish that skewness has no effect asymptotically.

We simulate 20 different samples from each error distribution because the value of  $\gamma_2$  varies with the sample. For each of the 20 samples drawn (for a given distribution

of  $u_i$ ), we compute the LS estimate  $\hat{\theta}$  and the ideal bootstrap standard error estimate  $\hat{se}_{\infty}$  defined in (2.2). We accomplish the latter by employing 250,000 bootstrap repetitions (each of sample size 25). We explicitly assume that 250,000 is close enough to infinity to accurately obtain  $\hat{se}_{\infty}$ .

Next, we run 2,500 Monte Carlo repetitions for each of the 20 samples, for a total of 50,000 repetitions. In each Monte Carlo repetition, we compute  $\widehat{se}_{B_1}$  and  $\widehat{se}_{B^*}$  for the LS estimate of the first slope coefficient following the three-step procedure outlined in Section 2.3. These calculations are made for several combinations of *pdb* (viz., 20%, 10%, and 5%) and  $1 - \tau$  (viz., .90, .95, and .975). For each repetition and each (*pdb*,  $\tau$ ) combination, we determine whether or not the estimate  $\widehat{se}_{B_1}$  satisfies

(2.20) 
$$100 \frac{|\widehat{se}_{B_1} - \widehat{se}_{\infty}|}{\widehat{se}_{\infty}} < pdb.$$

We call the fraction of times that this condition is satisfied, out of the 2,500 repetitions, the *empirical level* based on  $B_1$  bootstrap repetitions. The empirical level based on  $B^*$  bootstrap repetitions is defined analogously. For each  $(pdb, \tau)$  combination and each sample, we compute the empirical levels based on  $B_1$  and  $B^*$  bootstrap repetitions. The three-step method of Section 2.3 is considered to perform well if the empirical level based on  $B_1$  bootstrap repetitions is close to  $1 - \tau$ , or if the empirical level based on  $B^*$  bootstrap repetitions is close to, or greater than,  $1 - \tau$ .

The results from this set of experiments are reported in Table 3 for the N(0, 1)and  $t_5$  error distributions. The numbers reported in Table 3 are averages over the 20 samples. (For example, Med is the average median over the 20 samples.) Results for the  $\chi_5^2$  error distribution are almost the same as those for the  $t_5$ . In consequence, we do not report the  $\chi_5^2$  results. They indicate that asymmetry of the errors is not an important factor for the performance of the three-step method.

Table 3(A) shows that the empirical levels are very close to their asymptotic counterparts for the experiment with the N(0, 1) error distribution. This is true even though the bootstrap distribution of the LS estimate with only 25 observations in the sample can be far away from its asymptotic normal distribution. Note that the empirical levels for the more stringent bounds (i.e., smaller *pdb*'s) and higher probabilities (i.e., higher  $1 - \tau$ 's) are closer to the asymptotic levels. The reason is that the asymptotic approximation improves as  $B_1$ , or  $B^*$ , increases. Smaller *pdb* values and/or larger  $1 - \tau$  values lead to larger  $B_1$  and  $B^*$  values and, hence, better performance.

The average of the  $\gamma_2$  values over the 20 samples used in Table 3(A) (computed using 250,000 bootstrap repetitions for each sample) is .37. The mean (over 2,500 simulation repetitions) of the estimator  $\hat{\gamma}_{2B_0}$  averaged over the 20 samples, as reported in Table 3(A), is markedly lower than .37 when  $B_0$  is small (or equivalently, when *pdb* is large). This downward bias of  $\hat{\gamma}_{2B_0}$  leads to  $B_1$  and  $B^*$  values that are smaller than desired. In turn, this leads to empirical levels based on  $B_1$  and  $B^*$ bootstrap repetitions that are less than  $1 - \tau$  when  $B_0$  is small. For larger values of  $B_0$  (which occur with smaller *pdb* values), this bias vanishes and the empirical levels are closer to  $1 - \tau$ . The problem of underestimating  $\gamma_2$  stems from the fact that neither the numerator nor the denominator of the estimator  $\hat{\gamma}_{2B_0}$  in (2.6) is an unbiased estimator of its population counterpart, although both are consistent estimators.

Note that there is significant variation in the values of  $B_1$  over the various  $(pdb, \tau)$  combinations in Table 3(A). The mean values of  $B_1$  range between 37 and 11,257. The corresponding values for  $B^*$  are very similar, because  $\gamma_2 > 0$  for all 20 samples,  $\hat{\gamma}_{2B_0}$  is positive or close to zero for the vast majority of repetitions, and  $B^* = B_1$  whenever  $\hat{\gamma}_{2B_0} > 0$ . If one is satisfied with a modest percentage deviation (e.g., pdb = 10%), then the required number of bootstrap repetitions is not very large. On the other hand, if one sets a very stringent percentage deviation (e.g., pdb = 5%) and a very high probability (e.g.,  $1 - \tau = .975$ ), then the number of bootstrap repetitions needed to achieve this level of accuracy is large.

Table 3(B) presents the results based on  $t_5$  errors. The average value of  $\gamma_2$  over the 20 samples with  $t_5$  errors is 1.26, which is noticeably larger than the value of .37 for normal errors. In Table 3(B), the empirical levels based on  $B_1$  and  $B^*$  bootstrap repetitions are lower than  $1 - \tau$  and lower than their values in Table 3(A). Nevertheless, the same basic pattern is observed as in Table 3(A). That is, the difference between the empirical levels and  $1-\tau$  are largest when  $B_0$  is small, which corresponds to *pdb* being large. When  $B_0$  is small,  $\hat{\gamma}_{2B_0}$  is markedly downward biased and its bias is greater in magnitude than in Table 3(A). This causes  $B_1$  and  $B^*$  to be smaller than desired by a greater magnitude than in Table 3(A).

Overall, the empirical level results of Table 3(B) are not as good as those of Table 3(A). Nevertheless, the three-step method still performs quite well with  $t_5$  errors. The largest deviation of an empirical level based on  $B_1$  repetitions from its asymptotic counterpart is .052 and for all other  $(pdb, \tau)$  combinations the deviations are less than half as large. Furthermore, the deviations based on  $B^*$  are smaller than those based on  $B_1$ .

#### 2.5. A Bootstrap Bias-corrected Estimator of $\gamma_2$

The simulation results of Section 2.4 suggest that the performance of the threestep method of Section 2.3 could be improved, especially when  $\gamma_2$  is large, if a lessbiased estimator of  $\gamma_2$  than  $\hat{\gamma}_{2B_0}$  is employed. In this section, we specify such an estimator.

The iid sample of  $B_0$  bootstrap estimates of  $\theta_0$  in Step 2 of the three-step method of Section 2.3 is  $\Theta^* = (\hat{\theta}_1^*, ..., \hat{\theta}_{B_0}^*)$ . By definition,  $\gamma_2$  is the coefficient of excess kurtosis of the distribution of  $\hat{\theta}_b^*$  for any  $b = 1, ..., B_0$ . For present purposes, we think of  $(\hat{\theta}_1^*, ..., \hat{\theta}_{B_0}^*)$  as being an original sample and  $\hat{\gamma}_{2B_0}$  as being an estimator based on this sample that we want to bootstrap bias correct.

Let  $\widehat{G}$  denote the empirical distribution of  $(\widehat{\theta}_1^*, ..., \widehat{\theta}_{B_0}^*)$ . A bootstrap sample  $\Theta^{**} = (\widehat{\theta}_1^{**}, ..., \widehat{\theta}_{B_0}^{**})$  is a random sample of size  $B_0$  drawn from  $\widehat{G}$ . Let  $\widehat{\gamma}_2(\Theta^{**})$  denote the estimate  $\widehat{\gamma}_{2B_0}$  of  $\gamma_2$  computed using the bootstrap sample  $\Theta^{**}$ , rather than the

original sample  $\Theta^*$ . That is,

(2.21) 
$$\widehat{\gamma}_{2}(\Theta^{**}) = \frac{\frac{1}{B_{0}-1}\sum_{b=1}^{B_{0}}\left(\widehat{\theta}_{b}^{**} - \frac{1}{B_{0}}\sum_{j=1}^{B_{0}}\widehat{\theta}_{j}^{**}\right)^{4}}{\left(\frac{1}{B_{0}-1}\sum_{b=1}^{B_{0}}\left(\widehat{\theta}_{b}^{**} - \frac{1}{B_{0}}\sum_{j=1}^{B_{0}}\widehat{\theta}_{j}^{**}\right)^{2}\right)^{2}} - 3$$

Note that  $\widehat{\gamma}_{2B_0} = \widehat{\gamma}_2(\Theta^*)$ .

The "ideal" bootstrap estimate of the bias of  $\hat{\gamma}_{2B_0}$  for estimating  $\gamma_2$  is

(2.22) 
$$E^{**}\widehat{\gamma}_2(\Theta^{**}) - \widehat{\gamma}_{2B_0}$$

where  $E^{**}$  denotes expectation with respect to the randomness in  $\Theta^{**}$ , e.g., see Efron and Tibshirani (1993, eqn. (10.2), p. 125). The "ideal" bootstrap bias-corrected estimate  $\hat{\gamma}_{2B_0\infty}$  of  $\gamma_2$  is

(2.23) 
$$\hat{\gamma}_{2B_0\infty} = \hat{\gamma}_{2B_0} - (E^{**}\hat{\gamma}_2(\Theta^{**}) - \hat{\gamma}_{2B_0}) = 2\hat{\gamma}_{2B_0} - E^{**}\hat{\gamma}_2(\Theta^{**}).$$

Analytic calculation of the ideal bootstrap bias-corrected estimate of  $\gamma_2$  is intractable. Instead we approximate it using bootstrap simulations. Consider R independent bootstrap samples  $\{\Theta_r^{**} : r = 1, ..., R\}$ , where each bootstrap sample  $\Theta_r^{**} = (\hat{\theta}_{1r}^{**}, ..., \hat{\theta}_{B_0r}^{**})$  is a random sample of size  $B_0$  drawn from  $\hat{G}$ . The corresponding R bootstrap estimates of  $\gamma_2$  are  $\hat{\gamma}_2(\Theta_r^{**})$  for r = 1, ..., R. The bootstrap bias-corrected estimator  $\hat{\gamma}_{2B_0R}$  of  $\gamma_2$  for R bootstrap repetitions is

(2.24) 
$$\hat{\gamma}_{2B_0R} = 2\hat{\gamma}_{2B_0} - \frac{1}{R} \sum_{r=1}^R \hat{\gamma}_2(\Theta_r^{**}).$$

Now, the three-step method of Section 2.3 can be altered by (i) adding a step between Steps 2 and 3 in which  $\hat{\gamma}_{2B_0R}$  is calculated and (ii) replacing  $\hat{\gamma}_{2B_0}$  in Step 3 by  $\hat{\gamma}_{2B_0R}$ . The added step is summarized as follows:

Step 2(b). Simulate R bootstrap samples  $\{\Theta_r^{**} : r = 1, ..., R\}$ , compute R bootstrap estimates  $\{\widehat{\gamma}_2(\Theta_r^{**}) : r = 1, ..., R\}$  from these samples using (2.21), and compute  $\widehat{\gamma}_{2B_0R}$  from these bootstrap estimates and  $\widehat{\gamma}_{2B_0}$  using (2.24).

We refer to the new procedure as the *bias-corrected three-step method* for determining B for bootstrap standard error estimates.

The computational requirements of Step 2(b) are quite modest. Step 2(b) requires that one simulate R bootstrap samples and calculate the simple closed form expressions for  $\hat{\gamma}_2(\Theta_r^{**})$  for r = 1, ..., R. For example, when  $B_0$  is 192 (which corresponds to  $(pdb, \tau) = (10, .05)$ ) and R = 400, the computational time is only about four seconds using a Sun Sparc-20 computer. Note that the computational requirements of Step 2(b) are the same no matter how difficult the computation of  $\hat{\theta}$  is and no matter how large the original sample size n is. Thus, if a single bootstrap estimate of  $\hat{\theta}$  takes several minutes or several hours to compute, the time required to carry out Step 2(b) is a small fraction of the total computational time.

# 2.6. Monte Carlo Simulations for the Bias-corrected Three-step Method

Here we evaluate the performance of the bias-corrected three-step method of Section 2.5 via Monte Carlo simulation. Table 4 reports simulation results for the bias-corrected three-step method of determining B for the linear regression model of Section 2.4 with  $t_5$  errors. That is, the results of Table 4 are analogous to those of Table 3(B) except that the three-step method is replaced by the bias-corrected threestep method. We only consider the  $t_5$  errors because they yield the worst results of the three error distributions considered in Section 2.4. The number of repetitions, R, used in the bootstrap bias correction is taken to be 407. This number is chosen, somewhat arbitrarily, to be a value that yields a reasonable tradeoff between computational time for our simulation experiment and accuracy of the bootstrap bias-corrected estimator.

The results of Table 4 show a significant improvement in the performance of the three-step method when it is augmented by a bias-correction of  $\hat{\gamma}_{2B_0}$ . Most of the empirical levels are very close to their theoretical counterparts. The largest deviation is .025 and all the rest are about half as large or less. The results in the "Mean" column for  $\hat{\gamma}_{2B_0R}$  indicate that the bias of the bias-corrected estimator  $\hat{\gamma}_{2B_0R}$  is much smaller than that of  $\hat{\gamma}_{2B_0}$  in Table 3(B). The "Mean" numbers of bootstrap repetitions  $B_1$  are larger than in Table 3(B) due to the bias-correction, but the increase is not substantial. Analogous results hold for  $B^*$ .

We conclude that the bias-corrected three-step method yields a noticeable improvement over the three-step method in cases where  $\gamma_2$  is large. The computational cost of the bias-correction is minimal in absolute terms. Also, it is minimal relative to the total computational cost for calculating the bootstrap standard error estimate  $\widehat{se}_{B^*}$  whenever  $\widehat{\theta}$  is difficult to compute. Thus, we recommend use of the bias-corrected three-step method.

## **3.** Confidence Interval Results

In this section, we consider the problem of choosing the number of bootstrap repetitions B for percentile t confidence intervals. The first three subsections deal with symmetric two-sided confidence intervals and the last subsection extends the results to equal-tailed two-sided and one-sided confidence intervals.

#### **3.1.** Notation and Definitions

We begin by introducing some notation and definitions. As in the previous section, **X** denotes the observed data and  $\hat{\theta} = \hat{\theta}(\mathbf{X})$  is an estimator of an unknown scalar parameter  $\theta_0$ . We wish to construct a confidence interval for  $\theta_0$  of (approximate) confidence level  $100(1-\alpha)\%$  for some  $0 < \alpha < 1$ . Here we consider symmetric confidence intervals about  $\hat{\theta}$ . (Note that symmetric confidence intervals typically yield greater coverage accuracy as measured by higher order expansions than equal-tailed confidence intervals; see Hall (1992, Secs. 3.5 and 3.6).) We assume that the normalized estimator  $n^{\kappa}(\hat{\theta} - \theta_0)$  has an asymptotic normal distribution as  $n \to \infty$ . (Adjustments for the non-normal case are specified below.) In many cases of interest,  $\kappa = 1/2$ . We allow for  $\kappa \neq 1/2$ , however, to cover non-parametric estimators, such as nonparametric estimators of a density or regression function at a point. Let  $\hat{\sigma} = \hat{\sigma}(\mathbf{X})$  denote a consistent estimator of the asymptotic standard error of  $n^{\kappa}(\hat{\theta} - \theta_0)$ . Let

(3.1) 
$$T = n^{\kappa} (\hat{\theta} - \theta_0) / \hat{\sigma}$$

denote the t statistic for testing whether  $\theta = \theta_0$ . The t statistic has an asymptotic standard normal distribution when the true parameter is  $\theta_0$ .

The "theoretical" symmetric percentile t confidence interval of confidence level  $100(1-\alpha)\%$  is

(3.2) 
$$J_{SY} = [\widehat{\theta} - n^{-\kappa} \widehat{\sigma} k_{\alpha}, \widehat{\theta} + n^{-\kappa} \widehat{\sigma} k_{\alpha}],$$

where  $k_{\alpha}$  is the solution to

$$(3.3) P(|T| \le k_{\alpha}) = 1 - \alpha.$$

By definition of  $k_{\alpha}$ ,  $J_{SY}$  has exact confidence level  $100(1-\alpha)\%$ . In practice, however, one typically does not know  $k_{\alpha}$ . We consider using the bootstrap to estimate  $k_{\alpha}$ .

Define a bootstrap sample  $\mathbf{X}^* = (X_1^*, ..., X_n^*)'$  and a bootstrap estimator  $\widehat{\theta}^* = \widehat{\theta}(\mathbf{X}^*)$  as in the previous section. Let  $\widehat{\sigma}^* = \widehat{\sigma}(\mathbf{X}^*)$  denote the asymptotic standard error estimator based on the bootstrap sample  $\mathbf{X}^*$ . Let  $T^* = n^{\kappa}(\widehat{\theta}^* - \widehat{\theta})/\widehat{\sigma}^*$  denote the bootstrap t statistic based on  $\mathbf{X}^*$ . Let  $\widehat{k}_{\alpha,\infty}$  denote the *ideal bootstrap estimate* of  $k_{\alpha}$ . Because the bootstrap statistic  $T^*$  has a discrete distribution (at least for the nonparametric bootstrap), there typically is no value  $\widehat{k}_{\alpha,\infty}$  that satisfies the equation  $P^*(|T^*| \leq \widehat{k}_{\alpha,\infty}) = 1 - \alpha$  exactly, where  $P^*(\cdot)$  denotes probability with respect to the bootstrap sample  $\mathbf{X}^*$  conditional on the original sample  $\mathbf{X}$ . Thus, to be precise, we define  $\widehat{k}_{\alpha,\infty} = \inf\{k: P^*(|T^*| \leq k) \geq 1 - \alpha\}$ .

The ideal bootstrap symmetric percentile t confidence interval of approximate confidence level  $100(1-\alpha)\%$  is

(3.4) 
$$\widehat{J}_{SY,\infty} = [\widehat{\theta} - n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,\infty}, \widehat{\theta} + n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,\infty}].$$

Analytic calculation of the ideal bootstrap estimate  $k_{\alpha,\infty}$  of the critical point  $k_{\alpha}$  is usually intractable. Nevertheless, one can approximate  $\hat{k}_{\alpha,\infty}$  using bootstrap simulations.

As above, consider B iid bootstrap samples  $\{\mathbf{X}_b^* : b = 1, ..., B\}$ , each with the same distribution as  $\mathbf{X}^*$ , and the corresponding bootstrap statistics  $\widehat{\theta}_b^* (= \widehat{\theta}(\mathbf{X}_b^*))$ ,  $\widehat{\sigma}_b^* (= \widehat{\sigma}(\mathbf{X}_b^*))$ , and  $T_b^* = n^{\kappa}(\widehat{\theta}_b^* - \widehat{\theta})/\widehat{\sigma}_b^*$  for b = 1, ..., B. Let  $\{|T^*|_{B,b} : b = 1, ..., B\}$  denote the ordered sample of the absolute values of  $T_b^*$ .

Following Hall (1992, p. 307), we choose B not to be just any positive integer, but one that satisfies  $\nu/(B+1) = 1 - \alpha$  for some positive integer  $\nu$ . (This has advantages in terms of the unconditional coverage probability of the resultant confidence interval; see Hall (1992, p. 307).) Then, the bootstrap estimate of  $k_{\alpha}$  based on B bootstrap repetitions is defined to be

$$\widehat{k}_{\alpha,B} = |T^*|_{B,\nu}$$

That is,  $k_{\alpha,B}$  is the  $\nu$ -th order statistic of  $\{|T_b^*| : b = 1, ..., B\}$ . Furthermore, the bootstrap symmetric percentile t confidence interval of approximate confidence level  $100(1-\alpha)\%$  based on B bootstrap repetitions is

(3.6) 
$$\widehat{J}_{SY,B} = [\widehat{\theta} - n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,B}, \widehat{\theta} + n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,B}].$$

Note that B can be chosen as in the previous paragraph only if  $\alpha$  is rational. We assume therefore that

$$(3.7) \qquad \qquad \alpha = \alpha_1/\alpha_2$$

for some positive integers  $\alpha_1$  and  $\alpha_2$  (with no common integer divisors). Then,

(3.8) 
$$B = \alpha_2 a - 1 \text{ and } \nu = (\alpha_2 - \alpha_1)a$$

for some positive integer a. For example, if  $\alpha = .05$ , then  $\alpha_1 = 1$ ,  $\alpha_2 = 20$ , B = 20a-1, and  $\nu = 19a$  for some integer a > 0. That is, B = 19, 39, 59, etc. If  $\alpha = .10$ , then  $\alpha_1 = 1$ ,  $\alpha_2 = 10$ , B = 10a - 1, and  $\nu = 9a$  for some integer a > 0.

## 3.2. A Three-step Method for Determining the Number of Bootstrap Repetitions

In this section, we introduce a three-step method for determining B for the bootstrap confidence interval  $\hat{J}_{SY,B}$  defined above. Our main interest is determining Bsuch that  $\hat{J}_{SY,B}$  is close to the ideal bootstrap confidence interval  $\hat{J}_{SY,\infty}$ . A secondary interest is in the unconditional coverage probability of  $\hat{J}_{SY,B}$  (where "unconditional" refers to the randomness in both the data and the simulations).

Our primary interest is the former, because the simulated random variables are ancillary with respect to the parameter  $\theta_0$ . Hence, the principle of ancillarity or conditionality (e.g., see Kiefer (1982) and references therein) implies that we should seek a confidence interval that has confidence level that is (approximately)  $100(1 - \alpha)\%$ conditional on the simulation draws. To obtain such an interval, we need to choose Bto be sufficiently large that  $\hat{J}_{SY,B}$  is close to  $\hat{J}_{SY,\infty}$ . Otherwise, two researchers using the same data and the same statistical method could reach different conclusions due only to the use of different simulation draws.

We measure the closeness of  $\widehat{J}_{SY,B}$  to  $\widehat{J}_{SY,\infty}$  by comparing the endpoints of the two intervals. The percentage deviation of the endpoints of  $\widehat{J}_{SY,B}$  to the endpoints of  $\widehat{J}_{SY,\infty}$  is

(3.9) 
$$100\frac{|n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,B} - n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,\infty}|}{n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,\infty}} = 100\frac{|\widehat{k}_{\alpha,B} - \widehat{k}_{\alpha,\infty}|}{\widehat{k}_{\alpha,\infty}}.$$

We could also measure the closeness of  $\hat{J}_{SY,B}$  to  $\hat{J}_{SY,\infty}$  by comparing the lengths of the two intervals. This is a particularly appropriate measure in the present case because each interval is symmetric about the same value  $\hat{\theta}$ . Furthermore, the length of a two-sided confidence interval is of inherent interest because it directly reflects the precision of the interval estimate. Denote the length of a confidence interval J by L(J). We have

(3.10) 
$$L(\widehat{J}_{SY,B}) = 2n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,B} \text{ and } L(\widehat{J}_{SY,\infty}) = 2n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,\infty}.$$

The percentage deviation of  $L(J_{SY,B})$  to  $L(J_{SY,\infty})$  is

(3.11) 
$$100\frac{|L(\hat{J}_{SY,B}) - L(\hat{J}_{SY,\infty})|}{L(\hat{J}_{SY,\infty})} = 100\frac{|\hat{k}_{\alpha,B} - \hat{k}_{\alpha,\infty}|}{\hat{k}_{\alpha,\infty}}.$$

Thus, for the symmetric confidence interval, our measure of the closeness of  $\hat{J}_{SY,B}$  to  $\hat{J}_{SY,\infty}$ , based on the percentage deviation of the endpoints, is equivalent to a measure based on the percentage deviation of the length of the confidence interval. The former measure is applicable more generally, however, because in the case of one-sided confidence intervals the lengths of all confidence intervals are infinite.

As in the previous section, let  $1 - \tau$  denote a probability close to one, such as .95. Let *pdb* be a bound on the percentage deviation of the endpoints of  $\hat{J}_{SY,B}$  to the endpoints of  $\hat{J}_{SY,\infty}$ . We want to determine  $B = B(pdb, \tau)$  such that

(3.12) 
$$P^*\left(100\frac{|\widehat{k}_{\alpha,B}-\widehat{k}_{\alpha,\infty}|}{\widehat{k}_{\alpha,\infty}} \le pdb\right) = 1-\tau.$$

That is, we want to specify a method of determining B to obtain a desired level of accuracy pdb with probability (approximately) equal to  $1 - \tau$ .

We introduce a three-step method of doing so. The method relies on an estimator of the reciprocal of a density function at a point, which appears in the asymptotic distribution of the sample quantile  $\hat{k}_{\alpha,B}$ . For this, we use Siddiqui's (1960) estimator (analyzed by Bloch and Gastwirth (1968) and Hall and Sheather (1988)) with a plugin estimator of the bandwidth parameter that is chosen to maximize the higher order asymptotic coverage probability of the resultant confidence interval, as calculated by Hall and Sheather (1988). To reduce the noise of the plug-in estimator, we take advantage of the fact that we know the asymptotic value of the density and use it to generate our estimators of the unknown coefficients in the plug-in formula.

The three-step method is defined as follows:

Step 1. Compute a preliminary number of bootstrap repetitions  $B_0$  via

(3.13) 
$$B_{0} = \alpha_{2}a_{0} - 1, \text{ where}$$
$$a_{0} = \operatorname{int}\left(\frac{2,500\alpha(1-\alpha)\chi_{1-\tau}^{2}}{z_{1-\alpha/2}^{2}\phi^{2}(z_{1-\alpha/2})pdb^{2}\alpha_{2}}\right) \text{ and } \alpha = \alpha_{1}/\alpha_{2}.$$

Step 2. Simulate  $B_0$  bootstrap t statistics  $\{T_b^* : b = 1, ..., B_0\}$ ; order the absolute values of the bootstrap t statistics, which are denoted  $\{|T^*|_{B_0,b} : b = 1, ..., B_0\}$ ; and calculate  $\nu_0 = (\alpha_2 - \alpha_1)a_0$ ,  $\hat{m} = \operatorname{int}(c_{\alpha}B_0^{2/3})$ ,  $\hat{k}_{\alpha,B_0} = |T^*|_{B_0,\nu_0}$ ,  $|T^*|_{B_0,\nu_0-\widehat{m}}$ , and  $|T^*|_{B_0,\nu_0+\widehat{m}}$ , where

(3.14) 
$$c_{\alpha} = \left(\frac{6z_{1-\alpha/2}^{2}\phi^{2}(z_{1-\alpha/2})}{2z_{1-\alpha/2}^{2}+1}\right)^{1/3}$$

**Step 3.** Take the desired number of bootstrap repetitions,  $B^*$ , to equal  $B^* = \max\{B_0, B_1\}$ , where

$$B_{1} = \alpha_{2}a_{1} - 1 \text{ and}$$

$$(3.15) \ a_{1} = \operatorname{int}\left(\frac{10,000\alpha(1-\alpha)\chi_{1-\tau}^{2}}{\hat{k}_{\alpha,B_{0}}^{2}pdb^{2}\alpha_{2}}\left(\frac{B_{0}}{2\widehat{m}}\right)^{2}\left(|T^{*}|_{B_{0},\nu_{0}+\widehat{m}} - |T^{*}|_{B_{0},\nu_{0}-\widehat{m}}\right)^{2}\right).$$

Note that  $z_{1-\alpha/2}$  denotes the  $(1-\alpha/2)$ -th quantile of a standard normal distribution,  $\phi(\cdot)$  denotes the standard normal density function, and  $\chi^2_{1-\tau}$  denotes the  $(1-\tau)$ -th quantile of a chi-square distribution with one degree of freedom.

Having determined  $B^*$ , one simulates  $B^* - B_0 (\geq 0)$  additional bootstrap t statistics  $\{T_b^* : b = B_0 + 1, ..., B^*\}$  and orders the absolute values of the  $B^*$  bootstrap t statistics, which are denoted  $\{|T^*|_{B^*,b} : b = 1, ..., B^*\}$ . The desired cutoff value,  $\nu^*$ , and the desired critical point,  $\hat{k}_{\alpha,B^*}$ , are then given by

(3.16) 
$$\nu^* = \max\{\nu_0, \nu_1\}, \ \nu_1 = (\alpha_2 - \alpha_1)a_1, \text{ and} \\ \widehat{k}_{\alpha, B^*} = |T^*|_{B^*, \nu^*}.$$

The resulting bootstrap confidence interval, based on  $B^*$  bootstrap repetitions, is equal to

(3.17) 
$$\widehat{J}_{SY,B^*} = [\widehat{\theta} - n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,B^*}, \widehat{\theta} + n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,B^*}].$$

In Table 5, we provide the values of  $B_0$ ,  $a_0$ ,  $\nu_0$ ,  $c_\alpha$ , and  $\hat{m}$  that correspond to common values of  $\alpha$ ,  $\tau$ , and *pdb*. Table 5 indicates that  $B_0$  increases significantly as  $\tau$  decreases and even more so as *pdb* decreases. For example, the combination  $(\alpha, pdb, \tau) = (.05, 15, .10)$  requires  $B_0 = 119$ . In contrast,  $(\alpha, pdb, \tau) = (.05, 5, .01)$ requires  $B_0 = 2399$ . In addition,  $B_0$  increases as  $\alpha$  decreases. The pattern of variation of  $\nu_0$  and  $\hat{m}$  is the same as that of  $B_0$  except that  $\hat{m}$  decreases as  $\alpha$  decreases. This occurs because the height of the "density" that is being estimated decreases as  $\alpha$ decreases and it decreases quickly enough to offset the increase in  $B_0$ .

To assess the magnitude of the  $B_1$  values generated by our three-step method, we carried out the following procedure: (i) we assumed that the bootstrap distribution of  $T^*$  was some specified distribution, viz., N(0,1),  $t_{10}$ ,  $t_5$ , or  $\chi_5^2$ ; (ii) for each  $(\alpha, pdb, \tau)$  combination in Table 5, we took  $B_0$  draws from the specified distribution and calculated  $B_1$  according to Steps 2 and 3 of the three-step procedure; (iii) we repeated the simulation of part (ii) 5000 times; and (iv) we computed the median, mean, minimum, maximum, and standard deviation of the 5000 values of  $B_1$ . For brevity, we do not provide tables of the results, but just summarize them briefly.

The use of the N(0,1) distribution illustrates typical  $B_1$  values when the bootstrap distribution of  $T^*$  equals (or is close to) its asymptotic distribution, which is N(0,1). In this case, we found that the ratio of the median  $B_1$  value to  $B_0$  was in the range 1.0-1.1 for most  $(\alpha, pdb, \tau)$  combinations with  $\alpha = .05$  or .10. Thus, in this case, the initial choice of  $B_0$  is an accurate starting value to determine  $B_1$ . When we used the  $t_{10}$ ,  $t_5$ , and  $\chi_5^2$  distributions, which differ increasingly from the N(0,1) distribution, we found that the ratio of the median  $B_1$  value to  $B_0$  increased significantly. For example, for the  $t_5$  distribution, which has very thick tails, the ratio was in the range 2.3–3.5 for  $\alpha = .05$  and 1.8–2.1 for  $\alpha = .10$ . Thus, when the bootstrap distribution is far from its asymptotic normal distribution noticeably more bootstrap repetitions  $B_1$  are needed than  $B_0$ . This illustrates the importance of using a three-step method, which takes account of the actual bootstrap distribution of  $T^*$  in Steps 2 and 3 and does not rely on its asymptotic distribution.

To illustrate the magnitude of  $B_1$  for what may be a typical scenario, we consider the  $t_{10}$  distribution and specify  $(\alpha, pdb, \tau)$  to equal (.05, 10, .05). In this case, the median  $B_1$  value is 699. This is larger than the number of bootstrap repetitions often used in the econometrics literature.

As in the previous section, the three-step method introduced here is based on a scalar parameter  $\theta_0$ . When one is interested in separate confidence intervals for several parameters, say  $\omega$  parameters, one can apply the three-step method for each of the parameters to obtain  $B^*_{(1)}$ ,  $B^*_{(2)}$ , ...,  $B^*_{(\omega)}$  and take  $B^*$  to equal the maximum of these values.

If the asymptotic distribution of T is not normal, then  $a_0$  and  $c_{\alpha}$  in Steps 1 and 2 above have to be adjusted. Suppose the asymptotic distribution of |T| is F, the  $(1 - \alpha)$ -th quantile of F is  $q_{1-\alpha}$ , and F has a density  $f(\cdot)$  with respect to Lebesgue measure at  $q_{1-\alpha}$ , then  $a_0 = \operatorname{int}((10,000\alpha(1-\alpha)\chi_{1-\tau}^2)/(q_{1-\alpha}^2f^2(q_{1-\alpha})pdb^2\alpha_2))$  and  $c_{\alpha}$  is defined as in (5.31) of the Appendix of Proofs. If F depends on unknown parameters, then consistent estimates of these parameters can be used to provide estimates of  $q_{1-\alpha}$  and  $f(q_{1-\alpha})$  for use in the definitions of  $a_0$  and  $c_{\alpha}$ .

#### **3.3.** Asymptotic Justification of the Three-step Method

We now discuss the justification of the three-step method introduced above. The three-step method relies on the fact that  $\hat{k}_{\alpha,B}$  is a sample quantile based on an iid sample of random variables each with distribution given by the bootstrap distribution of  $|T^*|$ . If the bootstrap distribution of  $|T^*|$  was absolutely continuous at  $\hat{k}_{\alpha,\infty}$ , then  $B^{1/2}(\hat{k}_{\alpha,B}-\hat{k}_{\alpha,\infty})$  would be asymptotically normally distributed as  $B \to \infty$  for fixed n with asymptotic variance given by  $\alpha(1-\alpha)/f^2(\hat{k}_{\alpha,\infty})$ , where  $f(\cdot)$  denotes the density of  $|T^*|$ . (Here and below, we condition on the data and the asymptotics are based on the randomness of the simulations alone.)

But, the bootstrap distribution of  $|T^*|$  is a discrete distribution (at least for the nonparametric bootstrap, which is based on the empirical distribution). In consequence, the asymptotic distribution of  $B^{1/2}(\hat{k}_{\alpha,B} - \hat{k}_{\alpha,\infty})$  as  $B \to \infty$  for fixed n is a pointmass at zero for all  $\alpha$  values except for those in a set of Lebesgue measure zero. (The latter set is the set of values that the distribution function of  $|T^*|$  takes on at its points of support.)

Although  $|T^*|$  has a discrete distribution in the case of the nonparametric iid bootstrap, its distribution is very nearly continuous even for small values of n. The largest probability  $\pi_n$  of any of its atoms is very small:  $\pi_n = n!/n^n \sim (2\pi n)^{1/2} e^{-n}$ provided the original sample **X** consists of distinct vectors and distinct bootstrap samples  $\mathbf{X}^*$  give rise to distinct values of  $|T^*|$  (as is typically the case); see Hall (1992, Appendix I). This suggests that we should consider asymptotics as  $n \to \infty$ , as well as  $B \to \infty$ , in order to account for the essentially continuous nature of the distribution of  $|T^*|$ . If we do so, then  $B^{1/2}(\hat{k}_{\alpha,B} - \hat{k}_{\alpha,\infty})$  has a nondegenerate asymptotic distribution with asymptotic variance that depends on the value of a density at a point, just as in the case where the distribution of  $|T^*|$  is continuous. This is what we do. It is in accord with Hall's (1992, p. 285) view that "for many practical purposes the bootstrap distribution of a statistic may be regarded as continuous."

We note that the (potential) discreteness of  $T^*$  significantly increases the complexity of the asymptotic justification of the three-step method given below and its proof.

We now introduce a strengthening of the assumption of asymptotic normality of the t statistic T that is needed for the asymptotic justification of the three-step method. We assume: For some  $\xi > 0$  and all sequences of constants  $\{x_n : n \ge 1\}$  for which  $x_n \to z_{1-\alpha/2}$ , we have

(3.18) 
$$P(|T| \le x_n) = P(|Z| \le x_n) + O(n^{-\xi}) \text{ as } n \to \infty \text{ and}$$
$$P^*(|T^*| \le x_n) = P(|Z| \le x_n) + O(n^{-\xi}) \text{ as } n \to \infty,$$

where  $Z \sim N(0, 1)$ . (The assumption on  $|T^*|$  is assumed to hold with probability one with respect to the randomness in the data, i.e., with respect to  $P(\cdot)$ .)

Assumption (3.18) holds whenever the t statistic and the bootstrap t statistic have one-term Edgeworth expansions. This occurs in any context in which the bootstrap delivers higher order improvements in the coverage probability of confidence intervals based on T. The literature on the bootstrap is full of results that establish (3.18) for different t statistics. For example, see Hall (1992, Sec. 3.3 and Ch. 5), Hall and Horowitz (1996), and references therein. When  $\kappa = 1/2$  and  $\hat{\sigma}$  is an  $n^{1/2}$ -consistent estimator of the asymptotic standard error of  $\hat{\theta}$ , then (3.18) typically holds with  $\xi = 1$ . (The  $n^{-1/2}$  terms in the Edgeworth expansions of T and T<sup>\*</sup> typically are even functions of  $x_n$  and hence cancel out in the Edgeworth expansions of |T| and  $|T^*|$ , leaving the order of the first terms of the latter equal to  $n^{-1}$ .) One example where (3.18) holds with  $\kappa = 1/2$  and  $\xi < 1$  is when  $\hat{\theta}$  is a sample quantile and  $\hat{\sigma}$  is an estimator of its asymptotic standard error (which is not  $n^{1/2}$ -consistent because it involves the nonparametric estimation of a density at a point); see Hall and Sheather (1988) and Hall and Martin (1991). When  $\kappa < 1/2$ , as occurs with nonparametric estimators  $\theta$ , then (3.18) typically holds with  $\xi < 1$ ; see Hall (1992, Ch. 4) and references therein.

The discussion above considers letting  $B \to \infty$ . This is not really appropriate because we want B to be determined endogenously by the three-step method. Rather, we consider asymptotics in which the accuracy measure  $pdb \to 0$  and this, in turn, forces  $B \to \infty$ . Thus, the asymptotic justification of the three-step method of choosing  $B^*$  is in terms of the limit as both  $pdb \to 0$  and  $n \to \infty$ .

We assume that  $pdb \rightarrow 0$  sufficiently slowly that

$$(3.19) pdb \times n^{\xi} \to \infty \text{ as } n \to \infty,$$

where  $\xi$  is as in (3.18).

The asymptotic justification of the three-step method is that

$$P^*\left(100\frac{|\hat{k}_{\alpha,B_1} - \hat{k}_{\alpha,\infty}|}{\hat{k}_{\alpha,\infty}} \le pdb\right) \to 1 - \tau \text{ as } pdb \to 0 \text{ and } n \to \infty, \text{ where}$$

$$(3.20) \qquad \hat{k}_{\alpha,B_1} = |T^*|_{B_1,\nu_1} \text{ and } \hat{J}_{SY,B_1} = [\hat{\theta} - n^{-\kappa}\hat{\sigma}\hat{k}_{\alpha,B_1}, \hat{\theta} + n^{-\kappa}\hat{\sigma}\hat{k}_{\alpha,B_1}].$$

As above, the probability  $P^*(\cdot)$  denotes probability with respect to the simulation randomness conditional on the infinite sequence of data vectors. Under the assumptions above, this conditional result holds with probability one with respect to the randomness in the data. The proof of (3.20) is given in the Appendix of Proofs.

Equation (3.20) implies that the three-step method attains precisely the desired level of accuracy using "small *pdb* and large *n*" asymptotics when  $B^* = B_1 > B_0$ . When  $B^* = B_0 > B_1$ , then the accuracy of the three-step method exceeds the desired level of accuracy. (This is a consequence of the fact that it would be silly to throw away the extra  $B_0 - B_1$  bootstrap estimates in Step 3 that have already been calculated in Step 2.)

#### 3.4. Monte Carlo Simulations for Symmetric Confidence Intervals

In this section, we evaluate the performance of the three-step method introduced in Section 3.2. As in Section 2.4, the purpose of the Monte Carlo experiments reported here is to evaluate whether or not the limit result of (3.20) is indicative of finite sample behavior for a range of values of  $\alpha$ , pdb, and  $\tau$ . That is, we want to see how close  $P^*(100 \mid \hat{k}_{\alpha,B_1} - \hat{k}_{\alpha,\infty} \mid /\hat{k}_{\alpha,\infty} \leq pdb)$  is to  $1 - \tau$ .

As in Section 2.4, we focus our attention on  $B_1$  rather than on  $B^*$ , because equation (3.20) implies that for  $B_1$ ,  $P^*(100 | \hat{k}_{\alpha,B_1} - \hat{k}_{\alpha,\infty} | /\hat{k}_{\alpha,\infty} \leq pdb)$  should be approximately equal to  $1 - \tau$ , whereas for  $B^*$  equation (3.20) only implies that  $P^*(100 | \hat{k}_{\alpha,B^*} - \hat{k}_{\alpha,\infty} | /\hat{k}_{\alpha,\infty} \leq pdb)$  should be approximately greater than, or equal to,  $1 - \tau$ . Nevertheless, as above, the ultimate interest is in the performance of the three-step method based on  $B^*$ .

We consider the same linear regression model as in (2.19) with the same three error distributions : N(0,1),  $t_5$ , and  $\chi_5^2$ . Again, we estimate  $\beta$  by LS and focus our attention on the first slope coefficient. Thus, the parameter  $\theta$  of Sections 3.1–3.3 is  $\beta_2$  (the second element of  $\beta$ ). The standard error estimator  $\hat{\sigma}$  is defined using the standard formula. That is,  $\hat{\sigma}^2$  is the (2,2) term of the matrix  $\hat{\sigma}_u^2(\sum_{i=1,\dots,25} x_i x_i'/25)^{-1}$ , where  $\hat{\sigma}_u^2 = e'e/(n-6)$  and e is the vector of LS residuals.

We simulate 250 different samples from each of the three error distributions. For each of the 250 samples, we compute the LS estimate  $\hat{\theta}$  and the standard error estimate  $\hat{\sigma}$ . Then, we simulate  $\hat{k}_{\alpha,\infty}$  using 250,000 bootstrap repetitions (each of size 25). As in Section 2.4, we explicitly assume that 250,000 is close enough to infinity to accurately obtain  $\hat{k}_{\alpha,\infty}$ . Given  $\hat{\theta}$ ,  $\hat{\sigma}$ , and  $\hat{k}_{\alpha,\infty}$ , we calculate the ideal symmetric confidence interval  $\hat{J}_{SY,\infty}$  defined in (3.4) for each of the 250 samples for each error distribution. Next, we run 2,000 Monte Carlo repetitions for each of the 250 samples for a total of 500,000 repetitions. In each Monte Carlo repetition, we compute  $\hat{J}_{SY,B_1}$ ,  $\hat{J}_{SY,B^*}$ ,  $\hat{k}_{\alpha,B_1}$ , and  $\hat{k}_{\alpha,B^*}$  using the three-step method of Section 3.2. We make this calculation for several combinations of  $\alpha$  (viz., .10 and .05), pdb (viz., 15%, 10%, and 5%), and  $1 - \tau$  (viz., .10 and .05). For each repetition and each  $(\alpha, pdb, \tau)$  combination, we check whether  $\hat{k}_{\alpha,B_1}$  satisfies

(3.21) 
$$100\frac{|\hat{k}_{\alpha,B_1} - \hat{k}_{\alpha,\infty}|}{\hat{k}_{\alpha,\infty}} \le pdb,$$

or equivalently, whether  $L(\widehat{J}_{SY,B_1})$  satisfies

(3.22) 
$$100 \frac{|L(\hat{J}_{SY,B_1}) - L(\hat{J}_{SY,\infty})|}{L(\hat{J}_{SY,\infty})} \le pdb.$$

We call the fraction of times this condition is satisfied, out of the 2,000 repetitions, the empirical level based on  $B_1$ . The empirical level based on  $B^*$  bootstrap repetitions is computed analogously. In addition, we compute the fraction of times that  $\theta$  falls within the constructed confidence interval  $\hat{J}_{SY,B_1}$ . We call this fraction the *empirical unconditional coverage probability*. The empirical unconditional coverage probability based on  $B^*$  bootstrap repetitions is defined analogously.

The three-step method of Section 3.2 is considered to perform well if the empirical levels based on  $B_1$  bootstrap repetitions are close to  $1 - \tau$ . Based on  $B^*$  bootstrap repetitions, the method is considered to perform well if the empirical levels are close to, or greater than,  $1 - \tau$ .

The results from this set of experiments are reported in Table 6 for the N(0, 1)and  $t_5$  error distributions. The numbers reported in this table are averages over the 250 samples. The results for the  $\chi_5^2$  error distribution are very similar to those given in Table 6(B) for the  $t_5$  error distribution in terms of both the empirical levels obtained and the number of bootstrap repetitions  $B_1$  needed. These results show that the high skewness of the  $\chi_5^2$  error distribution does not have any effect on the performance of the three-step method. For brevity, we do not report these results.

Table 6(A) shows that the empirical levels are somewhat higher than the corresponding  $1 - \tau$  values for the experiments with the N(0, 1) error distribution. Nevertheless, with low *pdb* (5), the empirical levels are quite close to their asymptotic counterparts.

Table 6(A) indicates that the performance of the three-step method is determined by the number of bootstrap repetitions  $B_1$ , or  $B^*$ , employed. The  $(\alpha, pdb, \tau)$  combinations that yield the best results are those that induce a relatively large number of bootstrap repetitions. Thus, the smaller the bound pdb, the closer are the empirical levels to their asymptotic counterparts, and the more so, the higher the  $1 - \tau$  value. For example, for the (.10, 5, .10) combination, the median  $B_1$  value is 1348, while for the combination (.10, 15, .10), it is only 230. As a result, the empirical level for the former case is .907, which is quite close to .900, while for the latter it is .942.

Also, the empirical levels are closer to their asymptotic counterparts for the confidence intervals with lower confidence level  $1 - \alpha$ . This occurs because it is more difficult to estimate the .95 quantile of  $|T^*|$  needed for a 95% confidence interval than to estimate the .90 quantile of  $|T^*|$  needed for a 90% confidence interval.

Table 6(B) reports the results from the Monte Carlo simulations with the  $t_5$  error distribution. The general picture revealed by Table 6(B) is very similar to that of Table 6(A). The empirical levels are comparable to those reported in Table 6(A). They are somewhat higher than their asymptotic counterparts. The most pronounced difference between the two sets of experiments is that for all  $(\alpha, pdb, \tau)$  combinations, the number of bootstrap repetitions  $B_1$  is somewhat larger for the experiment with the  $t_5$  error distribution, but not by much. This indicates that even with a relatively small sample size (25 observations) the bootstrap distribution of  $T^*$  with a fat-tailed  $t_5$  error distribution is not much different than with a N(0, 1) error distribution. Certainly, the bootstrap distribution of  $T^*$  based on  $t_5$  errors is far from being a  $t_5$ distribution itself.

We conclude that the three-step method does pretty well in attaining the desired accuracy of the bootstrap endpoints and confidence interval length in relation to their ideal bootstrap counterpoints. The three-step method is slightly conservative, because the accuracy obtained is slightly greater than the nominal accuracy.

Lastly, we consider the empirical unconditional coverage probabilities. In all cases, they are the same whether based on  $B_1$  or  $B^*$  bootstrap repetitions. In Table 6(A), they equal .908 or .909 for all cases where  $\alpha = .900$  and they equal .957 for all cases where  $\alpha = .950$ . In Table 6(B), they are in the range .900–.902 for all cases where  $\alpha = .900$  and they are in the range .951–.953 for all cases where  $\alpha = .950$ . Thus, the empirical unconditional coverage probabilities are extremely close to their asymptotic counterparts. This is consistent with Hall's (1986) result that one need not employ a large number of bootstrap repetitions in order to obtain good unconditional coverage probabilities. Nevertheless, our results show that in order to construct confidence intervals whose endpoints, length, and conditional coverage probability are close to that of the ideal bootstrap confidence interval, one does need to employ a relatively large number of bootstrap repetitions.

#### **3.5.** Equal-tailed and One-sided Confidence Intervals

We now develop three-step methods for choosing B for the case of equal-tailed and one-sided bootstrap percentile t confidence intervals. We take  $\mathbf{X}, \hat{\theta}, \theta_0, \hat{\sigma}, T, \mathbf{X}^*, \hat{\theta}^*, \hat{\sigma}^*, T^*, \text{ and } \{(\mathbf{X}_b^*, \hat{\theta}_b^*, T_b^*) : b = 1, ..., B\}$  as in Section 3.1. We assume that the normalized estimator  $n^{\kappa}(\hat{\theta} - \theta_0)$  has an asymptotic normal distribution as  $n \to \infty$ for some  $\kappa > 0$ . (Adjustments for the non-normal case are provided below.)

The "theoretical" equal-tailed and one-sided percentile t confidence intervals with exact confidence levels  $100(1-2\alpha)\%$  and  $100(1-\alpha)\%$ , respectively, are

(3.23) 
$$J_2 = [\widehat{\theta} - n^{-\kappa} \widehat{\sigma} q_{1-\alpha}, \widehat{\theta} - n^{-\kappa} \widehat{\sigma} q_{\alpha}] \text{ and } J_1 = [\widehat{\theta} - n^{-\kappa} \widehat{\sigma} q_{1-\alpha}, \infty),$$

where  $q_{\alpha}$  is the solution to  $P(T \leq q_{\alpha}) = \alpha$  for any  $\alpha \in (0, 1)$ .

We use the bootstrap to estimate the quantiles  $q_{\alpha}$  and  $q_{1-\alpha}$ . Let  $\hat{q}_{\alpha,\infty}$  denote the *ideal bootstrap estimate* of  $q_{\alpha}$ , i.e., the  $\alpha$ -th quantile of the distribution of  $T^*$ .

Again, to be precise, we define  $\hat{q}_{\alpha,\infty} = \inf\{q : P^*(T^* \leq q) \geq \alpha\}$ . The ideal bootstrap equal-tailed and one-sided percentile t confidence intervals of approximate confidence levels  $100(1-2\alpha)\%$  and  $100(1-\alpha)\%$ , respectively, are

(3.24) 
$$\widehat{J}_{2,\infty} = [\widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{1-\alpha,\infty}, \widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{\alpha,\infty}] \text{ and}$$
$$\widehat{J}_{1,\infty} = [\widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{1-\alpha,\infty}, \infty).$$

We approximate  $\hat{q}_{1-\alpha,\infty}$  and  $\hat{q}_{\alpha,\infty}$  using bootstrap simulations. Let  $\{T^*_{B,b} : b = 1, ..., B\}$  denote the ordered sample of  $\{T^*_b : b = 1, ..., B\}$ . We assume that  $\alpha$  is rational. That is,  $\alpha = \alpha_1/\alpha_2$  for some positive integers  $\alpha_1$  and  $\alpha_2$  (with no common integer divisors). We choose B to be a positive integer that satisfies  $\nu/(B+1) = 1-\alpha$  and  $\eta/(B+1) = \alpha$  for some positive integers  $\nu$  and  $\eta$ . That is,  $B = \alpha_2 a - 1$ ,  $\nu = (\alpha_2 - \alpha_1)a$ , and  $\eta = \alpha_1 a$ , for some positive integer a. For example, if  $\alpha = .05$ , then  $\alpha_1 = 1$ ,  $\alpha_2 = 20$ , B = 20a - 1,  $\nu = 19a$ , and  $\eta = a$  for some integer a > 0.

The bootstrap estimates of  $q_{1-\alpha}$  and  $q_{\alpha}$  based on B bootstrap repetitions are defined to be

(3.25) 
$$\widehat{q}_{1-\alpha,B} = T^*_{B,\nu} \text{ and } \widehat{q}_{\alpha,B} = T^*_{B,\eta}.$$

That is,  $\hat{q}_{1-\alpha,B}$  and  $\hat{q}_{\alpha,B}$  are the  $\nu$ -th and  $\eta$ -th order statistics of  $\{T_b^*: b = 1, ..., B\}$ . Then, the bootstrap equal-tailed and one-sided percentile t confidence intervals of approximate confidence levels  $100(1-2\alpha)\%$  and  $100(1-\alpha)\%$ , respectively, based on B bootstrap repetitions are defined to be

(3.26) 
$$\widehat{J}_{2,B} = [\widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{1-\alpha,B}, \widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{\alpha,B}] \text{ and}$$
$$\widehat{J}_{1,B} = [\widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{1-\alpha,B}, \infty).$$

We now introduce three-step methods for determining B for the bootstrap confidence intervals  $\hat{J}_{2,B}$  and  $\hat{J}_{1,B}$ . We measure the closeness of  $\hat{J}_{h,B}$  to  $\hat{J}_{h,\infty}$  by comparing the endpoints of these intervals for h = 1, 2. The percentage deviation of the lower endpoint of  $\hat{J}_{h,B}$  to the lower endpoint of  $\hat{J}_{h,\infty}$  is

$$(3.27) 100 \frac{|n^{-\kappa}\widehat{\sigma}\widehat{q}_{1-\alpha,B} - n^{-\kappa}\widehat{\sigma}\widehat{q}_{1-\alpha,\infty}|}{n^{-\kappa}\widehat{\sigma}\widehat{q}_{1-\alpha,\infty}} = 100 \frac{|\widehat{q}_{1-\alpha,B} - \widehat{q}_{1-\alpha,\infty}|}{\widehat{q}_{1-\alpha,\infty}}$$

for h = 1, 2. The percentage deviation of the upper endpoint of  $\widehat{J}_{2,B}$  to the upper endpoint of  $\widehat{J}_{2,\infty}$  is defined analogously.

As above, let  $1 - \tau$  denote a probability close to one, such as .95. Let pdb be a bound on the percentage deviation of an endpoint of  $\widehat{J}_{h,B}$  to the corresponding endpoint of  $\widehat{J}_{h,\infty}$  for h = 1 or 2. For the lower endpoint, we want to determine  $B = B(pdb, \tau)$  such that

(3.28) 
$$P^*\left(100\frac{|\widehat{q}_{1-\alpha,B}-\widehat{q}_{1-\alpha,\infty}|}{\widehat{q}_{1-\alpha,\infty}} \le pdb\right) = 1-\tau.$$

For the upper endpoint, we want to determine an analogous value of B with  $1 - \alpha$  replaced by  $\alpha$ .

The three-step method of determining B for  $\widehat{J}_{2,B}$  is designed to obtain a given desired level of accuracy pdb for both endpoints, each with probability (approximately) equal to  $1-\tau$ . The three-step method for the equal-tailed confidence interval  $\widehat{J}_{2,B}$  is defined as follows:

Step 1. Compute a preliminary number of bootstrap repetitions  $B_0$  via

(3.29) 
$$B_{0} = \alpha_{2}a_{0} - 1, \text{ where} \\ a_{0} = \operatorname{int} \left( \frac{10,000\alpha(1-\alpha)\chi_{1-\tau}^{2}}{z_{1-\alpha}^{2}\phi^{2}(z_{1-\alpha})pdb^{2}\alpha_{2}} \right) \text{ and } \alpha = \alpha_{1}/\alpha_{2}.$$

Step 2. Simulate  $B_0$  bootstrap t statistics  $\{T_b^*: b = 1, ..., B_0\}$ ; compute the ordered bootstrap t statistics, which are denoted  $\{T_{B_0,b}^*: b = 1, ..., B_0\}$ ; and calculate  $\nu_0 = (\alpha_2 - \alpha_1)a_0, \ \eta_0 = \alpha_1a_0, \ \hat{m} = \operatorname{int}(c_{\alpha}B_0^{2/3}), \ \hat{q}_{1-\alpha,B_0} = T_{B_0,\nu_0}^*, \ T_{B_0,\nu_0-\widehat{m}}^*, \ T_{B_0,\nu_0+\widehat{m}}^*, \ \hat{q}_{\alpha,B_0} = T_{B_0,\eta_0}^*, \ T_{B_0,\eta_0-\widehat{m}}^*, \ T_{B_0,\eta_0+\widehat{m}}^*, \ \text{where}$ 

(3.30) 
$$c_{\alpha} = \left(\frac{1.5z_{1-\alpha/2}^2\phi^2(z_{1-\alpha})}{2z_{1-\alpha}^2 + 1}\right)^{1/3}$$

Step 3. Take the desired number of bootstrap repetitions,  $B^*$ , to equal  $B^* = \max\{B_0, B_{1\ell}, B_{1u}\}$ , where

$$B_{1\ell} = \alpha_2 a_{1\ell} - 1, \ B_{1u} = \alpha_2 a_{1u} - 1,$$
  

$$a_{1\ell} = \operatorname{int} \left( \frac{10,000\alpha(1-\alpha)\chi_{1-\tau}^2}{\hat{q}_{1-\alpha,B_0}^2 p db^2 \alpha_2} \left( \frac{B_0}{2\hat{m}} \right)^2 \left( T^*_{B_0,\nu_0+\hat{m}} - T^*_{B_0,\nu_0-\hat{m}} \right)^2 \right), \text{ and}$$
  

$$(3.31) \ a_{1u} = \operatorname{int} \left( \frac{10,000\alpha(1-\alpha)\chi_{1-\tau}^2}{\hat{q}_{\alpha,B_0}^2 p db^2 \alpha_2} \left( \frac{B_0}{2\hat{m}} \right)^2 \left( T^*_{B_0,\eta_0+\hat{m}} - T^*_{B_0,\eta_0-\hat{m}} \right)^2 \right).$$

Note that the term in (3.30) that depends on  $z_{1-\alpha/2}$  rather than  $z_{1-\alpha}$  follows from the formula of Hall and Sheather (1988); see (5.31). It is not a typographical error.

Having determined  $B^*$ , one simulates  $B^* - B_0 (\geq 0)$  additional bootstrap t statistics  $\{T_b^* : b = B_0 + 1, ..., B^*\}$  and orders the values of the  $B^*$  bootstrap t statistics, which are denoted  $\{T_{B^*,b}^* : b = 1, ..., B^*\}$ . For the equal-tailed confidence interval  $\widehat{J}_{2,B}$ , the desired cutoff values,  $\nu^*$  and  $\eta^*$ , and the desired critical points,  $\widehat{q}_{1-\alpha,B^*}$  and  $\widehat{q}_{\alpha,B^*}$ , are then given by

$$\nu^* = \max\{\nu_0, \nu_{1\ell}, \nu_{1u}\}, \ \nu_{1\ell} = (\alpha_2 - \alpha_1)a_{1\ell}, \ \nu_{1u} = (\alpha_2 - \alpha_1)a_{1u}, \eta^* = \max\{\eta_0, \eta_{1\ell}, \eta_{1u}\}, \ \eta_{1\ell} = \alpha_1 a_{1\ell}, \ \eta_{1u} = \alpha_1 a_{1u}, (3.32) \ \widehat{q}_{1-\alpha,B^*} = T^*_{B^*,\nu^*}, \ \text{and} \ \widehat{q}_{\alpha,B^*} = T^*_{B^*,\eta^*}.$$

The three-step method of determining B for the one-sided confidence interval  $\hat{J}_{1,B}$  is the same as that for  $\hat{J}_{2,B}$  except that one does not need to calculate  $\eta_0$ ,  $\hat{q}_{\alpha,B_0}$ ,

 $T^*_{B_0,\eta_0-\widehat{m}}$ , or  $T^*_{B_0,\eta_0+\widehat{m}}$  in Step 2 and one defines  $B^* = \max\{B_0, B_{1\ell}\}$  in Step 3. (For the one-sided confidence interval  $(-\infty, \widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{\alpha,B}]$  that has a finite upper bound, rather than lower bound, the three-step method is the same as that for  $\widehat{J}_{2,B}$  except that one does not need to calculate  $\nu_0$ ,  $\widehat{q}_{1-\alpha,B_0}$ ,  $T^*_{B_0,\nu_0-\widehat{m}}$ , or  $T^*_{B_0,\nu_0+\widehat{m}}$  in Step 2 and one defines  $B^* = \max\{B_0, B_{1u}\}$  in Step 3.) The desired cutoff value,  $\nu^*$ , and the desired critical point,  $\widehat{q}_{1-\alpha,B^*}$ , for the one-sided confidence interval  $J_{1,B}$  are given by (3.32) with  $\nu_{1u}$  deleted in the definition of  $\nu^*$ .

The equal-tailed and one-sided bootstrap confidence intervals based on  $B^*$  bootstrap repetitions, then, are equal to

(3.33) 
$$\begin{aligned} \widehat{J}_{2,B^*} &= [\widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{1-\alpha,B^*}, \widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{\alpha,B^*}] \text{ and} \\ \widehat{J}_{1,B^*} &= [\widehat{\theta} - n^{-\kappa} \widehat{\sigma} \widehat{q}_{1-\alpha,B^*}, \infty). \end{aligned}$$

Table 7 provides the values of  $B_0$  for equal-tailed and one-sided confidence intervals that correspond to different  $(\alpha, pdb, \tau)$  combinations, along with corresponding values of  $\nu_0$ ,  $\eta_0$ ,  $c_\alpha$ , and  $\hat{m}$ . The pattern of Table 7 as  $(\alpha, pdb, \tau)$  varies is exactly the same as that of Table 5 for symmetric confidence intervals, as is expected from the formulae.

Tables 5 and 7 indicate that the  $B_0$  values for equal-tailed and one-sided confidence intervals are noticeably larger than those for symmetric two-sided confidence intervals with the same confidence level. The ratio of the  $B_0$  value for equal-tailed or one-sided confidence intervals to that for symmetric confidence intervals only depends on the confidence level and not on pdb or  $\tau$  (except for rounding effects from the int(·) function.) For equal-tailed confidence intervals, this ratio is 2.0 and 2.1 for confidence levels .95 and .90 respectively. For one-sided confidence intervals, this ratio is 1.8 and 2.3 for confidence levels .95 and .90 respectively. (Note that to make these comparisons correctly one has to take account of the fact that the confidence levels of symmetric and one-sided confidence intervals are both  $1 - \alpha$ , whereas the confidence level of equal-tailed confidence intervals is  $1 - 2\alpha$ .) The reason fewer repetitions are needed for symmetric confidence intervals is that the asymptotic density of  $|T^*|$  is twice as large as that of  $T^*$  at any positive value.

As in Section 3.2, we computed the magnitude of  $B_1$  values generated by the three-step method for equal-tailed and one-sided confidence intervals by specifying certain distributions for  $T^*$ . In this case, we considered the distributions N(0, 1),  $t_5$ , and  $\chi_5^2$ . The results (in terms of the ratios of the median  $B_1$  values to the  $B_0$  values) and their implications are quite similar to those for symmetric confidence intervals, so we do not repeat them here.

The asymptotic justifications of the three-step methods introduced above are analogous to the asymptotic justification given for the symmetric percentile t confidence intervals. Details are given in Section 5.3 of the Appendix.

As in previous sections, when one is interested in separate confidence intervals for several parameters, say  $\omega$  parameters, one can apply the three-step method for each of the parameters to obtain  $B^*_{(1)}$ ,  $B^*_{(2)}$ , ...,  $B^*_{(\omega)}$  and take  $B^*$  to equal the maximum of these values.

If the asymptotic distribution of T is not normal, then Steps 1 and 2 of the threestep method have to be adjusted. Suppose the asymptotic distribution of T is F, the  $\alpha$ -th and the  $(1 - \alpha)$ -th quantiles of F are  $\overline{q}_{\alpha}$  and  $\overline{q}_{1-\alpha}$ , and F has a density  $f(\cdot)$  with respect to Lebesgue measure at  $\overline{q}_{\alpha}$  and  $\overline{q}_{1-\alpha}$ . To allow for the case where F is not symmetric about zero, we have to define two pairs of values  $(B_{0\ell}, B_{0u})$  and  $(a_{0\ell}, a_{0u})$  in place of  $B_0$  and  $a_0$  in Step 1 and four pairs of values  $(\nu_{0\ell}, \nu_{0u}), (\eta_{0\ell}, \eta_{0u}),$  $(\widehat{m}_{\ell}, \widehat{m}_u)$ , and  $(c_{\alpha\ell}, c_{\alpha u})$  in place of  $\nu_0, \eta_0, \widehat{m}$ , and  $c_{\alpha}$ , respectively, in Step 2. Then, in Step 3,  $a_{0\ell}$  is defined with  $B_0, \nu_0, \eta_0$ , and  $\widehat{m}$  replaced by  $B_{0\ell}, \nu_{0\ell}, \eta_{0\ell}$ , and  $\widehat{m}_{\ell}$ , respectively, and  $a_{0u}$  is defined with  $B_0, \nu_0, \eta_0$ , and  $\widehat{m}$  replaced by  $B_{0u}, \nu_{0u}, \eta_{0u}$ , and  $\widehat{m}_u$ , respectively.

It suffices to define  $(a_{0\ell}, a_{0u})$  and  $(c_{\alpha\ell}, c_{\alpha u})$ . The other new terms above follow from these via the same definitions as in Steps 1 and 2 above. We define  $a_{0\ell} = int((10,000\alpha(1-\alpha)\chi_{1-\tau}^2) / (\bar{q}_{1-\alpha}^2 f^2(\bar{q}_{1-\alpha})pdb^2\alpha_2))$  and  $a_{0u}$  the same way except with  $\bar{q}_{\alpha}$  in place of  $\bar{q}_{1-\alpha}$  twice in the formula. We define  $c_{\alpha\ell}$  as in (5.31) with  $q_{1-\alpha}$  replaced by  $\bar{q}_{1-\alpha}$  and  $c_{\alpha u}$  as in (5.31) with  $q_{1-\alpha}$  replaced by  $\bar{q}_{\alpha}$ .

If F depends on unknown parameters, then consistent estimates of these parameters can be used to provide estimates of  $\bar{q}_{1-\alpha}$ ,  $\bar{q}_{\alpha}$ ,  $f(\bar{q}_{1-\alpha})$ , and  $f(\bar{q}_{\alpha})$  for use in the definitions of  $a_{0\ell}$ ,  $a_{0u}$ ,  $c_{\alpha\ell}$ , and  $c_{\alpha u}$ .

#### 4. Test Results

In this section, we consider the problem of choosing the number of bootstrap repetitions B for tests. First, we provide a method of doing so when a specific significance level  $\alpha$  is of interest. Next, we provide a method of doing so for *p*-values. We recommend the use of the p-value results in most circumstances, because they convey more information.

#### 4.1. Tests of Significance Level $\alpha$

We begin by introducing some notation and definitions. As above, X denotes the observed data. We wish to construct a test of some null hypothesis of (approximate) significance level  $\alpha$  for some  $0 < \alpha < 1$ . Our results apply to a wide variety of tests, such as tests of parametric restrictions and of model specification in parametric, semiparametric, and nonparametric models. Let T denote a test statistic based on X. For example, T could be a t-statistic, a Wald statistic, a Lagrange multiplier statistic, a likelihood ratio statistic, etc.

We assume that the test statistic T has an asymptotic distribution, G, under the null hypothesis. For example, G could be a normal distribution, the distribution of the absolute value of a normal random variable, a chi-squared distribution with d degrees of freedom for some positive integer d, etc. We assume that G has a unique  $(1-\alpha)$ -th quantile, denoted  $q_{G,1-\alpha}$ , and that G has a density with respect to Lebesgue measure at  $q_{G,1-\alpha}$ , denoted  $g(q_{G,1-\alpha})$ .

The "theoretical" test of significance level  $\alpha$  rejects the null hypothesis if  $T > k_{\alpha}$ , where  $k_{\alpha}$  is the solution to  $P(T > k_{\alpha}) = \alpha$ . By definition of  $k_{\alpha}$ , the "theoretical" test has exact signifiance level  $\alpha$ . In practice, however, one typically does not know  $k_{\alpha}$ . We consider using the bootstrap to approximate  $k_{\alpha}$ .

Let  $\mathbf{X}^* = (X_1^*, ..., X_n^*)'$  denote a bootstrap sample based on  $\mathbf{X}$ . Depending upon the circumstances, the bootstrap employed could be a variant of a nonparametric iid bootstrap, a moving block bootstrap for time series data, a parametric or semiparametric bootstrap for iid or time series data, or a bootstrap for regression models based on bootstrapping residuals. Let  $T^*$  denote a bootstrap version of the test statistic T based on  $\mathbf{X}^*$ . We assume that  $T^*$  is defined such that its asymptotic distribution conditional on the data is G with probability one (with respect to the randomness in the data). It is important for purposes of power of the test to define  $T^*$  such that the latter holds whether or not the null hypothesis is true; see Hall and Wilson (1991), Hall and Horowitz (1996), and Li and Maddala (1996).

If T is an asymptotically pivotal statistic (i.e., the asymptotic distribution G of T is the same for all distributions in the null), then the significance level of the bootstrap test typically exhibits higher order improvements (in terms of the closeness of its exact and nominal significance levels) over the standard test that results from using the delta method to estimate  $k_{\alpha}$ ; e.g., see Beran (1988) and Hall (1992).

Let  $k_{\alpha,\infty}$  denote the *ideal bootstrap estimate* of  $k_{\alpha}$ , i.e., the  $(1-\alpha)$ -th quantile of the distribution of  $T^*$ . To be precise, we define  $\hat{k}_{\alpha,\infty} = \inf\{k : P^*(T^* \leq k) \geq 1-\alpha\}$ , where  $P^*(\cdot)$  denotes probability with respect to  $\mathbf{X}^*$  conditional on the data  $\mathbf{X}$ . The ideal bootstrap test of approximate significance level  $\alpha$  rejects the null hypothesis if  $T > \hat{k}_{\alpha,\infty}$ . Analytic calculation of  $\hat{k}_{\alpha,\infty}$  is usually intractable. In consequence, one typically approximates  $\hat{k}_{\alpha,\infty}$  using bootstrap simulations.

As above, consider B iid bootstrap samples  $\{\mathbf{X}_b^* : b = 1, ..., B\}$ , each with the same distribution as  $\mathbf{X}^*$ . The corresponding B bootstrap test statistics are  $\{T_b^* : b = 1, ..., B\}$ . Let  $\{T_{B,b}^* : b = 1, ..., B\}$  denote the ordered sample of  $\{T_b^* : b = 1, ..., B\}$ .

We assume that  $\alpha = \alpha_1/\alpha_2$  for some positive integers  $\alpha_1$  and  $\alpha_2$  (with no common integer divisors). We choose B to be a positive integer that satisfies  $\nu/(B+1) = 1-\alpha$  for some positive integer  $\nu$ . That is,  $B = \alpha_2 a - 1$  and  $\nu = (\alpha_2 - \alpha_1)a$  for some positive integer a.

The bootstrap estimate of  $k_{\alpha}$  based on B bootstrap repetitions is defined to be

(4.1) 
$$\widehat{k}_{\alpha,B} = T^*_{B,\nu}$$

That is,  $\hat{k}_{\alpha,B}$  is the  $\nu$ -th order statistic of  $\{T_b^* : b = 1, ..., B\}$ . Then, the bootstrap test of approximate significance level  $\alpha$  based on B bootstrap repetitions rejects the null hypothesis if

$$(4.2) T > \hat{k}_{\alpha,B}.$$

We now introduce the three-step method for determining B for the bootstrap test. The percentage deviation of the simulated critical value  $\hat{k}_{\alpha,B}$  from the ideal bootstrap critical value  $\hat{k}_{\alpha,\infty}$  is

(4.3) 
$$100\frac{|\hat{k}_{\alpha,B} - \hat{k}_{\alpha,\infty}|}{\hat{k}_{\alpha,\infty}}$$

As above, let  $1 - \tau$  denote a probability close to one, such as .95. Let pdb be a bound on the percentage deviation of the critical value  $\hat{k}_{\alpha,B}$  from the critical value  $\hat{k}_{\alpha,\infty}$ . We want to determine  $B = B(pdb, \tau)$  such that

(4.4) 
$$P^*\left(100\frac{|\hat{k}_{\alpha,B}-\hat{k}_{\alpha,\infty}|}{\hat{k}_{\alpha,\infty}} \le pdb\right) = 1-\tau.$$

The three-step method of determining B is designed to do so. It is defined as follows:

Step 1. Compute a preliminary number of bootstrap repetitions  $B_0$  via

(4.5) 
$$B_{0} = \alpha_{2}a_{0} - 1, \text{ where}$$
$$a_{0} = \operatorname{int}\left(\frac{10,000\alpha(1-\alpha)\chi_{1-\tau}^{2}}{q_{G,1-\alpha}^{2}g^{2}(q_{G,1-\alpha})pdb^{2}\alpha_{2}}\right) \text{ and } \alpha = \alpha_{1}/\alpha_{2}$$

Step 2. Simulate  $B_0$  bootstrap test statistics  $\{T_b^* : b = 1, ..., B_0\}$ ; compute the ordered bootstrap test statistics, which are denoted  $\{T_{B_0,b}^* : b = 1, ..., B_0\}$ ; and calculate  $\nu_0 = (\alpha_2 - \alpha_1)a_0$ ,  $\hat{m} = \operatorname{int}(c_{\alpha}B_0^{2/3})$ ,  $\hat{k}_{\alpha,B_0} = T_{B_0,\nu_0}^*$ ,  $T_{B_0,\nu_0-\hat{m}}^*$ , and  $T_{B_0,\nu_0+\hat{m}}^*$ , where

(4.6) 
$$c_{\alpha} = \left(\frac{1.5\chi_{1-\alpha}^{2}g^{4}(q_{G,1-\alpha})}{3g'(q_{G,1-\alpha})^{2} - g(q_{G,1-\alpha})g''(q_{G,1-\alpha})}\right)^{1/3}$$

Step 3. Take the desired number of bootstrap repetitions,  $B^*$ , to equal  $B^* = \max\{B_0, B_1\}$ , where

(4.7) 
$$B_{1} = \alpha_{2}a_{1} - 1 \text{ and} \\ \left(\frac{10,000\alpha(1-\alpha)\chi_{1-\tau}^{2}}{\widehat{k}_{\alpha,B_{0}}^{2}pdb^{2}\alpha_{2}} \left(\frac{B_{0}}{2\widehat{m}}\right)^{2} \left(T_{B_{0},\nu_{0}+\widehat{m}}^{*} - T_{B_{0},\nu_{0}-\widehat{m}}^{*}\right)^{2}\right).$$

Steps 1 and 2 require the calculation of  $q_{G,1-\alpha}$ ,  $g(q_{G,1-\alpha})$ ,  $g'(q_{G,1-\alpha})$ , and  $g''(q_{G,1-\alpha})$ , where  $g'(\cdot)$  and  $g''(\cdot)$  denote the first and second derivatives of  $g(\cdot)$ . If G is a standard normal distribution, then these quantities equal  $z_{1-\alpha}$ ,  $\phi(z_{1-\alpha})$ ,  $-z_{1-\alpha}\phi(z_{1-\alpha})$ , and  $(z_{1-\alpha}^2-1)\phi(z_{1-\alpha})$ , respectively, where  $z_{1-\alpha}$  denotes the  $(1-\alpha)$ -th quantile of a standard normal distribution. If G is the distribution of the absolute value of a standard normal random variable and  $\alpha < .5$ , then these quantities equal  $z_{1-\alpha/2}$ ,  $2\phi(z_{1-\alpha/2})$ ,  $-2z_{1-\alpha/2}\phi(z_{1-\alpha/2})$ , and  $2(z_{1-\alpha/2}^2-1)\phi(z_{1-\alpha/2})$  respectively. If G is a chi-squared distribution with d degrees of freedom, then these quantities equal q,  $g(q) = (2^{d/2}\Gamma(d/2))^{-1}q^{\psi}\exp(-q/2)$ ,  $g'(q) = (\psi/q - 1/2)g(q)$ , and  $g''(q) = (\psi(\psi-1)/q^2 - \psi/q + 1/4)g(q)$ , respectively, where  $\psi = d/2 - 1$  and q denotes the  $(1-\alpha)$ -th quantile of a chi-squared distribution with d degrees of freedom.

If G depends on unknown parameters, then consistent estimates of these parameters can be used to provide estimates of  $q_{G,1-\alpha}$  and  $f(q_{G,1-\alpha})$  for use in Steps 1 and 2. Having determined  $B^*$ , one simulates  $B^* - B_0 (\geq 0)$  additional bootstrap test statistics  $\{T_b^* : b = B_0 + 1, ..., B^*\}$  and orders the values of the  $B^*$  bootstrap test statistics, which are denoted  $\{T_{B^*,b}^* : b = 1, ..., B^*\}$ . The desired cutoff value,  $\nu^*$ , and the desired critical value,  $\hat{k}_{\alpha,B^*}$ , are given by

(4.8) 
$$\nu^* = \max\{\nu_0, \nu_1\}, \ \nu_1 = (\alpha_2 - \alpha_1)a_1, \ \text{and} \ \widehat{k}_{\alpha, B^*} = T^*_{B^*, \nu^*}.$$

The bootstrap test based on  $B^*$  bootstrap repetitions, then, rejects the null hypothesis if

$$(4.9) T > k_{\alpha,B^*}.$$

To assess the computational burden of the three-step procedure for tests with specified significance levels, Table 8 provides values for  $B_0$ , as well as  $a_0$ ,  $\nu_0$ , and  $\hat{m}$ , for a variety of  $(\alpha, \tau)$  combinations when pdb = 10 and the asymptotic null distribution of the test statistic is absolute N(0, 1), N(0, 1),  $\chi_5^2$ , and  $\chi_{15}^2$ . (Results for the  $\chi_{10}^2$  distribution are intermediate between those of the  $\chi_5^2$  and  $\chi_{15}^2$  distributions, but are somewhat closer to the  $\chi_{15}^2$  results.)

Table 8 shows that for tests with absolute N(0,1) asymptotic null distribution the same number of initial bootstrap repetitions  $B_0$  are needed as for symmetric confidence intervals. For tests with N(0,1) asymptotic null distribution, noticeably larger  $B_0$  values are required—the ratio of  $B_0$  values for N(0,1) to absolute N(0,1)tests is in the range 1.8–2.3 for  $\alpha = .05$  or  $\alpha = .10$ . For tests with  $\chi_5^2$  asymptotic null distribution, similar  $B_0$  values are required as for absolute N(0,1) tests—the ratio of  $B_0$  values for  $\chi_5^2$  to absolute N(0,1) tests is in the range 1.0–1.2 for  $\alpha = .05$ or  $\alpha = .10$ . For tests with  $\chi_{15}^2$  asymptotic null distribution, noticeably smaller  $B_0$ values are required than for absolute N(0,1) tests—the ratio of  $B_0$  values for  $\chi_{15}^2$ to absolute N(0,1) tests is in the range .38–.50 for  $\alpha = .05$  or  $\alpha = .10$ . Thus, there is considerable variation in suitable values of  $B_0$  for test statistics with different asymptotic null distributions.

In all cases,  $B_0$  increases quickly as  $\alpha$  or  $\tau$  decreases. It is also true that  $B_0$  increases very quickly as *pdb* decreases, but Table 8 only reports results for pdb = 10. For most combinations reported, the number of bootstrap repetitions required is greater than that commonly used in empirical econometric applications.

The asymptotic justification of the three-step method introduced above is analogous to the asymptotic justification given for symmetric percentile t confidence intervals in Section 3.3. See Section 5.4 of the Appendix of Proofs for details.

#### 4.2. p-values

We now consider choosing the number of bootstrap repetitions B for a testing problem in which one wants to report a p-value. By definition, the p-value is the infimum of the significance levels for which the test rejects the null hypothesis given the observed value of the test statistic T. We view the reporting of a p-value to be an efficient method of communicating the result of hypothesis tests for all significance levels  $\alpha \in (0, 1)$ . The use of a bootstrap p-value exploits the higher-order improvements of the bootstrap, because given the p-value and a significance level  $\alpha$  of interest (which may vary across individuals), one can determine whether the test rejects the null hypothesis and the significance level of the test is accurate to the level obtained by the bootstrap test.

We use the same notation, definitions, and assumptions as in Section 4.1 except that assumptions (5.36) and (5.37) are not needed and n is treated as fixed. We consider probabilities with respect to the bootstrap simulation randomness conditional on the sample **X**.

The ideal bootstrap *p*-value is defined to be

(4.10) 
$$\widehat{p}_{\infty} = P^*(T^* > T),$$

where  $P^*(\cdot)$  denotes probability with respect to  $\mathbf{X}^*$  (and hence  $T^*$ ) conditional on  $\mathbf{X}$  (and hence T). We assume that  $\hat{p}_{\infty}$  does not equal zero or one. (This holds with probability one with respect to the randomness in the sample  $\mathbf{X}$  except in pathological cases.) We estimate  $\hat{p}_{\infty}$  using bootstrap simulations. Given B bootstrap repetitions, the bootstrap p-value is

(4.11) 
$$\widehat{p}_B = \frac{1}{B} \sum_{b=1}^B \mathbb{1}(T_b^* > T).$$

We now introduce a three-step method for determining B for the bootstrap p-value. The percentage deviation of the simulated p-value  $\hat{p}_B$  from the ideal bootstrap p-value  $\hat{p}_{\infty}$  is

(4.12) 
$$100\frac{|\hat{p}_B - \hat{p}_{\infty}|}{\hat{p}_{\infty}}.$$

Let  $1 - \tau$  denote a probability close to one, such as .95. Let pdb be a bound on the percentage deviation of  $\hat{p}_B$  from  $\hat{p}_{\infty}$ . We want to determine  $B = B(pdb, \tau)$  such that

(4.13) 
$$P^*\left(100\frac{|\widehat{p}_B - \widehat{p}_{\infty}|}{\widehat{p}_{\infty}} \le pdb\right) = 1 - \tau.$$

The three-step method of determining B is designed to do this. It is defined as follows:

Step 1. Compute a preliminary number of bootstrap repetitions  $B_0$  via

(4.14) 
$$B_0 = \operatorname{int}\left(\frac{10,000\chi_{1-\tau}^2G(T)}{(1-G(T))pdb^2}\right).$$

**Step 2.** Simulate  $B_0$  bootstrap test statistics  $\{T_b^* : b = 1, ..., B_0\}$  and compute

(4.15) 
$$\widehat{p}_{B_0} = \frac{1}{B_0} \sum_{b=1}^{B_0} \mathbb{1}(T_b^* > T).$$

Step 3. Take the desired number of bootstrap repetitions,  $B^*$ , to equal  $B^* = \max\{B_0, B_1\}$ , where

(4.16) 
$$B_1 = \operatorname{int}\left(\frac{10,000\chi_{1-\tau}^2(1-\hat{p}_{B_0})}{\hat{p}_{B_0}pdb^2}\right).$$

In Step 1, the term 1-G(T) is an initial estimate of the *p*-value that is obtained by using the asymptotic null distribution G of the test statistic T. For example, if G is a standard normal distribution, then  $G(T) = \Phi(T)$ , where  $\Phi(\cdot)$  is the standard normal distribution function. If G is the distribution of the absolute value of a standard normal random variable, then  $G(T) = 2\Phi(T) - 1$ . If G is a chi-squared distribution, then G(T) is the corresponding chi-squared distribution function evaluated at T.

If G depends on unknown parameters, then consistent estimates of these parameters can be used to provide estimates of G(T) for use in Step 1.

We note that one should adjust one's choice of pdb in light of the initial *p*-value estimates 1 - G(T) and/or  $\hat{p}_{B_0}$ , because the level of accuracy needed depends on the *p*-value. In particular, when the *p*-value is small or large, e.g., .001 or .70, then one does not need to take pdb to be as small as when the *p*-value is of intermediate magnitude, e.g., .075. This is quite important in terms of minimizing the computational burden.

If one or more significance levels  $\alpha$  are of particular interest, then one should choose  $B_0$  and  $B_1$  (by rounding up) such that  $\nu/(B+1) = 1 - \alpha$  for some positive integer  $\nu$  for each  $\alpha$  of interest. For example, if significance levels .05 and .10 are of particular interest, then  $B_0$  and  $B_1$  should be rounded up to the nearest value B = 20a - 1 for some a = 1, 2, ... (i.e., B = 19, 39, 59, etc.). If .01, .05, and .10 are of particular interest, then  $B_0$  and  $B_1$  should be rounded up to the nearest value B = 100a - 1 for some a = 1, 2, ... The reason for doing this is that it has advantages in terms of the unconditional significance level for the values of  $\alpha$  of particular interest; see Hall (1992, p. 307).

Having determined  $B^*$ , one simulates  $B^* - B_0 (\geq 0)$  additional bootstrap test statistics  $\{T_b^* : b = B_0 + 1, ..., B^*\}$  and computes the bootstrap *p*-value

(4.17) 
$$\widehat{p}_{B^*} = \frac{1}{B^*} \sum_{b=1}^{B^*} \mathbb{1}(T_b^* > T).$$

Table 9 provides representative values of  $B_0$  for the three-step method for pvalues. Three different values of  $\tau$  are considered, viz., .01, .05 and .10. A range of values of the initial p-value estimate 1 - G(T) and the accuracy bound *pdb* are considered. For clarity, the Table only provides (1 - G(T), pdb) combinations that are of some interest. For example, it is not of interest to consider the combination (.001,5), because this combination yields excessive accuracy and, hence, requires an excessively large value of  $B_0$ .

Table 9 indicates that the required magnitude of  $B_0$  depends on the initial p-value estimate 1 - G(T). If it is quite small or large, then one does not need a small value of *pdb* and the required magnitude of  $B_0$  is not large. On the other hand, if 1 - G(T) is in an intermediate range, such as (.01, .15), then one may want to employ a relatively small value of *pdb* and the required magnitude of  $B_0$  may be quite large.

The asymptotic justification of the three-step method of choosing  $B^*$  is in terms of the limit as  $pdb \rightarrow 0$  with n fixed:

(4.18) 
$$P^*\left(100\frac{|\hat{p}_{B_1} - \hat{p}_{\infty}|}{\hat{p}_{\infty}} \le pdb\right) \to 1 - \tau \quad \text{as } pdb \to 0,$$

where  $\hat{p}_{B_1} = \frac{1}{B_1} \sum_{b=1}^{B_1} (T_b^* > T)$ . This conditional result holds provided  $\hat{p}_{\infty}$  does not equal zero or one. The proof is given in the Appendix of Proofs.

Equation (4.18) implies that the three-step method attains precisely the desired level of accuracy using "small pdb" asymptotics when  $B^* = B_1 \ge B_0$ . When  $B^* = B_0 > B_1$ , then the accuracy of the three-step method exceeds the desired level of accuracy.

# 5. Appendix of Proofs

#### 5.1. Proofs of the Standard Error Results

First, we prove (2.11). We rewrite  $\widehat{se}_B$  of (2.3) as

$$\widehat{se}_{B} = \left(\frac{1}{B}\Sigma_{b=1}^{B}\left(\widehat{\theta}_{b}^{*}-\mu\right)^{2}-\left(\frac{1}{B}\Sigma_{b=1}^{B}\widehat{\theta}_{b}^{*}-\mu\right)^{2}\right)^{1/2}$$
$$= m(A_{B}), \text{ where}$$
$$(5.1) \quad A_{B} = \left(\frac{1}{B}\Sigma_{b=1}^{B}\left(\widehat{\theta}_{b}^{*}-\mu\right)^{2}\right) \text{ and } m(a) = \left(a_{1}-a_{2}^{2}\right)^{1/2} \text{ for } a = (a_{1}, a_{2})'.$$

For convenience, we have replaced B-1 in the denominator of  $\widehat{se}_B$  by B. By the central limit theorem,

(5.2) 
$$B^{1/2}(A_B - A) \xrightarrow{d} N(\mathbf{0}, \Omega) \text{ as } B \to \infty, \text{ where}$$
$$A = \begin{pmatrix} \widehat{se}_{\infty}^2 \\ 0 \end{pmatrix} \text{ and } \Omega = \begin{pmatrix} E^* \left( (\widehat{\theta}_b^* - \mu)^2 - \widehat{se}_{\infty}^2 \right)^2 & E^* (\widehat{\theta}_b^* - \mu)^3 \\ E^* (\widehat{\theta}_b^* - \mu)^3 & \widehat{se}_{\infty}^2 \end{pmatrix}.$$

We have  $\frac{\partial}{\partial a}m(a) = \frac{1}{2}(a_1 - a_2^2)^{-1/2}(1, -2a_2)'$  and  $\frac{\partial}{\partial a}m(A) = (1/(2\widehat{se}_{\infty}), 0)'$ . The delta method now gives

(5.3) 
$$B^{1/2}(\widehat{se}_B - \widehat{se}_\infty) = B^{1/2}(m(A_B) - m(A)) \xrightarrow{d} N(0, V), \text{ where}$$
$$V = \frac{1}{4\widehat{se}_\infty^2} E^* \left( (\widehat{\theta}_b^* - \mu)^2 - \widehat{se}_\infty^2 \right)^2 = \frac{\widehat{se}_\infty^2}{4} (2 + \gamma_2).$$

In turn, this gives

(5.4) 
$$\left(100\frac{|\widehat{se}_B - \widehat{se}_{\infty}|}{\widehat{se}_{\infty}}\right)^2 / (2, 500(2+\gamma_2)/B) \xrightarrow{d} \chi^2,$$

where  $\chi^2$  denotes a chi-squared random variable with one degree of freedom, which establishes (2.11).

Next, we prove (2.17). Let  $B_{11} = 2,500\chi_{1-\tau}^2(2+\gamma_2)/pdb^2$ . Note that  $B_{11}$  is nonrandom. Equations (5.2)–(5.4) hold with *B* replaced by  $B_{11}$  throughout and with the limit as  $B \to \infty$  replaced by the limit as  $pdb \to 0$  (because the latter forces  $B_{11} \to \infty$ ). Now, by the central limit theorem of Doeblin–Anscombe for a sum of independent random variables with a random number of terms in the sum (e.g., see Chow and Teicher (1978, Thm. 9.4.1, p. 317)), provided  $B_1/B_{11} \to_p 1$  as  $pdb \to 0$ , the result of (5.2) holds with *B* replaced by  $B_1$  and with the limit as  $B \to \infty$  replaced by the limit as  $pdb \to 0$ . In turn, this implies that (5.3) and (5.4) hold with the same changes. The latter can be rewritten using (2.16) as

(5.5) 
$$\left(100\frac{|\widehat{se}_{B_1} - \widehat{se}_{\infty}|}{\widehat{se}_{\infty}}\right)^2 (\chi^2_{1-\tau}/pdb^2)(2+\widehat{\gamma}_{2B_0})/(2+\gamma_2) \xrightarrow{d} \chi^2 \text{ as } pdb \to 0.$$

(The effect of the int(·) function in (2.16) is asymptotically negligable and, hence, is ignored in obtaining the previous equation from (5.4).) By (2.7) and the fact that  $B_0 \to \infty$  as  $pdb \to 0$ , this yields

(5.6) 
$$\left(100\frac{|\widehat{se}_{B_1} - \widehat{se}_{\infty}|}{\widehat{se}_{\infty}}\right)^2 \chi^2_{1-\tau}/pdb^2 \xrightarrow{d} \chi^2 \text{ as } pdb \to 0,$$

which establishes (2.17).

It remains to show that  $B_1/B_{11} \rightarrow_p 1$  as  $pdb \rightarrow 0$ . This follows from (2.7) because  $B_1/B_{11} = (2 + \hat{\gamma}_{2B_0})/(2 + \gamma_2)$ .

## 5.2. Proofs of the Symmetric Confidence Interval Results

We now prove (3.20). First we show that (3.20) holds with  $B_1$  replaced by the non-random quantity  $B_{11}$ . By definition,

(5.7) 
$$B_{11} = \alpha_2 a_{11} - 1, \ \nu_{11} = (\alpha_2 - \alpha_1) a_{11}, \text{ and} a_{11} = \operatorname{int} \left( \frac{10,000\alpha(1-\alpha)\chi_{1-\tau}^2}{z_{1-\alpha/2}^2 p db^2 \alpha_2} \left( \frac{1}{2\phi(z_{1-\alpha/2})} \right)^2 \right).$$

Note that  $B_{11} \to \infty$  as  $pdb \to 0$  and  $B_{11}$  does not depend on n.

We establish the asymptotic distribution of  $B_{11}^{1/2}(\hat{k}_{\alpha,B_{11}} - \hat{k}_{\alpha,\infty})$  as  $pdb \to 0$  and  $n \to \infty$ , where  $\hat{k}_{\alpha,B_{11}} = |T^*|_{B_{11},\nu_{11}}$ , using an argument developed for proving the asymptotic distribution of the sample median based on an iid sample of random variables that are absolutely continuous at their population median; see Lehmann (1983, Thm. 5.3.2, p. 354). (In contrast, recall that  $\hat{k}_{\alpha,B_{11}}$  is the sample  $(1 - \alpha)$ -th quantile of iid observations each with the bootstrap distribution of  $|T^*|$ , which depends on n and may be discrete.)

We have: For any  $x \in R$ ,

(5.8) 
$$P^*(B_{11}^{1/2}(\hat{k}_{\alpha,B_{11}}-\hat{k}_{\alpha,\infty}) \le x) = P^*(|T^*|_{B_{11},\nu_{11}} \le \hat{k}_{\alpha,\infty}+x/B_{11}^{1/2}).$$

Let  $S_B$  be the number of  $|T_b^*|$ 's for b = 1, ..., B that exceed  $\hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}$ . Presently, we consider  $S_{B_{11}}$ . Below, we consider  $S_{B_1}$ . (In both cases, the cutoff point  $\hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}$  depends on  $B_{11}$ .) We have

(5.9) 
$$|T^*|_{B_{11},\nu_{11}} \leq \hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}$$
 if and only if  $S_{B_{11}} \leq B_{11} - \nu_{11} = B_{11}\alpha - (1-\alpha)$ .

The random variable  $S_{B_{11}}$  has a binomial distribution with parameters  $(B_{11}, p_{B_{11},n})$ , where

(5.10) 
$$p_{B_{11},n} = 1 - P^*(|T^*| \le \hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}).$$

The probability in (5.8) equals

$$P^* \left( S_{B_{11}} \le B_{11}\alpha - (1-\alpha) \right)$$

$$(5.11) = P^* \left( \frac{S_{B_{11}} - B_{11}p_{B_{11},n}}{(B_{11}p_{B_{11},n}(1-p_{B_{11},n}))^{1/2}} \le \frac{B_{11}\alpha - (1-\alpha) - B_{11}p_{B_{11},n}}{(B_{11}p_{B_{11},n}(1-p_{B_{11},n}))^{1/2}} \right)$$

Note that the random variable in the right-hand side probability has mean zero and variance one and satisfies the conditions of the Lindeberg central limit theorem (applied with  $pdb \rightarrow 0$  and  $n \rightarrow \infty$ ).

Using the assumption of (3.18), we obtain

$$\widehat{k}_{\alpha,\infty} = \inf\{k : P^*(|T^*| \le k) \ge 1 - \alpha\} = \inf\{k : P(|Z| \le k) \ge 1 - \alpha\} + o(1)$$
  
=  $z_{1-\alpha/2} + o(1)$  as  $n \to \infty$  and

(5.12)  $p_{B_{11},n} = 1 - P^*(|T^*| \le \hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}) \to \alpha \text{ as } pdb \to 0 \text{ and } n \to \infty.$ 

The upper bound in the right-hand side probability of (5.11) can be written as

(5.13)  

$$w_{B_{11},n} = \frac{B_{11}^{1/2}(\alpha - p_{B_{11},n}) - (1-\alpha)/B_{11}^{1/2}}{(p_{B_{11},n}(1-p_{B_{11},n}))^{1/2}} = \left( (\alpha(1-\alpha))^{-1/2} + o(1) \right) B_{11}^{1/2}(\alpha - p_{B_{11},n}) + o(1)$$

as  $pdb \to 0$  and  $n \to \infty$ . In addition, we have

$$\begin{split} B_{11}^{1/2}(\alpha - p_{B_{11},n}) &= B_{11}^{1/2}(P^*(|T^*| \le \hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}) - (1 - \alpha)) \\ &= B_{11}^{1/2}(P(|T| \le \hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}) - P(|T| \le \hat{k}_{\alpha,\infty})) + o(1) \\ &= B_{11}^{1/2}(P(|Z| \le \hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}) - P(|Z| \le \hat{k}_{\alpha,\infty})) + o(1) \\ &= B_{11}^{1/2}2\phi(\zeta_{B_{11},n})x/B_{11}^{1/2} + o(1) \\ &\to 2\phi(z_{1-\alpha/2})x \text{ as } pdb \to 0 \text{ and } n \to \infty. \end{split}$$

The first equality of 5.14 holds by the definition of  $p_{B_{11},n}$ . The second and third equalities hold by (3.18) and (3.19) (using the fact that the latter and the definition of  $B_{11}$  imply that  $B_{11}^{1/2} = O(1/pdb) = n^{\xi}O(1/(pdb \times n^{\xi})) = o(n^{\xi})$ ). The fourth equality holds for some  $\zeta_{B_{11},n}$  that lies between  $\hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}$  and  $\hat{k}_{\alpha,\infty}$  by a mean value expansion using the fact that the density at y > 0 of the absolute value of a standard normal random variable is  $2\phi(y)$ . The convergence result of 5.14 holds because  $\zeta_{B_{11},n} \to z_{1-\alpha/2}$  as  $pdb \to 0$  and  $n \to \infty$ .

Equations (5.13) and (5.14) give

(5.15) 
$$\lim_{pdb\to 0, n\to\infty} w_{B_{11},n} = 2\phi(z_{1-\alpha/2})/(\alpha(1-\alpha))^{1/2}.$$

Equations (5.8), (5.11), and (5.15) plus the Lindeberg central limit theorem applied to (5.11) yield

(5.16) 
$$P^*(B_{11}^{1/2}(\hat{k}_{\alpha,B_{11}} - \hat{k}_{\alpha,\infty}) \le x) \to \Phi(x2\phi(z_{1-\alpha/2})/(\alpha(1-\alpha))^{1/2}) \text{ and}$$
$$B_{11}^{1/2}(\hat{k}_{\alpha,B_{11}} - \hat{k}_{\alpha,\infty}) \xrightarrow{d} N\left(0, \frac{\alpha(1-\alpha)}{(2\phi(z_{1-\alpha/2}))^2}\right)$$

as  $pdb \to 0$  and  $n \to \infty$ .

This result, (3.11), and (5.7) imply that

$$P^* \left( 100 \frac{|\hat{k}_{\alpha,B_{11}} - \hat{k}_{\alpha,\infty}|}{\hat{k}_{\alpha,\infty}} \le pdb \right)$$
  
=  $P^* \left( 100 \frac{|\hat{k}_{\alpha,B_{11}} - \hat{k}_{\alpha,\infty}|}{\hat{k}_{\alpha,\infty}} \le \frac{100(\alpha(1-\alpha))^{1/2}\chi_{1-\tau}}{z_{1-\alpha/2}B_{11}^{1/2}} \left( \frac{1}{2\phi(z_{1-\alpha/2})} \right) (1+o(1)) \right)$   
 $\rightarrow 1-\tau \text{ as } pdb \rightarrow 0 \text{ and } n \rightarrow \infty, \text{ where}$ 

(5.17) 
$$\widehat{J}_{SY,B_{11}} = [\widehat{\theta} - n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,B_{11}}, \widehat{\theta} + n^{-\kappa}\widehat{\sigma}\widehat{k}_{\alpha,B_{11}}].$$

Thus, (3.20) holds with  $B_1$  replaced with  $B_{11}$ .

Next, we show that

(5.18) 
$$(B_1 - B_{11})/B_{11} \xrightarrow{p} 0 \text{ as } pdb \to 0 \text{ and } n \to \infty$$

(with respect to the simulation randomness conditional on the data). This follows from

(5.19) 
$$\widehat{k}_{\alpha,B_0} \xrightarrow{p} z_{1-\alpha/2}$$
 and  $\left(\frac{B_0}{2\widehat{m}}\right) \left( |T^*|_{B_0,\nu_0+\widehat{m}} - |T^*|_{B_0,\nu_0-\widehat{m}} \right) \xrightarrow{p} \frac{1}{2\phi(z_{1-\alpha/2})}$ 

as  $pdb \to 0$  and  $n \to \infty$ . The former holds by (5.12) and (5.16) with  $B_{11}$  replaced by  $B_0$ . The latter is established as follows.

Define the inverse of a distribution function F to be  $F^{-1}(t) = \inf\{x: F(x) \ge t\}$ . Let  $\widehat{F}_{|T^*|}(\cdot)$  denote the distribution function of the bootstrap distribution of  $|T^*|$ . Let  $\{U_b: b = 1, ..., B_0\}$  denote iid uniform [0,1] random variables. Let  $\{U_{B_0,b}: b = 1, ..., B_0\}$  denote the ordered sample of  $\{U_b: b = 1, ..., B_0\}$ . Then,  $\widehat{F}_{|T^*|}^{-1}(U_b)$  has the same distribution as  $|T_b^*|$  and  $\widehat{F}_{|T^*|}^{-1}(U_{B_0,b})$  has the same distribution as  $|T^*|_{B_0,b}$ . It suffices to show that

(5.20) 
$$\left(\frac{B_0}{2\hat{m}}\right) \left(\widehat{F}_{|T^*|}^{-1}(U_{B_0,\nu_0+\hat{m}}) - \widehat{F}_{|T^*|}^{-1}(U_{B_0,\nu_0-\hat{m}})\right) \xrightarrow{p} \frac{1}{2\phi(z_{1-\alpha/2})}$$

as  $pdb \to 0$  and  $n \to \infty$ . (Note that  $B_0 \to \infty$  as  $pdb \to 0$ .) Let

(5.21) 
$$\Psi(x) = P(|Z| \le x) = \Phi(x) - \Phi(-x), \text{ where } Z \sim N(0, 1).$$

The left-hand side of (5.20) equals

$$\left(\frac{\widehat{F}_{|T^{*}|}^{-1}(U_{+}) - \widehat{F}_{|T^{*}|}^{-1}(U_{-})}{U_{+} - U_{-}}\right) \left(\frac{B_{0}}{2\widehat{m}}\right) (U_{+} - U_{-}) = \left(\frac{\widehat{F}_{|T^{*}|}^{-1}(U_{+}) - \widehat{F}_{|T^{*}|}^{-1}(U_{-})}{U_{+} - U_{-}}\right) (1 + o_{p}(1))$$
(5.22)

where  $U_+$  and  $U_-$  abbreviate  $U_{B_0,\nu_0+\widehat{m}}$  and  $U_{B_0,\nu_0-\widehat{m}}$  respectively. Equation (5.22) holds by the argument of Bloch and Gastwirth (1968, Pf. of Thm. 1) (which relies on the fact that the spacings of the order statistics of uniform random variables have

beta distributions). The first term in parentheses on the right-hand side of (5.22) equals

$$\frac{\Psi^{-1}(U_{+}) - \Psi^{-1}(U_{-})}{U_{+} - U_{-}} + \frac{B_{0}^{1/3}(\widehat{F}_{|T^{*}|}^{-1}(U_{+}) - \Psi^{-1}(U_{+}))}{B_{0}^{1/3}(U_{+} - U_{-})} - \frac{B_{0}^{1/3}(\widehat{F}_{|T^{*}|}^{-1}(U_{-}) - \Psi^{-1}(U_{-}))}{B_{0}^{1/3}(U_{+} - U_{-})}.$$
(5.23)

The first summand of (5.23) satisfies

$$U_+ \xrightarrow{p} 1-\alpha, \ U_- \xrightarrow{p} 1-\alpha, \ \text{and}$$

(5.24) 
$$\frac{\Psi^{-1}(U_{+}) - \Psi^{-1}(U_{-})}{U_{+} - U_{-}} \xrightarrow{p} \frac{\partial}{\partial x} \Psi^{-1}(1 - \alpha) = \frac{1}{\psi(\Psi^{-1}(1 - \alpha))} = \frac{1}{2\phi(z_{1 - \alpha/2})}$$

as  $pdb \to 0$  and  $n \to \infty$ , where  $\psi(\cdot) = \Psi'(\cdot)$ . The first two results of (5.24) hold by standard results for the sample quantiles of iid uniform random variables. The third result follows from the first two results using the definition of differentiability of  $\Psi^{-1}(\cdot)$  and an almost sure representation argument.

Next, we show that the second and third summands of (5.23) are  $o_p(1)$ . By the argument of Bloch and Gastwirth referred to above,  $B_0^{1/3}(U_+ - U_-) \xrightarrow{p} 2c_{\alpha} > 0$ . Thus, it suffices to show that

(5.25) 
$$B_0^{1/3}(\widehat{F}_{|T^*|}^{-1}(U_+) - \Psi^{-1}(U_+)) \xrightarrow{p} 0 \text{ as } pdb \to 0 \text{ and } n \to \infty$$

and likewise with " $U_+$ " replaced by " $U_-$ ". The proofs of these two results are the same, so we just prove the former.

It suffices to prove (5.25) with  $B_0^{1/3}$  replaced by  $n^{2\xi/3}$  because  $B_0^{1/3} = o(n^{2\xi/3})$  by the assumption of (3.19). For any distribution function F,  $x_1 < F^{-1}(t) \le x_2$  if and only if  $F(x_1) < t \le F(x_2)$ ; see Shorack and Wellner (1986, p. 5). Thus, for any  $\varepsilon > 0$ ,

(5.26)  
$$n^{2\xi/3} |\widehat{F}_{|T^*|}^{-1}(U_+) - \Psi^{-1}(U_+)| \le \varepsilon$$
$$\text{iff } \Psi^{-1}(U_+) - n^{-2\xi/3}\varepsilon < F_{|T^*|}^{-1}(U_+) \le \Psi^{-1}(U_+) + n^{-2\xi/3}\varepsilon$$
$$\text{iff } F_{|T^*|}(\Psi^{-1}(U_+) - n^{-2\xi/3}\varepsilon) < U_+ \le F_{|T^*|}(\Psi^{-1}(U_+) + n^{-2\xi/3}\varepsilon).$$

We have

$$\begin{split} F_{|T^{\bullet}|}(\Psi^{-1}(U_{+}) - n^{-2\xi/3}\varepsilon) \\ &= (F_{|T^{\bullet}|}(\Psi^{-1}(U_{+}) - n^{-2\xi/3}\varepsilon) - \Psi(\Psi^{-1}(U_{+}) - n^{-2\xi/3}\varepsilon)) + \Psi(\Psi^{-1}(U_{+}) - n^{-2\xi/3}\varepsilon) \\ &= O_{p}(n^{-\xi}) + \left(U_{+} + 2\phi(\gamma_{B_{0},n})(-n^{-2\xi/3}\varepsilon)\right) \end{split}$$

 $(5.27) < U_+$  with probability that goes to one as  $pdb \to 0$  and  $n \to \infty$ ,

where the second equality holds by (i) the assumption of (3.18), the fact that  $\Psi^{-1}(U_+) - n^{-2\xi/3} \varepsilon \rightarrow_p z_{1-\alpha/2}$ , and the use of an almost sure representation argument and (ii) a mean value expansion, where  $\gamma_{B_0,n}$  lies between  $\Psi^{-1}(U_+) - n^{-2\xi/3}\varepsilon$ 

and  $\Psi^{-1}(U_+)$  and, hence,  $\gamma_{B_0,n} \to_p z_{1-\alpha/2}$ . An analogous result (with the inequality reversed) holds for  $F_{|T^*|}(\Psi^{-1}(U_+) + n^{-2\xi/3}\varepsilon)$ . Hence, the right-hand side of (5.26) holds with probability that goes to one, which establishes (5.25), and the proof of the second result of (5.19) is complete.

Now we use equation (5.18) and the above proof that (3.20) holds with the random quantity  $B_1$  replaced by the non-random quantity  $B_{11}$  to establish (3.20) as is.

First, we have: For any  $x \in R$ ,

(5.28) 
$$P^*(B_{11}^{1/2}(\hat{k}_{\alpha,B_1} - \hat{k}_{\alpha,\infty}) \le x) = P^*(|T^*|_{B_1,\nu_{11}} \le \hat{k}_{\alpha,\infty} + x/B_{11}^{1/2}).$$

(Note that we take the normalization factor to be  $B_{11}$  not  $B_{1.}$ ) Let  $S_{B_1}$  be as defined above. We have

(5.29) 
$$|T^*|_{B_1,\nu_{11}} \le \hat{k}_{\alpha,\infty} + x/B_{11}^{1/2} \text{ iff } S_{B_1} \le B_1 - \nu_1 = B_1\alpha - (1-\alpha).$$

The random variable  $S_{B_1}$  has a binomial distribution with parameters  $(B_1, p_{B_{11},n})$ , where  $p_{B_{11},n}$  is the same as above. The probability in (5.28) equals

(5.30) 
$$P^* \left( S_{B_1} \le B_1 \alpha - (1 - \alpha) \right) = P^* \left( \frac{S_{B_1} - B_1 p_{B_{11,n}}}{(B_1 p_{B_{11,n}} (1 - p_{B_{11,n}}))^{1/2}} \le \frac{B_1 \alpha - (1 - \alpha) - B_1 p_{B_{11,n}}}{(B_1 p_{B_{11,n}} (1 - p_{B_{11,n}}))^{1/2}} \right).$$

The random variable depending on  $S_{B_1}$  in the right-hand side probability is a normalized sum of independent random variables with a random number,  $B_1$ , of terms in the sum. By the central limit theorem of Doeblin-Anscombe (e.g., see Chow and Teicher (1978, Thm. 9.4.1, p. 317)), it has a standard normal asymptotic distribution, because (i) it has a standard normal asymptotic distribution when  $B_1$ is replaced by the non-random quantity  $B_{11}$  and (ii)  $B_1/B_{11} \rightarrow_p 1$  by (5.18).

Now, for present purposes, equation (5.12) holds without any changes. In addition, by the same argument as in (5.13)–(5.15), coupled with (5.18), the upper bound in the right-hand side of (5.30) converges in probability to  $z_{1-\alpha/2}$  as  $pdb \rightarrow 0$  and  $n \rightarrow \infty$ . These results and the result of the previous paragraph combine to verify (5.16) and (5.17) with  $B_{11}$  replaced by  $B_1$ . That is, (3.20) holds, as desired.

We finish by showing that our formula for the bandwidth parameter  $\hat{m}$  used with the Siddiqui estimator corresponds to that given by Hall and Sheather (1988). In our notation, Hall and Sheather's formula is

(5.31) 
$$\widehat{m} = \operatorname{int}(c_{\alpha}B_0^{2/3}) \text{ and } c_{\alpha} = \left(\frac{1.5z_{1-\alpha/2}^2f^4(q_{1-\alpha})}{3f'(q_{1-\alpha})^2 - f(q_{1-\alpha})f''(q_{1-\alpha})}\right)^{1/3},$$

where  $f(\cdot)$  denotes the density of the iid random variables upon which the sample quantile is based,  $f'(\cdot)$  and  $f''(\cdot)$  denote the first two derivatives of  $f(\cdot)$ ,  $q_{1-\alpha}$  denotes the population quantile, and  $z_{1-\alpha/2}$  is as above. In our case, we use the asymptotic analogues of  $f(\cdot)$  and  $q_{1-\alpha}$ , viz.,  $2\phi(\cdot)$  and  $z_{1-\alpha/2}$ , in the formula. Note that  $\phi'(x) = -x\phi(x)$  and  $\phi''(x) = (x^2 - 1)\phi(x)$ . Hence, our constant  $c_{\alpha}$  satisfies

$$(5.32)c_{\alpha} = \left(\frac{6z_{1-\alpha/2}^{2}\phi^{2}(z_{1-\alpha/2})}{2z_{1-\alpha/2}^{2}+1}\right)^{1/3} = \left(\frac{6z_{1-\alpha/2}^{2}\phi^{4}(z_{1-\alpha/2})}{3\phi'(z_{1-\alpha/2})^{2}-\phi(z_{1-\alpha/2})\phi''(z_{1-\alpha/2})}\right)^{1/3},$$

which corresponds to Hall and Sheather's constant  $c_{\alpha}$ .

# 5.3. Asymptotic Justification for the Three-step Methods for Equal-tailed and One-sided Confidence Intervals

The asymptotic justification of the three-step methods introduced in Section 3.5 for equal-tailed and one-sided confidence intervals is analogous to that given for the symmetric percentile t confidence intervals in Section 3.3. First, we introduce an analogous strengthening of the assumption of asymptotic normality of the t statistic T. For  $\hat{J}_{2,B^*}$ , we assume: For some  $\xi > 0$  and all sequences of constants  $\{x_n : n \ge 1\}$  for which  $x_n \to z_{1-\alpha/2}$  or  $x_n \to -z_{1-\alpha/2}$ , we have

(5.33) 
$$P(T \le x_n) = P(Z \le x_n) + O(n^{-\xi}) \text{ as } n \to \infty \text{ and}$$
$$P^*(T^* \le x_n) = P(Z \le x_n) + O(n^{-\xi}) \text{ as } n \to \infty,$$

where  $Z \sim N(0, 1)$ . For  $\hat{J}_{1,B^*}$ , we make the same assumption except that we do not need it to hold for sequences for which  $x_n \to -z_{1-\alpha/2}$ . (As above, the assumption on  $T^*$  is assumed to hold with probability one with respect to the randomness in the data.)

Assumption (5.33) holds whenever the t statistic and the bootstrap t statistic have one-term Edgeworth expansions, just as in the case of symmetric confidence intervals. When  $\kappa = 1/2$  and  $\hat{\sigma}$  is an  $n^{1/2}$ -consistent estimator of the asymptotic standard error of  $\hat{\theta}$ , then (5.33) typically holds with  $\xi = 1/2$  rather than  $\xi = 1$ , however, because there is no cancelling out of the  $n^{-1/2}$  terms in the Edgeworth expansions of T and  $T^*$  as there are in the Edgeworth expansions of |T| and  $|T^*|$ .

The asymptotic justifications of the three-step method of choosing  $B^*$  are in terms of the limit as  $pdb \to 0$  and  $n \to \infty$ . We assume that  $pdb \to 0$  sufficiently slowly that

$$(5.34) pdb \times n^{\xi} \to \infty \text{ as } n \to \infty,$$

where  $\xi$  is as in (5.33).

The asymptotic justifications of the three-step methods for  $\hat{J}_{2,B^*}$  and  $\hat{J}_{1,B^*}$  are that

$$P^*\left(100\frac{|\hat{q}_{1-\alpha,B_{1\ell}}-\hat{q}_{1-\alpha,\infty}|}{\hat{q}_{1-\alpha,\infty}} \le pdb\right) \to 1-\tau \text{ as } pdb \to 0 \text{ and } n \to \infty \text{ and}$$
$$P^*\left(100\frac{|\hat{q}_{\alpha,B_{1u}}-\hat{q}_{\alpha,\infty}|}{\hat{q}_{\alpha,\infty}} \le pdb\right) \to 1-\tau \text{ as } pdb \to 0 \text{ and } n \to \infty, \text{ where}$$

(5.35) 
$$\begin{aligned} \widehat{q}_{1-\alpha,B_{1h}} &= T^*_{B_{1h},\nu_{1h}}, \ \widehat{q}_{\alpha,B_{1h}} = T^*_{B_{1h},\eta_{1h}}, \\ \widehat{J}_{2,B_{1h}} &= [\widehat{\theta} - n^{-\kappa}\widehat{\sigma}\widehat{q}_{1-\alpha,B_{1h}}, \widehat{\theta} - n^{-\kappa}\widehat{\sigma}\widehat{q}_{\alpha,B_{1h}}] \text{ for } h = \ell, u, \text{ and} \\ \widehat{J}_{1,B_{1\ell}} &= [\widehat{\theta} - n^{-\kappa}\widehat{\sigma}\widehat{q}_{1-\alpha,B_{1\ell}}, \infty). \end{aligned}$$

As above, the probability  $P^*(\cdot)$  denotes probability with respect to the simulation randomness conditional on the infinite sequence of data vectors. Under the assumptions, this conditional result holds with probability one with respect to the randomness in the data.

Equation (5.35) implies that the three-step method for  $\widehat{J}_{2,B^*}$  attains precisely the desired level of accuracy using "small pdb and large n" asymptotics when  $B^* = \max(B_{1\ell}, B_{1u}) > B_0$ . When  $B^* = B_0 > \max(B_{1\ell}, B_{1u})$ , then the accuracy of the three-step method exceeds the desired level of accuracy. An analogous statement holds for the three-step method for  $\widehat{J}_{1,B^*}$ .

The proof of (5.35) is the same as that given in Section 5.2 for symmetric percentile t confidence intervals except that |T| and  $|T^*|$  are replaced throughout by T and  $T^*$ ,  $\hat{k}_{\alpha,B}$  and  $\hat{k}_{\alpha,\infty}$  are replaced throughout by either  $\hat{q}_{1-\alpha,B}$  and  $\hat{q}_{1-\alpha,\infty}$  or  $\hat{q}_{\alpha,B}$  and  $\hat{q}_{\alpha,\infty}$ , and the formulae for  $a_0, B_0, c_\alpha$ , and  $\hat{m}$  are changed to reflect the fact that we are estimating a density that asymptotically equals either  $\phi(z_{1-\alpha})$  or  $\phi(z_\alpha)$  rather than  $2\phi(z_{1-\alpha/2})$ .

## 5.4. Asymptotic Justification for the Three-step Method for Tests with a Specified Significance Level

The asymptotic justification of the three-step method for tests of significance level  $\alpha$  introduced in Section 4.1 is analogous to the asymptotic justification given for symmetric percentile *t* confidence intervals in Section 3.3. First, we introduce an analogous strengthening of the assumption of convergence in distribution to *G* of the test statistic *T* under the null hypothesis. We assume: For some  $\xi > 0$  and all sequences of constants  $\{x_n : n \geq 1\}$  for which  $x_n \to q_{G,1-\alpha}$ , we have

(5.36) 
$$P(T \le x_n) = G(x_n) + O(n^{-\xi}) \text{ as } n \to \infty \text{ and}$$
$$P^*(T^* \le x_n) = G(x_n) + O(n^{-\xi}) \text{ as } n \to \infty$$

when the null hypothesis is true. (The assumption on  $T^*$  is assumed to hold with probability one with respect to the randomness in the data.) Assumption (5.36) holds whenever the test statistic and the bootstrap test statistic have one-term Edgeworth expansions, just as in the case of symmetric confidence intervals. This assumption is widely applicable. See Hall and Horowitz (1996) for an example in which (5.36) holds with the asymptotic distribution G being a chi-squared distribution.

The asymptotic justification of the three-step method of choosing  $B^*$  is in terms of the limit as  $pdb \rightarrow 0$  and  $n \rightarrow \infty$ . We assume that  $pdb \rightarrow 0$  sufficiently slowly that

$$(5.37) pdb \times n^{\xi} \to \infty \text{ as } n \to \infty,$$

where  $\xi$  is as in (5.36).

The asymptotic justification of the three-step method is that

(5.38) 
$$P^*\left(100\frac{|\hat{k}_{\alpha,B_1} - \hat{k}_{\alpha,\infty}|}{\hat{k}_{\alpha,\infty}} \le pdb\right) \to 1 - \tau \text{ as } pdb \to 0 \text{ and } n \to \infty,$$

where  $\hat{k}_{\alpha,B_1} = T^*_{B_1,\nu_1}$ . Under the assumptions, the conditional result above holds with probability one with respect to the randomness in the data.

Equation (5.38) implies that the three-step method attains precisely the desired level of accuracy using "small pdb and large n" asymptotics when  $B^* = B_1 \ge B_0$ . When  $B^* = B_0 > B_1$ , then the accuracy of the three-step method exceeds the desired level of accuracy.

The proof of (5.38) is the same as that given in Section 5.2 for symmetric percentile t confidence intervals except that |T| and  $|T^*|$  are replaced throughout by T and  $T^*$  and the formulae for  $a_0, B_0, c_\alpha$ , and  $\hat{m}$  are changed to reflect the fact that we are estimating a density that asymptotically equals  $g(q_{G,1-\alpha})$  rather than  $2\phi(z_{1-\alpha/2})$ .

## 5.5. Proof of the p-value Results

All of the probabilistic statements below refer to the bootstrap simulation randomness conditional on the sample  $\mathbf{X}$ . First, by the central limit theorem for iid random variables,

(5.39) 
$$\frac{B(\hat{p}_B - \hat{p}_\infty)^2}{\hat{p}_\infty(1 - \hat{p}_\infty)} \xrightarrow{d} \chi^2 \text{as } B \to \infty,$$

because  $\widehat{p}_{\infty}$  does not equal zero or one.

Next, let  $B_{11} = 10,000\chi_{1-\tau}^2(1-\hat{p}_{\infty})/(\hat{p}_{\infty}pdb^2)$ . Note that  $B_{11}$  is non-random. Equation (5.39) holds with B replaced by  $B_{11}$  and with the limit as  $B \to \infty$  replaced by the limit as  $pdb \to 0$  (because the latter forces  $B_{11} \to \infty$ ). Now, by the central limit theorem of Doeblin–Anscombe for a sum of independent random variables with a random number of terms in the sum (e.g., see Chow and Teicher (1978, Thm. 9.4.1, p. 317)), provided  $B_1/B_{11} \to_p 1$  as  $pdb \to 0$ , the result of (5.39) holds with B replaced by  $B_1$  and with the limit as  $B \to \infty$  replaced by the limit as  $pdb \to 0$ . With these changes, (5.39) can be rewritten using (4.16) as

(5.40) 
$$\left(100\frac{|\widehat{p}_{B_1} - \widehat{p}_{\infty}|}{\widehat{p}_{\infty}}\right)^2 \left(\frac{\chi_{1-\tau}^2}{pdp^2}\right) \left(\frac{\widehat{p}_{\infty}(1 - \widehat{p}_{B_0})}{(1 - \widehat{p}_{\infty})\widehat{p}_{B_0}}\right) \xrightarrow{d} \chi^2 \text{ as } pdb \to 0.$$

(The effect of the int(·) function in (4.16) is asymptotically negligible and, hence, is ignored in obtaining the previous equation from (5.39).) By the law of large numbers for iid bounded random variables,  $\hat{p}_{B_0} \rightarrow_p \hat{p}_{\infty}$  as  $pdb \rightarrow 0$  because  $B_0 \rightarrow \infty$  as  $pdb \rightarrow 0$ . This and (5.40) yield

(5.41) 
$$\left(100\frac{|\hat{p}_{B_1} - \hat{p}_{\infty}|}{\hat{p}_{\infty}}\right)^2 \chi_{1-\tau}^2 / pdp^2 \xrightarrow{d} \chi^2 \text{ as } pdb \to 0,$$

which establishes (4.18).

It remains to show that  $B_1/B_{11} \to_p 1$  as  $pdb \to 0$ . This follows from  $\hat{p}_{B_0} \to_p \hat{p}_{\infty}$ , because  $B_1/B_{11} = (\hat{p}_{\infty}(1-\hat{p}_{B_0}))/((1-\hat{p}_{\infty})\hat{p}_{B_0})$ .

# 6. Footnotes

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<sup>2</sup>We received the following comment on an earlier version of this paper, which only considered bootstrap standard errors: "This paper addresses the wrong bootstrap statistics. Standard errors are not interesting quantities for statistical inference. A standard error is useful only if it can be used to obtain a confidence interval or test statistic."

We disagree with this comment. It is not in accord with standard statistical theory or practice. Point estimation accompanied by a measure dispersion of the distribution of the estimator, usually its standard error, is a perfectly valid and widely used method of statistical inference. For example, see Dawid's (1983) entry on "Statistical Inference" in the *Encyclopedia of Statistical Science* and Efron and Tibshirani's (1993, Ch. 6) discussion of the use of the bootstrap for estimating standard errors.

Point estimation with standard errors, confidence intervals, and tests are the three most commonly used forms of statistical inference. Each is a special case of statistical decision theory. None is right or wrong. Each is just more or less suitable for a given application. In practice, point estimation is probably the most common form of statistical inference used in econometrics and many other fields.

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						B				
$\widehat{\gamma}_{2B}$	10	25	50	100	200	350	500	750	1,000	2,000
0	44	28	20	14	10	7.4	6.2	5.1	4.4	3.1
1	54	34	24	17	12	9.1	7.6	6.2	5.4	3.8
2	62	39	28	20	14	10.5	8.8	7.2	6.2	4.4
3	69	44	31	22	15	11.7	10.0	8.0	6.9	4.9

Table 1. Values of pdb as a function of  $\hat{\gamma}_{2B}$  and B when  $\tau = .05$  for Standard Errors

**Table 2.** Values of  $B_1$  as a function of  $\hat{\gamma}_{2B_0}$  and pdb when  $\tau = .05$  for Standard Errors

		pdb	
$\widehat{\gamma}_{2B_0}$	20	10	5
0	48	192	768
1	72	288	1,152
2	96	384	1,536
3	120	480	$ \begin{array}{c c} 1,152\\ 1,536\\ 1,920 \end{array} $

Table 3. Monte Carlo Simulation Results for Standard Errors

	1- au	-	irical vel	$B_0$		E	B <sub>1</sub>			$\widehat{\gamma}_2$	B <sub>0</sub>	
*		$B^*$	$B_1$	_	Mean	Med	Min	Max	Mean	Med	Min	Max
20	.900	.891	.870	34	37	33	12	222	0.15	-0.07	-1.34	11.07
10	.900	.897	.890	136	158	148	76	1,297	0.32	0.17	-0.89	17.13
5	.900	.896	.894	542	645	620	417	4,449	0.38	0.28	-0.46	14.42
20	.950	.945	.931	48	54	49	19	386	0.21	0.01	-1.24	14.06
.10	.950	.947	.944	192	225	213	120	1,805	0.34	0.21	-0.76	16.80
5	.950	.951	.950	768	917	884	630	6,901	0.39	0.30	-0.36	15.97
20	.975	.973	.964	63	71	65	27	545	0.25	0.07	-1.14	15.35
10	.975	.973	.972	251	297	281	165	2,440	0.36	0.24	-0.69	17.44
5	.975	.975	.974	1,004	1,204	1,161	854	11,257	0.40	0.31	-0.30	20.42

A. Error Distribution N(0,1)

**B.** Error Distribution  $t_5$ 

pdb	$1-\tau$		irical vel	$B_0$		1	31			$\widehat{\gamma}_2$	<i>B</i> <sub>0</sub>	
-		B*	$B_1$		Mean	Med	Min	Max	Mean	Med	Min	Max
20	.900	.859	.848	34	45	39	13	276	0.65	0.29	-1.28	14.24
10	.900	.878	.876	136	208	189	88	1,568	1.07	0.78	-0.71	21.14
5	.900	.889	.889	542	874	828	516	6,885	1.22	1.05	-0.10	23.40
20	.950	.925	.917	48	67	59	21	456	0.79	0.43	-1.14	16.97
10	.950	.934	.934	192	300	276	135	2,227	1.12	0.87	-0.60	21.20
5	.950	.944	.944	768	1,244	1,189	781	9,516	1.24	1.10	0.03	22.78
20	.975	.960	.955	63	91	80	31	657	0.88	0.54	-1.03	18.92
10	.975	.966	.966	251	397	368	196	2,727	1.16	0.93	-0.44	19.73
5	.975	.971	.971	1,004	1,631	1,567	1,044	11,264	1.25	1.12	0.08	20.44

**Note:** The reported numbers are the averages over the simulations performed for 20 samples, each of which consists of 25 observations. For each sample, we carry out 2,500 Monte Carlo repetitions.  $\gamma_2$  is calculated for each of the 20 samples using 250,000 bootstrap repetitions. The average of the 20  $\gamma_2$  values is .37 in part A of the Table and 1.26 in part B of the Table.

pdb	$1-\tau$	-	irical vel	B <sub>0</sub>		I	31			$\widehat{\gamma}_{21}$	3 <sub>0</sub> R	
1		<i>B</i> *	$B_1$		Mean	Med	Min	Max	Mean	Med	Min	Max
20	.900	.887	.875	34	54	49	13	349	1.03	0.75	-1.31	17.98
10	.900	.892	.890	136	217	209	83	1,710	1.19	0.90	-0.84	23.01
5	.900	.899	.897	542	91 <b>3</b>	849	505	7,327	1.20	0.96	-0.27	24.77
20	.950	.945	.939	48	79	77	19	511	1.08	0.79	-1.20	18.85
10	.950	.947	.945	192	324	290	139	2,463	1.19	0.92	-0.67	23.37
5	.950	.949	.949	768	1,334	1,203	766	10,186	1.24	0.98	-0.18	24.34
20	.975	.972	.970	63	110	99	31	696	1.12	0.80	-1.08	18.59
10	.975	.973	.971	251	439	395	192	3,305	1.21	0.98	-0.55	24.39
5	.975	.974	.974	1,004	1,645	1,595	1,032	14,267	1.25	1.03	-0.07	24.36

**Table 4.** Monte Carlo Simulation Results for the Bias-corrected Three-stepMethod for Standard Errors with Error Distribution  $t_5$ 

**Note:** The reported numbers are the averages over the simulations performed for 20 samples, each of which consists of 25 observations. For each sample we carry out 2,500 Monte Carlo repetitions.  $\gamma_2$  is calculated for each of the 20 samples using 250,000 bootstrap repetitions. The average of the 20  $\gamma_2$  values is 1.26. The value of R is 407.

$\alpha, c_{\alpha}$		01, .083	7	.0	5, .2086	5	.1	0, .2993	3
au	.01	.05	.10	.01	.05	.10	.01	.05	.10
pdb = 5:									
$a_0$	48	28	20	120	70	49	208	121	85
$B_0$	4799	2799	1999	2399	1399	979	2079	1209	849
$\nu_0$	4752	2772	1980	2280	1330	931	1872	1089	765
$\widehat{m}$	24	17	14	38	27	21	49	34	27
pdb = 10:									
$a_0$	12	7	5	30	18	13	52	31	22
$B_0$	1199	699	499	599	359	259	519	309	219
$ u_0$	1188	693	495	570	342	247	468	279	198
$\widehat{m}$	10	7	6	15	11	9	20	14	11
pdb = 15:									
$a_0$	6	4	3	14	8	6	24	14	10
$B_0$	599	399	299	279	159	119	239	139	99
$ u_0$	594	396	297	266	152	114	216	126	90
$\widehat{m}$	6	5	4	9	7	6	12	9	7

**Table 5.** Values of  $a_0$ ,  $B_0$ ,  $\nu_0$ ,  $c_{\alpha}$ , and  $\hat{m}$  as a Function of  $\alpha$ ,  $\tau$ , and pdb for Symmetric Confidence Intervals

Note: All quantities are defined in the three-step procedure of Section 3.2.

Table 6. Monte Carlo Simulation Results for Symmetric Confidence Intervals

$1-\alpha$	pdb	$1-\tau$	Empirical Level		B <sub>0</sub>		E	31	
			B*	$B_1$		Mean	Med	Min	Max
.90	15	.90	.946	.943	99	258	216	28	1837
.90	10	.90	.924	.920	219	394	364	74	1482
.90	5	.90	.907	.905	849	1317	1280	481	3003
.90	15	.95	.970	.968	139	309	273	47	1532
.90	10	.95	.960	.957	309	524	493	124	1652
.90	5	.95	.952	.951	1209	1825	1785	756	3829
.95	15	.90	.952	.949	119	564	360	31	16709
.95	10	.90	.947	.946	259	754	654	104	4346
.95	5	.90	.915	.915	979	1920	1843	591	5104
.95	15	.95	.989	.989	159	1228	804	69	35579
.95	10	.95	.969	.968	359	884	801	159	3809
.95	5	.95	.955	.955	1399	2611	2531	947	6046

**A.** Error Distribution N(0, 1)

**B.** Error Distribution  $t_5$ 

$1-\alpha$	pdb	1- au	Empirical Level		$B_0$	<i>B</i> <sub>1</sub>					
			$B^*$	$B_1$		Mean	Med	Min	Max		
.90	15	.90	.945	.942	99	275	230	29	1927		
.90	10	.90	.924	.920	219	418	385	79	1560		
.90	5	.90	.908	.907	849	1388	1348	505	3196		
.90	15	.95	.969	.967	139	329	291	48	1686		
.90	10	.95	.959	.957	309	555	521	130	1792		
.90	5	.95	.953	.952	1209	1922	1878	792	4048		
.95	15	.90	.950	.948	119	587	377	32	18426		
.95	10	.90	.947	.946	259	800	696	107	4439		
.95	. 5	.90	.917	.916	979	2055	1972	635	5320		
.95	15	.95	.989	.989	159	1274	839	75	39633		
.95	10	.95	.969	.968	359	941	854	163	3958		
.95	5	.95	.957	.956	1399	2799	2714	1007	6530		

Note: The reported numbers are the averages over the simulations performed for 250 samples, each of which consists of 25 observations. For each sample we carry out 2,000 Monte Carlo repetitions.

$\alpha, c_{\alpha}$		01, .083	8	).	25, .143	36		05, .212	2		10, .307	4
$\overline{\tau}$	.01	.05	.10	.01	.05	.10	.01	.05	.10	.01	.05	.10
pdb = 5:												
$a_0$	69	40	29	124	72	51	219	127	90	473	274	194
$B_0$	6899	3999	2899	4959	2879	2039	4379	2539	1799	4729	2739	1939
$ u_0$	6831	3960	2871	4836	2808	1989	4161	2413	1710	4257	2466	1746
$\eta_0$	69	40	29	124	72	51	219	127	90	473	274	194
$\hat{\eta}_0 \ \widehat{m}$	31	22	18	42	30	24	57	40	32	87	61	48
pdb = 10:												
$\dot{a}_0$	18	10	8	31	18	13	55	32	23	119	69	49
$B_0$	1799	999	799	1239	719	519	1099	639	459	1189	689	489
$ u_0$	1782	990	792	1209	702	507	1045	608	437	1071	621	441
$\eta_0$	18	10	8	31	18	13	55	32	23	119	69	49
$\hat{\eta}_0 \ \widehat{m}$	13	9	8	17	12	10	23	16	13	35	24	20
pdb = 15:												
$a_0$	8	5	4	14	8	6	25	15	10	53	31	22
$B_0$	799	499	399	559	319	239	499	299	199	529	309	219
$ u_0$	792	495	396	546	312	234	475	285	190	477	279	198
$\eta_0$	8	5	4	14	8	6	25	15	10	53	31	22
$\hat{\eta}_0$ $\widehat{m}$	8	6	5	10	7	6	14	10	8	21	15	12

**Table 7.** Values of  $a_0$ ,  $B_0$ ,  $\nu_0$ ,  $\eta_0$ ,  $c_{\alpha}$ , and  $\hat{m}$  as a Function of  $\alpha$ ,  $\tau$ , and pdb for Equal-tailed and One-sided Confidence Intervals

Note: All quantities are defined in the three-step procedure of Section 3.5.

# **Table 8.** Values of $a_0$ , $B_0$ , $\nu_0$ , $c_\alpha$ , and $\hat{m}$ as a Function of $\alpha$ and $\tau$ for pdb = 10 for Tests with Significance Level $\alpha$

$\alpha, c_{\alpha}$	.0	1, .083	7	.0	5, .208	36	.1	0, .299	)3
$\overline{\tau}$	.01	.05	.10	.01	.05	.10	.01	.05	.10
pdb = 10:									
$a_0$	12	7	5	30	18	13	52	31	22
$B_0$	1199	699	499	599	359	259	519	309	219
$\nu_0$	1188	693	495	570	342	247	468	279	198
$\widehat{m}$	10	7	6	15	11	9	20	14	11

## A. Test Statistics with Absolute N(0, 1)Asymptotic Null Distribution

#### **B.** Test Statistics with N(0,1) Asymptotic Null Distribution

$\alpha, c_{\alpha}$	.0	1, .083	8	.0.	5, .212	2	.1	0, .307	4
$\overline{\tau}$	.01	.05	.10	.01	.05	.10	.01	.05	.10
pdb = 10:									
$a_0$	18	10	8	55	32	23	119	69	49
$B_0$	1799	999	799	1099	639	459	1189	689	489
$ u_0$	1782	990	792	1045	608	437	1071	621	441
$\widehat{m}$	13	9	8	23	16	13	35	24	20

C. Test Statistics with  $\chi^2_5$  Asymptotic Null Distribution

$\alpha, c_{\alpha}$	.0	1, .080	0	.0	5, .196	63	.1	0, .282	20
au	.01	.05	.10	.01	.05	.10	.01	.05	.10
pdb = 10:									
$a_0$	18	10	7	35	21	15	52	30	22
$B_0$	1799	999	699	699	419	299	519	299	219
$ u_0$	1782	990	693	665	399	285	468	270	198
$\hat{m}^{ u_0}$	12	8	7	16	11	9	19	13	11

**D.** Test Statistics with  $\chi^2_{15}$  Asymptotic Null Distribution

$\alpha, c_{\alpha}$	.01, .0811				5, .202	22	.10, 2912			
au	.01	.05	.10	.01	.05	.10	.01	.05	.10	
pdb = 10:										
$a_0$	8	5	4	14	9	6	20	12	9	
$B_0$	799	499	399	279	179	119	199	119	89	
$\nu_0$	792	495	396	266	171	114	180	108	81	
$\widehat{m}$	7	6	5	9	7	5	10	8	6	

Note: All quantities are defined in the three-step method of Section 4.1.

1-G(T)	pdb										
- Ale 100	5	10	15	20	30	40	50	100	150	200	300
$\begin{array}{c} \tau = .01;\\ .001\\ .005\\ .010\\ .025\\ .050\\ .10\\ .15\\ .20\\ .30\\ .50\\ .70\\ .90 \end{array}$	50388 23869 15028 10609	12597 5968 3757 2653	11492 5599 2653 1670 1179 688	6465 3150 1492 940 664 387 166	7293 2873 1400 664 418 295 172 74 32 9	4103 1617 788 97 42 18 5	5278 2626 1035 62 27 12 3	6624 1320 657	2944 587 292	1656 330	736 147
$\begin{array}{c} \tau = .05;\\ .001\\ .005\\ .010\\ .025\\ .050\\ .10\\ .15\\ .20\\ .30\\ .50\\ .70\\ .90 \end{array}$	29184 13825 8704 6145	7296 3457 2176 1537	6656 3243 1537 968 683 399 171	3744 1824 865 544 385 224 96	4224 1664 811 385 242 171 100 43 19 5	2376 936 456 56 24 11 3	3057 1521 600 36 16 7 2	3837 765 381	1705 340 169	960 192	427 85
$\begin{array}{c} \tau = .10;\\ .001\\ .005\\ .010\\ .025\\ .050\\ .10\\ .15\\ .20\\ .30\\ .50\\ .70\\ .90 \end{array}$	20596 9757 6143 4337	5149 2440 1536 1085	4698 2289 1085 683 482 282	2643 1288 610 384 272 159 68	2981 1175 573 272 171 121 71 31 13 4	1677 661 322 40 17 8 2	2158 1074 423 26 11 5 2	2708 540 269	1204 240 120	677 135	301 60

**Table 9.** Values of  $B_0$  as a Function of  $\tau$ , pdb, and 1 - G(T) for p-values

Note: All quantities are defined in the three-step method of Section 4.2.