Size Distortion of Bootstrap Unit Root Tests

by

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Abstract

Testing for a unit root in a series obtained by summing a stationary MA(1) process with a parameter close to -1 leads to serious size distortions under the null, on account of the near cancellation of the unit root by the MA component in the driving stationary series. The situation is analysed from the point of view of bootstrap testing, and an exact quantitative account is given of the error in rejection probability of a bootstrap test. A particular method of estimating the MA parameter is recommended, and a new bootstrap procedure with improved properties is proposed. While more computationally demanding than the usual bootstrap, it is much less so than the double bootstrap.

Keywords: Unit root test, bootstrap, MA(1), size distortion

JEL codes: C10, C12, C22

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1. Introduction

There are well-known difficulties in testing for a unit root in a series obtained by summing a stationary series that is a moving average process with a parameter close to -1. Size distortions under the null lead to gross over-rejection of the null hypothesis of a unit root, on account of the near cancellation of the unit root by the MA component in the driving stationary series. We may cite Schwert (1989) and Perron and Ng (1996) in this regard. Galbraith and Zinde-Walsh (1999) introduce a method based on feasible GLS in order to reduce the size distortions induced by an MA(1) driving series. Recently, Richard (2007a) has extended their approach to ARMA(p, q) using explicit bias correction. In this paper, I investigate the properties of a variety of parametric bootstrap unit root tests, and see that quite reliable inference is possible if the bootstrap procedure is chosen carefully.

Sieve bootstraps of one sort or another have been proposed for unit root testing when one wishes to be quite agnostic as to the nature of the driving process. One of the first papers to propose a sieve bootstrap is Bühlmann (1997). The idea was further developed in Bühlmann (1998), Choi and Hall (2000), and Park (2002). In Park (2003), it was shown that under certain conditions a sieve bootstrap test benefits from asymptotic refinements. The sieve in question is an AR sieve, whereby one seeks to model the stationary driving series by a finite-order AR process, the chosen order being data driven.

Sieves based on a set of finite-order MA or ARMA processes are considered in Richard (2007b), and many of Park's results are shown to carry over to these sieve bootstraps. In particular, as might be expected, the MA sieve has better properties than the more usual AR sieve when the driving process is actually MA(1).

The problem considered in this paper is very specific. The unit root test on which the bootstrap tests are based is the augmented Dickey-Fuller test. It is supposed that it is known that the driving stationary process is MA(1), so that the only unknown quantity is the MA parameter. The bootstrap is a parametric bootstrap, for which it is assumed that the innovations of the MA(1) process are Gaussian. Thus no sieve is used in the bootstrap procedure; the bootstrap samples are always drawn from an MA(1) process. In addition, no mention is made in the paper of asymptotic theory or asymptotic refinements. Rather, simulations are used in order to elucidate the finite-sample behaviour of the various tests considered.

Although it is straightforward to estimate the parameters of an AR(p) process by a linear regression, estimating the parameter(s) of an MA or ARMA process is much less simple. In Galbraith and Zinde-Walsh (1994) and (1997), estimators are proposed that are easy to compute, as they are based on running the sort of linear regression used for estimation of AR parameters. However, I show that their estimators are too inefficient for them to be used effectively in the bootstrap context when the MA parameter is close to -1. The maximum likelihood estimator is easy enough to program, but computation time is much longer than for the Galbraith and Zinde-Walsh (GZW) techniques. Further, the MLE has the odd property that its distribution sometimes has an atom with positive probability located at the point where the parameter is exactly equal to -1. A bootstrap DGP with parameter equal to -1 violates a basic principle of bootstrapping, since such a DGP does not have a unit root, whereas the null hypothesis of a unit root test is that one does exist. Here, I propose estimators based on nonlinear least squares (NLS) that are faster to compute than the MLE, although slower than the GZW estimators. They seem almost as efficient as maximum likelihood, and have no atom at -1. It is shown that they work very well for bootstrapping.

The fact that the bootstrap data-generating process (DGP) is completely determined by one single parameter makes it possible to implement a theoretical formula for the **bootstrap discrepancy**, that is, the difference between the true rejection probability of a bootstrap test and the nominal significance level of the test. This makes it possible to estimate the bootstrap discrepancy much more cheaply than usual. It also makes it possible to devise a **discrepancy-corrected** bootstrap test, in which the estimated discrepancy is used to estimate the true rejection probability, and thus adjust the bootstrap P value.

In Section 2, the NLS estimators of the parameters of MA and ARMA processes are described, and given in specific detail for MA(1) and ARMA(1,1). In Section 3, the distributions of these estimators are compared with those of the MLE and the GZW estimators in a set of simulation experiments. Then, in Section 4, the bootstrap discrepancy is studied theoretically, and shown to depend on the joint bivariate distribution of two random variables. In Section 5, simulation-based methods for estimating the bootstrap discrepancy, and approximations to the discrepancy, are studied and compared in another set of simulation experiments. Section 6 studies three possible corrected bootstrap tests: the double bootstrap of Beran (1988), the fast double bootstrap of Davidson and MacKinnon (2007), and a new bootstrap, dubbed the discrepancy-corrected bootstrap, that is a good deal less computationally intensive than the double bootstrap while more so than the fast double bootstrap. It is seen to be at least as good as the other two corrected bootstraps. Some concluding remarks are offered in Section 7.

2. Estimating ARMA models by Nonlinear Least Squares

Suppose that the times series u_t is generated by an ARMA(p,q) process, that we write as

$$(1+\rho(\mathrm{L}))u_t = (1+\theta(\mathrm{L}))\varepsilon_t, \tag{1}$$

where L is the lag operator, ρ and θ are polynomials of degree p and q respectively:

$$\rho(z) = \sum_{i=1}^{p} \rho_i z^i \quad \text{and} \quad \theta(z) = \sum_{j=1}^{q} \theta_j z^j.$$

Note that neither polynomial has a constant term. We wish to estimate the coefficients ρ_i, $i = 1,\ldots,p$, and θ_j, $j = 1,\ldots,q$, from an observed sample u_t, $t = 1,\ldots,n$, under the assumption that the series ε_t is white noise, with variance σ^2.

In a model to be estimated by least squares, the dependent variable, here u_t, is expressed as the sum of a regression function, which in this pure time-series case is a function of lags of u_t, and a white-noise disturbance. The disturbance is ε_t, and so we solve for it in (1) to get

$$\varepsilon = (1+\theta(\mathrm{L}))^{-1}(1+\rho(\mathrm{L}))u.$$

Here, we may omit the subscript t, and interpret u and ε as the whole series. Since ρ and θ have no constant term, the current value, u_t, appears on the right-hand side only once, with coefficient unity. Thus we have

$$\begin{aligned}\varepsilon &= u + \big((1+\theta(\mathrm{L}))^{-1}(1+\rho(\mathrm{L}))-1\big)u\\ &= u + (1+\theta(\mathrm{L}))^{-1}\big(1+\rho(\mathrm{L})-(1+\theta(\mathrm{L}))\big)u.\end{aligned}$$

The nonlinear regression we use for estimation is then

$$u = (1+\theta(\mathrm{L}))^{-1}(\theta(\mathrm{L})-\rho(\mathrm{L}))u+\varepsilon. \tag{2}$$

The regression function is a nonlinear function of the ARMA parameters, the ρ_i and the θ_j.

In order to use the Gauss-Newton algorithm for solving nonlinear least-squares problems, we want the derivatives of the regression function with respect to the ρ_i and θ_j. Note that

$$\partial\rho(\mathrm{L})/\partial\rho_i = \mathrm{L}^i \quad\text{and}\quad \partial\theta(\mathrm{L})/\partial\theta_j = \mathrm{L}^j.$$

Write $R(\mathrm{L}) = (1+\theta(\mathrm{L}))^{-1}(\theta(\mathrm{L})-\rho(\mathrm{L}))$. Then we see at once that

$$\partial R(\mathrm{L})/\partial\rho_i = -(1+\theta(\mathrm{L}))^{-1}\mathrm{L}^i.$$

For the MA parameters, we have that

$$\begin{aligned}\partial R(\mathrm{L})/\partial\theta_j &= (1+\theta(\mathrm{L}))^{-1}\mathrm{L}^j - (1+\theta(\mathrm{L}))^{-2}\mathrm{L}^j(\theta(\mathrm{L})-\rho(\mathrm{L}))\\ &= (1+\theta(\mathrm{L}))^{-1}\mathrm{L}^j(1-R(\mathrm{L})).\end{aligned}$$

A good way to compute series like $R(\mathrm{L})u$ or its derivatives is to make use of the operation of convolution. For two series a and b, the convolution series c is defined by

$$c_t = \sum_{s=0}^{t} a_s b_{t-s}. \tag{3}$$

The definition is messier if the first index of a series is 1 rather than 0. Convolution is symmetric in a and b and is linear with respect to each argument. In fact, the c_t are just the coefficients of the polynomial $c(z)$ given by the product $a(z)b(z)$, with $a(z) = \sum_t a_t z^t$, and similarly for $b(z)$ and $c(z)$.

Define the convolution operator C in the obvious way: $\mathrm{C}(a,b) = c$, where c is the series with c_t given by (3). Although the coefficients of the inverse of a polynomial can be computed using the binomial theorem, it is easier to define an inverse convolution function C^{-1} such that

$$a = \mathrm{C}^{-1}(c, b) \quad \text{iff} \quad c = \mathrm{C}(a, b).$$

Inverse convolution is *not* symmetric with respect to its arguments. It is linear with respect to its first argument, but not the second. It is easy to compute an inverse convolution recursively. If the relation is (3), then, if $b_0 = 1$ as is always the case here, we see that

$$a_0 = c_0 \quad \text{and} \quad a_t = c_t - \sum_{s=0}^{t-1} a_s b_{t-s}.$$

Note that $\mathrm{C}(a, e_0) = a$ and $\mathrm{C}^{-1}(a, e_0) = a$ where $(e_0)_t = \delta_{t0}$. This corresponds to the fact that the polynomial 1 is the multiplicative identity in the algebra of polynomials. In addition, $\mathrm{C}(a, e_j) = \mathrm{L}^j a$, where e_j has element t equal to δ_{tj}.

Let a be the series the first element (element 0) of which is 1, element i of which is the AR parameter ρ_i, for $i = 1, \ldots, p$, and elements a_t for $t > p$ are zero. Define b similarly with the MA parameters. Then the series r containing the coefficients of $R(\mathrm{L})$ is given by

$$r = \mathrm{C}^{-1}(b - a, b),$$

and the series $R(\mathrm{L})u$ is just $\mathrm{C}(u, r)$. The derivatives are

$$\partial r/\partial \rho_i = -\mathrm{C}^{-1}(e_i, b) \quad \text{and} \quad \partial r/\partial \theta_j = \mathrm{C}^{-1}(\mathrm{C}(e_0 - r, e_j), b),$$

The series $\partial R(\mathrm{L})/\partial \rho_i u$ and $\partial R(\mathrm{L})/\partial \theta_j u$ are

$$-\mathrm{C}^{-1}(\mathrm{L}^i u, b) \quad \text{and} \quad \mathrm{C}^{-1}(\mathrm{L}^j(u - \mathrm{C}(u, r)), b).$$

MA(1)

It is useful to specialise the above results for the case of an MA(1) process. The series a is then e_0, and b is $e_0 + \theta e_1$, where we write θ instead of θ_1, since there are no other parameters. Then $R(\mathrm{L}) = \theta(1 + \theta\mathrm{L})^{-1}\mathrm{L}$, and the coefficients of the polynomial R are the elements of the series $r = R(\mathrm{L})e_0 = \theta\mathrm{C}^{-1}(\mathrm{L}e_0, b)$. Consequently, $\mathrm{C}(u, r) = \theta\mathrm{C}^{-1}(\mathrm{L}u, b)$. The only derivative of interest is with respect to θ; it is $\mathrm{C}^{-1}\big(\mathrm{L}(u - \mathrm{C}(u, r)), b\big)$.

The regression (2), which we write as $u = R(\mathrm{L})u + \varepsilon$, is not in fact accurate for a finite sample, because the convolution operation implicitly sets the elements with negative indices of all series equal to 0. For the first element, the regression says therefore that $u_0 = \varepsilon_0$, whereas what should be true is rather that $u_0 = \varepsilon_0 + \theta\varepsilon_{-1}$. Thus the relation $u - \theta\varepsilon_{-1}e_0 = (1 + \theta\mathrm{L})\varepsilon$ is true for all its elements if the lag of ε_0 is treated as zero. We write $\phi = \theta\varepsilon_{-1}$, and treat ϕ as an unknown parameter. The regression model (2) is replaced by

$$u = \phi e_0 + \theta(1 + \theta\mathrm{L})^{-1}\mathrm{L}(u - \phi e_0) + \varepsilon. \tag{4}$$

Although it is perfectly possible to estimate (4) by nonlinear least squares, with two parameters, θ and ϕ, it is faster to perform two nonlinear regressions, each with only one parameter θ. When there is only one parameter, the least-squares problem can be solved as a one-dimensional minimisation. The first stage sets $\phi = 0$, and, for the second stage, ϕ is estimated from the first-stage result, and the result used as a constant in the second stage. The first-order condition for ϕ in the regression (4) is

$$\bigl((1 - R(\mathrm{L})e_0\bigr)^\top\bigl((1 - R(\mathrm{L})\bigr)(u - \phi e_0)\bigr) = 0,$$

Recalling that $R(\mathrm{L})e_0 = r$ and writing $e_0 - r = s$, we can write this condition as

$$s^\top\bigl((1 - R(\mathrm{L}))u - \phi s\bigr) = 0 \quad \text{whence} \quad \phi = \frac{s^\top(1 - R(\mathrm{L}))u}{s^\top s}.$$

In order to compute the estimate of ϕ from the first stage, the series s is set up with $s_0 = 1$, $s_t = -r_t$ for $t > 0$, and we note that $(1 - R(\mathrm{L}))u$ is just the vector of residuals from the first stage regression.

ARMA(1,1)

The ARMA(1,1) model can be written as $(1 + \rho\mathrm{L})u = (1 + \theta\mathrm{L})\varepsilon$. The polynomial $R(\mathrm{L})$ is $(\theta - \rho)(1 + \theta\mathrm{L})^{-1}\mathrm{L}$. Again, the regression $u = R(\mathrm{L})u + \varepsilon$ is not accurate when certain elements with negative indices are set to 0. However, as we will see, the regression

$$u = R(\mathrm{L})u + z(u_0 - \varepsilon_0) + \varepsilon, \tag{5}$$

where $z_t = (-\theta)^t$, turns out to be correct for all its elements. We show this by induction. For $t = 0$, (5) gives $u_0 = u_0 - \varepsilon_0 + \varepsilon_0$, which is obviously true. Suppose that the relation is true for element t, that is, $u_t = (R(\mathrm{L})u)_t + (-\theta)^t(u_0 - \varepsilon_0) + \varepsilon_t$. Then the right-hand side of (5) for element $t + 1$ is

$$\begin{aligned}
&(R(\mathrm{L})u)_{t+1} + (-\theta)^{t+1}(u_0 - \varepsilon_0) + \varepsilon_{t+1}\\
&= (\theta - \rho)((1 + \theta\mathrm{L})^{-1}u)_t + (-\theta)^{t+1}(u_0 - \varepsilon_0) + \varepsilon_{t+1}\\
&= -\rho u_t + \theta u_t + (\theta - \rho)\bigl((1 + \theta\mathrm{L})^{-1} - 1)u_t + (-\theta)^{t+1}(u_0 - \varepsilon_0) + \varepsilon_{t+1}\\
&= -\rho u_t + \theta\Bigl(u_t - (\theta - \rho)(1 + \theta\mathrm{L})^{-1}u_{t-1} - (\theta)^t(u_0 - \varepsilon_0)\Bigr) + \varepsilon_{t+1}\\
&= -\rho u_t + \theta\varepsilon_t + \varepsilon_{t+1} = u_{t+1}.
\end{aligned}$$

This completes the induction proof.

Again we can treat $\phi \equiv u_0 - \varepsilon_0$ as an unknown parameter, and apply nonlinear least squares to (5). Alternatively, we can again use a two-stage procedure, setting $\phi = 0$ in the first stage, and treating an estimate of ϕ from the first stage as a constant in the second stage. In each step, there are then only two parameters, θ and ρ. The first-order condition for ϕ is

$$z^\top\bigl((1 - R(\mathrm{L}))u - \phi z\bigr) = 0 \quad \text{whence} \quad \phi = \frac{z^\top(1 - R(\mathrm{L}))u}{z^\top z}.$$

Once more we note that $(1 - R(\mathrm{L}))u$ is the series of residuals from the first stage.

3. Comparison of Estimators for MA(1) and ARMA(1,1)

Asymptotic efficiency in the estimation of the parameter θ of an MA(1) process is achieved by Gaussian maximum likelihood (ML) if the disturbances are Gaussian. But ML is a rather costly procedure in this case, and so it is of interest to see how much efficiency is lost by using other, more computationally friendly, methods.

The loglikelihood function for the MA(1) model is

$$\ell(\theta, \sigma^2) = -\frac{n}{2} \log 2\pi\sigma^2 - \frac{1}{2} \log \det \boldsymbol{\Sigma}(\theta) - \frac{1}{2\sigma^2} \boldsymbol{u}^\top \boldsymbol{\Sigma}^{-1}(\theta) \boldsymbol{u}, \tag{6}$$

where $\sigma^2 = \text{Var}(\varepsilon_t)$ and $\boldsymbol{\Sigma}(\theta)$ is an $n \times n$ Toeplitz matrix with all diagonal elements equal to $1 + \theta^2$ and all elements of the diagonals immediately below and above the principal diagonal equal to θ. The notation $\boldsymbol{u}$ is just vector notation for the series u.

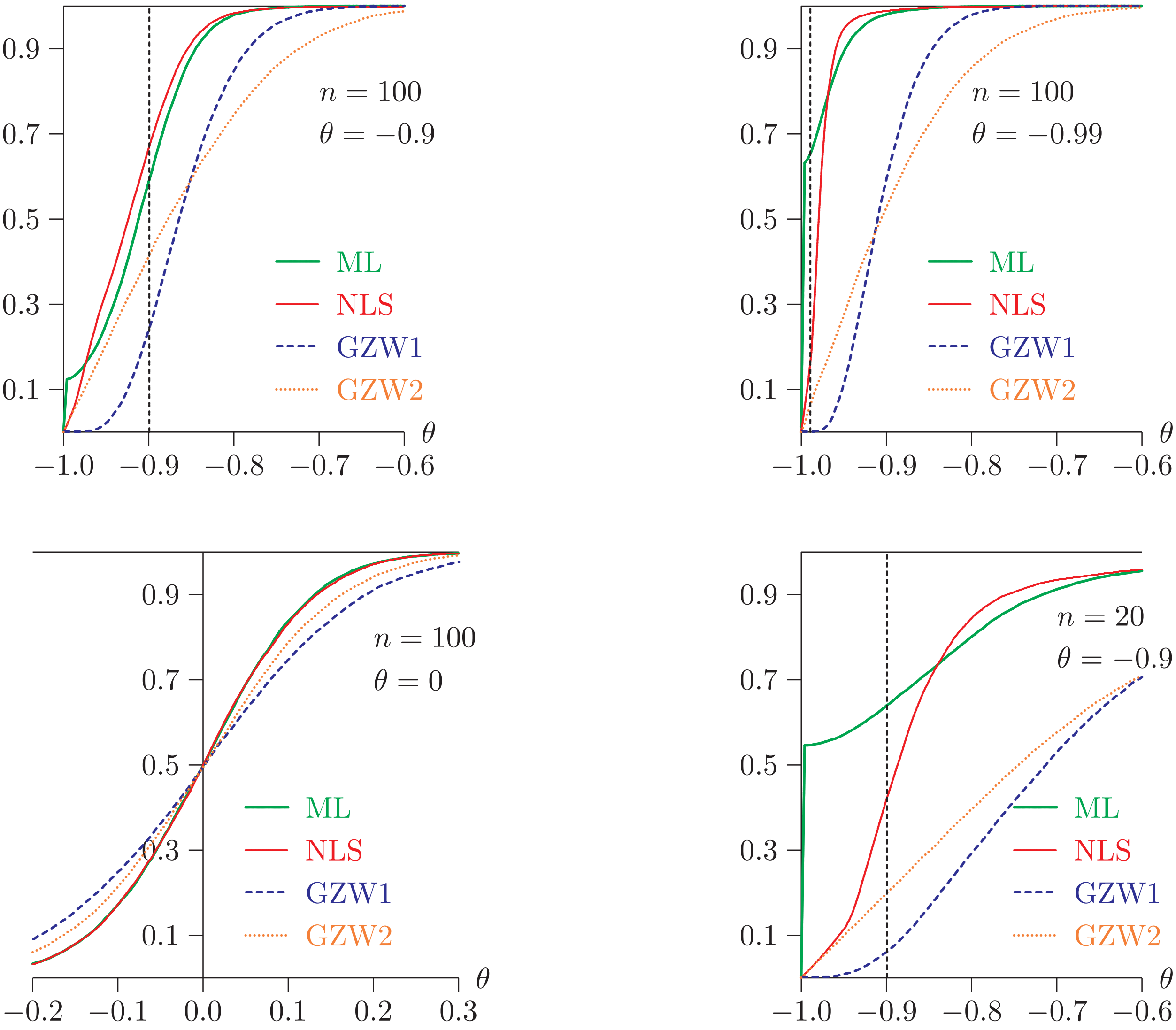


Figure 1: Comparison of MA(1) estimators

We may concentrate the loglikelihood (6) by maximising with respect to σ^2. For given θ, the value of σ^2 that maximises (6) is

$$\hat{\sigma}^2(\theta) = \tfrac{1}{n}\boldsymbol{u}^\top\boldsymbol{\Sigma}^{-1}(\theta)\boldsymbol{u}.$$

Thus the concentrated loglikelihood is

$$\tfrac{n}{2}(\log n - \log 2\pi - 1) - \tfrac{n}{2}\log \boldsymbol{u}^\top\boldsymbol{\Sigma}^{-1}(\theta)\boldsymbol{u} - \tfrac{1}{2}\log\det\boldsymbol{\Sigma}(\theta). \tag{7}$$

This expression can be maximised with respect to θ by minimising

$$\ell(\theta) \equiv n\log \boldsymbol{u}^\top\boldsymbol{\Sigma}^{-1}(\theta)\boldsymbol{u} + \log\det\boldsymbol{\Sigma}(\theta), \tag{8}$$

and this can be achieved by use of any suitable one-dimensional minimisation algorithm, including Newton's method, since it is straightforward to compute the derivative of (8) with respect to θ:

$$\frac{\partial\ell(\theta)}{\partial\theta} = -\frac{n}{Q(\theta)}\boldsymbol{u}^\top\boldsymbol{\Sigma}^{-1}(\theta)\frac{\partial\boldsymbol{\Sigma}(\theta)}{\partial\theta}\boldsymbol{\Sigma}^{-1}(\theta)\boldsymbol{u} + \operatorname{tr}\boldsymbol{\Sigma}^{-1}(\theta)\frac{\partial\boldsymbol{\Sigma}(\theta)}{\partial\theta},$$

where $Q(\theta) \equiv \boldsymbol{u}^\top\boldsymbol{\Sigma}^{-1}(\theta)\boldsymbol{u}$. Note that the matrix $\partial\boldsymbol{\Sigma}(\theta)/\partial\theta$ is a Toeplitz matrix with 2θ on the principal diagonal, and 1 on the two adjacent diagonals. It remains true, however, that this minimisation is considerably slower than the nonlinear least-squares method developed in the previous section.

Other methods for estimating MA models have been proposed by Galbraith and Zinde-Walsh (1994) and for ARMA models by the same authors (1997). Their methods are based on estimating the following AR(k) model by ordinary least squares:

$$u_t = \sum_{i=1}^{k} a_i u_{t-i} + \text{residual}, \quad t = k+1,\ldots,n. \tag{9}$$

For an ARMA(p,q) model, k is chosen considerably greater than $p+q$. The estimators are consistent as $k \to \infty$ while $k/n \to 0$, but are not asymptotically efficient. They are however simple and fast to compute, as they involve no iterative procedure.

Let the OLS estimates of the parameters a_i in (9) be denoted as $\hat{a}_i$. For the MA(1) model $u_t = \varepsilon_t + \theta\varepsilon_{t-1}$, the simplest estimator of θ is just $\hat{a}_1$. Another estimator, that can be traced back to Durbin (1959), is the parameter estimate from the OLS regression of the vector $[\hat{a}_1 \ldots \hat{a}_k]^\top$, on the vector $[1 \quad -\hat{a}_1 \ldots -\hat{a}_{k-1}]^\top$. For the ARMA(1,1) model $u_t = \rho u_{t-1} + \varepsilon_t + \theta\varepsilon_{t-1}$, an estimator analogous to the simplest estimator in the MA(1) case is not available. For the other method, first θ is estimated by regressing $[\hat{a}_2 \ldots \hat{a}_k]^\top$ on $-[\hat{a}_1 \ldots \hat{a}_{k-1}]$ – essentially the regression used for MA(1) but without the first observation. Then, for ρ, the residuals $\hat{v}_t$ from (9) are used to construct the series $u_t^* = u_t - \hat{\theta}\hat{v}_{t-1}$, which is then regressed on the first lag of u_t, with the k initial observations omitted. The estimate $\hat{\rho}$ is the parameter estimated from this last regression.

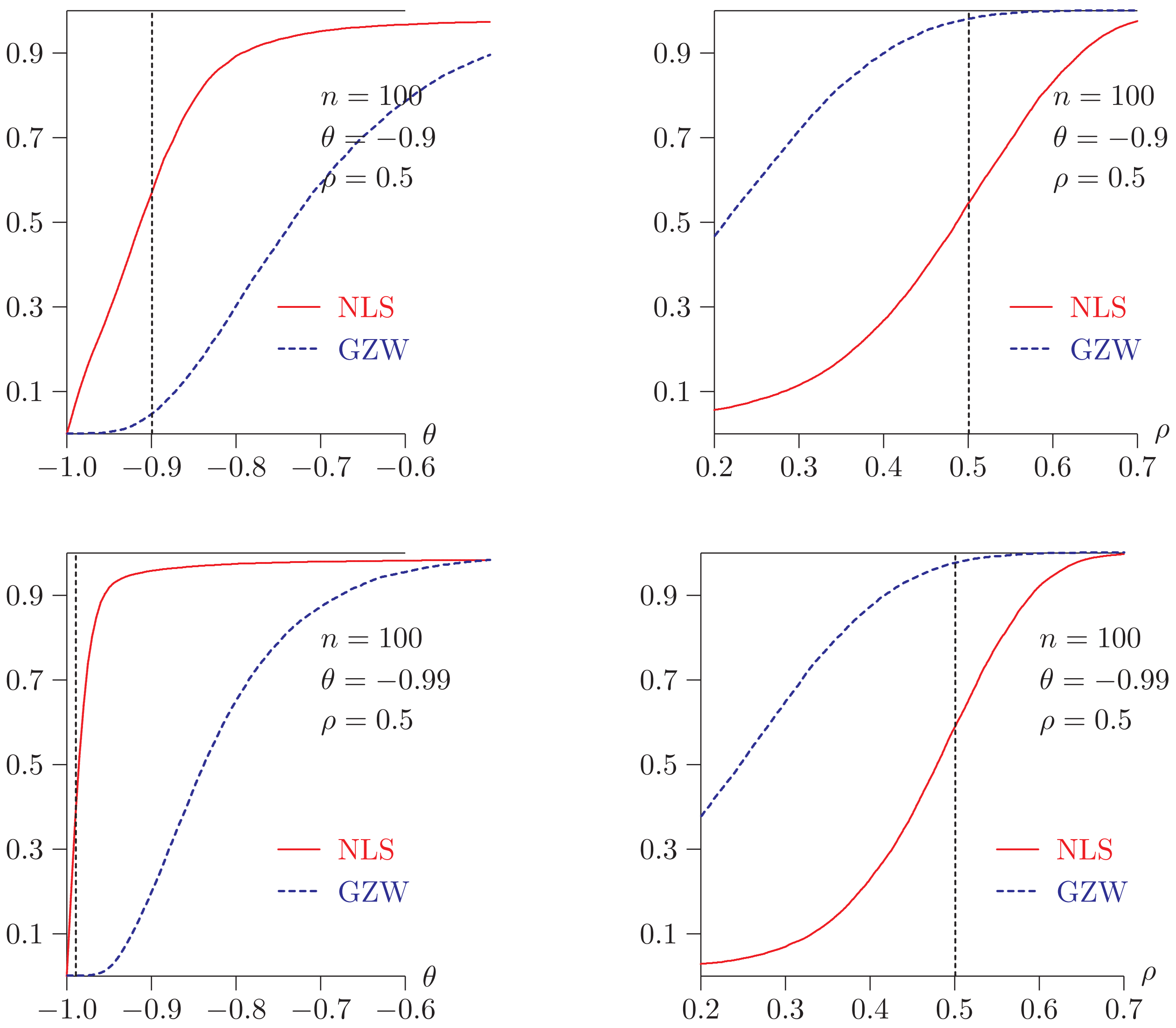


Figure 2a: Comparison of ARMA(1,1) estimators

We focus first on the MA(1) model. Any of the estimation methods so far discussed can give an estimate of θ outside the interval $[-1, 1]$. But the processes with parameters θ and $1/\theta$ are observationally equivalent. Thus whenever an estimate outside $[-1, 1]$ is obtained, it is simply replaced by its reciprocal. In Figure 1 are shown estimated CDFs of four estimators, (Gaussian) maximum likelihood (ML), nonlinear least-squares using the two-stage procedure based on (4), with $\rho(z) = 0$, $\theta(z) = \theta z$ (NLS), Galbraith and Zinde-Walsh's first estimator $\hat{a}_1$ (GZW1), and their second estimator (GZW2). In all but the bottom right panel of the figure the sample size is $n = 100$. The distributions are shown for values of θ of -0.9, -0.99, and 0. The length of the GZW preliminary autoregression (9) is $k = 20$. In the bottom right panel, $n = 20$, $\theta = -0.9$, and $k = 6$. It is well known that the greatest challenge for estimators of the MA(1) parameter arises when θ is close to -1. The overall picture is clear enough. Both ML and NLS outperform the GZW estimators except when $\theta = 0$, or, more generally, when θ is distant from -1. GZW1 has much greater

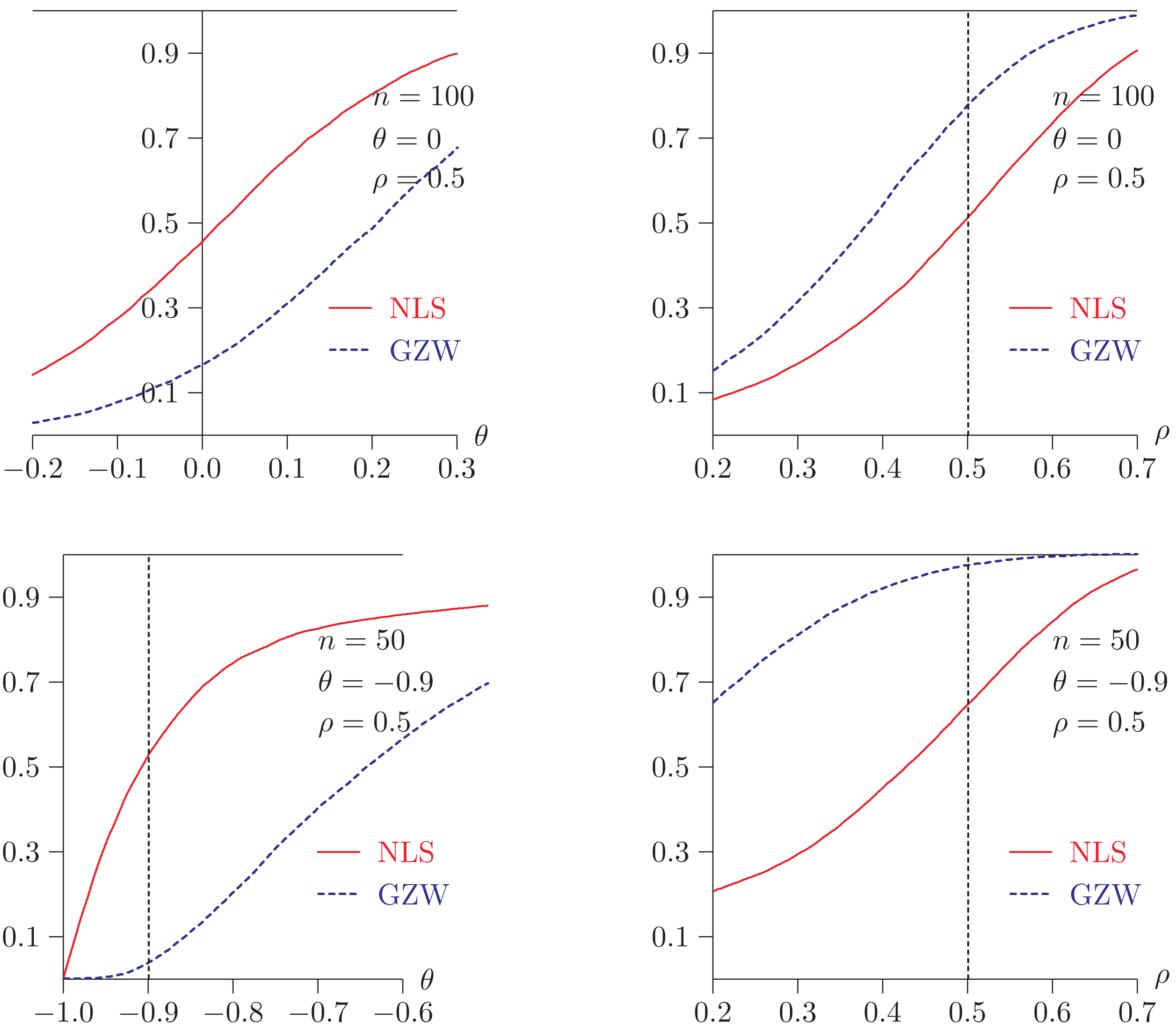


Figure 2b: Comparison of ARMA(1,1) estimators

variance than the other estimators, and GZW2 is heavily biased to the right. For $n = 20$, the concentration of ML estimates close to -1 is seen; the other estimators do not exhibit this feature, which is much less visible for ML itself for the larger sample size. ML and NLS are almost unbiased for $n = 100$, and do not greatly differ. Experiments with other values of θ show that the four estimators have similar distributions when n is large enough and θ is greater than around -0.5

Results for the ARMA(1,1) model are shown in Figures 2a and 2b for the NLS and GZW2 estimators. Since GZW1 was obviously inferior to all the other estimators for MA(1), there is no need to consider it here. Since ML and NLS gave very similar results with MA(1), while NLS is easier and faster to compute, we have limited attention to it here. It is obtained by the two-stage procedure based on regression (5). Again, estimates of θ outside the interval $[-1, 1]$ are replaced by their reciprocals.

Setups like those of Figure 1 are examined, but with an AR parameter $\rho = 0.5$. Both ρ and θ have to be estimated, and so the (marginal) distributions of each are shown for each configuration, the distribution of the estimated θ on the left, and of ρ on the right. As before, NLS is reasonably reliable, while GZW is biased and has greater variance. The inescapable conclusion is that using the GZW estimator in a bootstrap procedure will give rise to serious size distortion.

4. The Bootstrap Discrepancy

Suppose that a test statistic τ is designed to test a particular null hypothesis. The set of all DGPs that satisfy that hypothesis is denoted as $\mathbb{M}_0$; this set constitutes what we may call the null model. A bootstrap test based on the statistic τ approximates the distribution of τ under a DGP $\mu \in \mathbb{M}_0$ by its distribution under a bootstrap DGP that also belongs to $\mathbb{M}_0$ and can be thought of as an estimate of the true DGP μ.

We define the **bootstrap discrepancy** as the difference, as a function of the true DGP and the nominal level, between the actual rejection probability of the bootstrap test and the nominal level. In order to study it, we suppose, without loss of generality, that the test statistic is already in approximate P value form, so that the rejection region is to the left of a critical value.

The **rejection probability function**, or RPF, depends both on the nominal level α and the DGP μ. It is defined as

$$R(\alpha, \mu) \equiv \Pr_\mu(\tau < \alpha). \tag{10}$$

We assume that, for all $\mu \in \mathbb{M}_0$, the distribution of τ has support $[0, 1]$ and is absolutely continuous with respect to the uniform distribution on that interval. For given μ, $R(\alpha, \mu)$ is just the CDF of τ evaluated at α. The inverse of the RPF is the **critical value function**, or CVF, which is defined implicitly by the equation

$$\Pr_\mu\bigl(\tau < Q(\alpha, \mu)\bigr) = \alpha. \tag{11}$$

It is clear from (11) that $Q(\alpha, \mu)$ is the α-quantile of the distribution of τ under μ. In addition, the definitions (10) and (11) imply that

$$R\bigl(Q(\alpha, \mu), \mu\bigr) = Q\bigl(R(\alpha, \mu), \mu\bigr) = \alpha \tag{12}$$

for all α and μ.

In what follows, we ignore simulation randomness in the estimate of the distribution of τ under the bootstrap DGP, which we denote by μ^*. The bootstrap critical value for τ at level α is $Q(\alpha, \mu^*)$. If τ is approximately (for example, asymptotically) pivotal relative to the model $\mathbb{M}_0$, realisations of $Q(\alpha, \mu^*)$ should be close to α. This is true whether or not the true DGP belongs to the null model, since the bootstrap DGP μ^* always does so. The bootstrap discrepancy arises from the fact that, in a finite sample, $Q(\alpha, \mu^*) \neq Q(\alpha, \mu)$ even when $\mu \in \mathbb{M}$.

Rejection by the bootstrap test is the event $\tau < Q(\alpha, \mu^*)$. Applying the increasing transformation $R(\cdot, \mu^*)$ to both sides and using (12), we see that the bootstrap test rejects whenever

$$R(\tau, \mu^*) < R\big(Q(\alpha, \mu^*), \mu^*\big) = \alpha.$$

Thus the bootstrap P value is just $R(\tau, \mu^*)$, which can therefore be interpreted as a bootstrap test statistic.

If instead we apply the increasing transformation $R(\cdot, \mu)$ to the inequality $\tau < Q(\alpha, \mu^*)$, it follows that rejection by the bootstrap test can also be expressed as $R(\tau, \mu) < R\big(Q(\alpha, \mu^*), \mu\big)$. We define two random variables, one a deterministic function of τ, the other a deterministic function of μ^*, the other random element involved in the bootstrap test. The first variable is $p \equiv R(\tau, \mu)$. It is distributed as U(0,1) under μ, because $R(\cdot, \mu)$ is the CDF of τ under μ and because we have assumed that the distribution of τ is absolutely continuous on the unit interval for all $\mu \in \mathbb{M}$. The second random variable is $q \equiv R(Q(\alpha, \mu^*), \mu) - \alpha = R(Q(\alpha, \mu^*), \mu) - R(Q(\alpha, \mu), \mu)$. Thus rejection by the bootstrap test is the event $p < \alpha + q$. Let the CDF of q under μ conditional on the random variable p be denoted as $F(q \mid p)$. Then it is shown in Davidson and MacKinnon (2006) that the bootstrap discrepancy can be expressed as

$$\int_{-\alpha}^{1-\alpha} x \, \mathrm{d}F(x \mid \alpha + x). \tag{13}$$

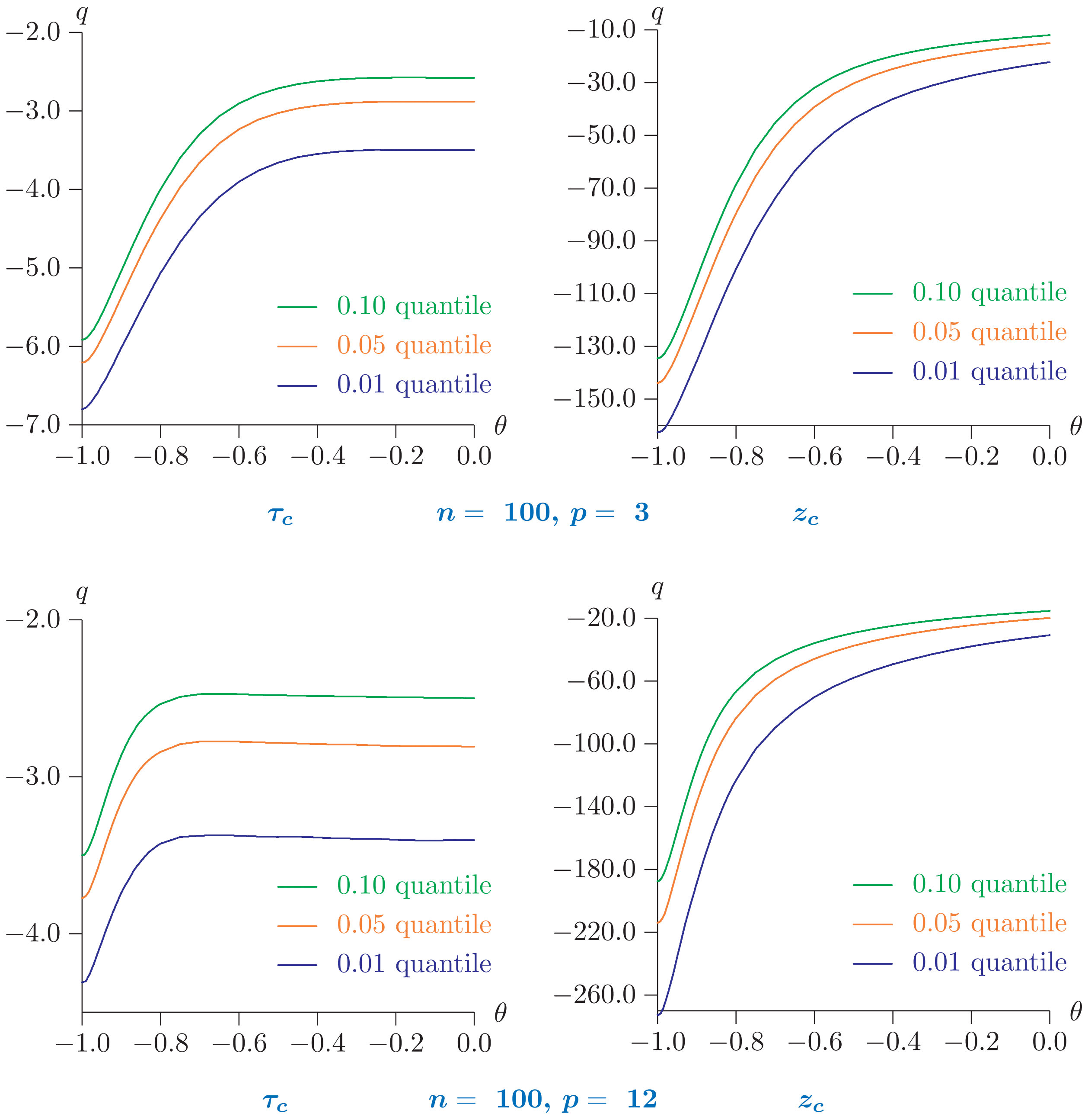
The random variable $q+\alpha$ is the probability that a statistic generated by the DGP μ is less than the α-quantile of the bootstrap distribution, conditional on that distribution. The expectation of q can thus be interpreted as the bias in rejection probability when the latter is estimated by the bootstrap. The actual bootstrap discrepancy, which is a nonrandom quantity, is the expectation of q conditional on being at the margin of rejection.

In order to understand, and, if possible, control for the size distortion of a bootstrap unit-root test when the innovation process is MA(1) with α close to -1, we study the critical value function of the test statistic most frequently used to test the null hypothesis of a unit root, namely the augmented Dickey-Fuller (ADF) test. The DGPs used to generate the data of the simulation experiment take the form

$$u_t = \varepsilon_t + \theta\varepsilon_{t-1}, \quad y_t = y_0 + \sum_{s=1}^{t} u_t, \tag{14}$$

where the ε_t are IID N(0,1). The test statistics are computed using the ADF testing regression

$$\Delta y_t = \beta_0 + \beta_1 y_{t-1} + \sum_{i=1}^{p} \gamma_i \Delta y_{t-1} + \text{residual}. \tag{15}$$



τ_c $\quad n = 100, p = 3 \quad$ z_c

τ_c $\quad n = 100, p = 12 \quad$ z_c

Figure 3: Critical value functions

The z_c statistic is $n\hat{\beta}_1$; the τ_c statistic is the conventional t statistic for the hypothesis that $\beta_1 = 0$. Under the null hypothesis that the series y_t has a unit root, these two statistics have well-known but nonstandard asymptotic distributions.

The variance of the ε_t is set to 1 without loss of generality, since both statistics are scale invariant. In fact, both statistics are also numerically invariant to changes in the value of the starting value y_0, and so we can without loss of generality set $y_0 = 0$ in our simulations. We vary the MA parameter θ from 0 to -0.8 by steps of 0.05, and from -0.8 to -0.99 by steps of 0.01. For each value we estimate the 0.01, 0.05, and 0.10 quantiles of the distribution of each statistic, using 99,999 replications. The same random numbers are used for each value of θ in order to achieve a smoother estimate of the critical value function, which is the quantile of the statistic as a function of θ.

Figure 3 shows the CVFs for the τ_c and z_c statistics for the 0.01, 0.05, and 0.1 quantiles. In the upper panels, the sample size $n = 100$ and the number p of lags of Δy_t is 3. In the lower panels, the functions are graphed for $n = 100$ and $p = 12$. The choice of the statistic τ_c and of $p = 12$ gives the smallest variation of the CVF, and so, for the rest of this study, we examine the consequences of making this choice.

5. Estimating the Bootstrap Discrepancy

The formula (13) cannot be implemented unless one knows the function F, the CDF of q conditional on p. This function can be estimated arbitrarily well by simulation if we can generate IID joint realisations of p and q. But that is made difficult by the fact that, for a given DGP μ, both p and q are defined in terms of the functions R and Q, which are in general unknown. Estimating R and Q by simulation is also quite possible, for a given μ. But q is defined using the bootstrap DGP μ^*, and, since this is random, we cannot estimate $Q(\cdot, \mu^*)$ for all possible realisations of μ^* in a single experiment.

The case of the model with DGPs of the form (14) is much more tractable than most, however, since the bootstrap DGP is completely determined by a single parameter. The bootstrap procedure for this model with MA(1) disturbances is as follows. First, a data set is used to obtain an estimate $\hat{\theta}$ of the MA(1) parameter, and also to compute the ADF τ_c statistic using (15). Then the bootstrap DGP is given by (14), with $y_0 = 0$, and $\theta = \hat{\theta}$. A sufficient number of bootstrap samples are generated, for each of which a bootstrap ADF τ_c statistic is computed. The bootstrap P value is estimated by the proportion of bootstrap statistics more extreme than the statistic computed from the original data.

Since any DGP of model (14) is uniquely characterised by the parameter θ, it is convenient to replace the notation μ by θ. Simulations of the sort used to obtain the data graphed in Figure 3 can be used for simulation-based estimates of $Q(\alpha, \theta)$ for any given α and θ. For a set of values of α and a set of values of θ, we can construct a table giving the values of $Q(\alpha, \theta)$ for the chosen arguments. There are as many experiments as there are argument pairs, but, as for Figure 3, it is advisable to use the same random numbers for each experiment.

Next, we can perform another set of experiments in which we obtain simulation-based estimates of $R(Q(\alpha, \theta_1), \theta_2)$ for the set of values chosen for α, and for any pair (θ_1, θ_2) of values in the set chosen for θ. Here we need only as many experiments as there are values of θ, since, after fixing θ_2, we generate a large number of τ_c statistics using the DGP characterised by θ_2, and then, for each value of $Q(\alpha, \theta_1)$ in the set, estimate $R(Q(\alpha, \theta_1), \theta_2)$ as the proportion of the generated statistics less than $Q(\alpha, \theta_1)$.

Now suppose that a single realisation from the DGP characterised by a value of θ in the chosen set gives rise to an estimate $\hat{\theta}$. For given α, we can then use the simulated values of $R(Q(\alpha, \theta_1), \theta)$ in order to interpolate the value of $R(Q(\alpha, \hat{\theta}), \theta)$. As Figure 3 shows, the quantiles vary quite smoothly as functions of θ, and so interpolation should work well. In the experiments to be described, cubic splines were used for this purpose.

If we now repeat the operation of the previous paragraph many times, we get a set of realisations of the random variable q by subtracting α from the simulated $R(Q(\alpha,\hat{\theta}),\theta)$. But for each repetition, we also compute the value of the τ_c statistic, and keep the pair (τ_c, q). When all the repetitions have been completed, we sort the pairs in increasing order of τ_c. For each repetition, then, we estimate the random variable p by the index of the associated pair in the sorted set, divided by the number of repetitions. This is equivalent to using the set of generated τ_c values to estimate $R(\cdot,\theta)$, and evaluating the result at the particular τ_c for each repetition. We end up with a set of IID joint realisations of p and q.

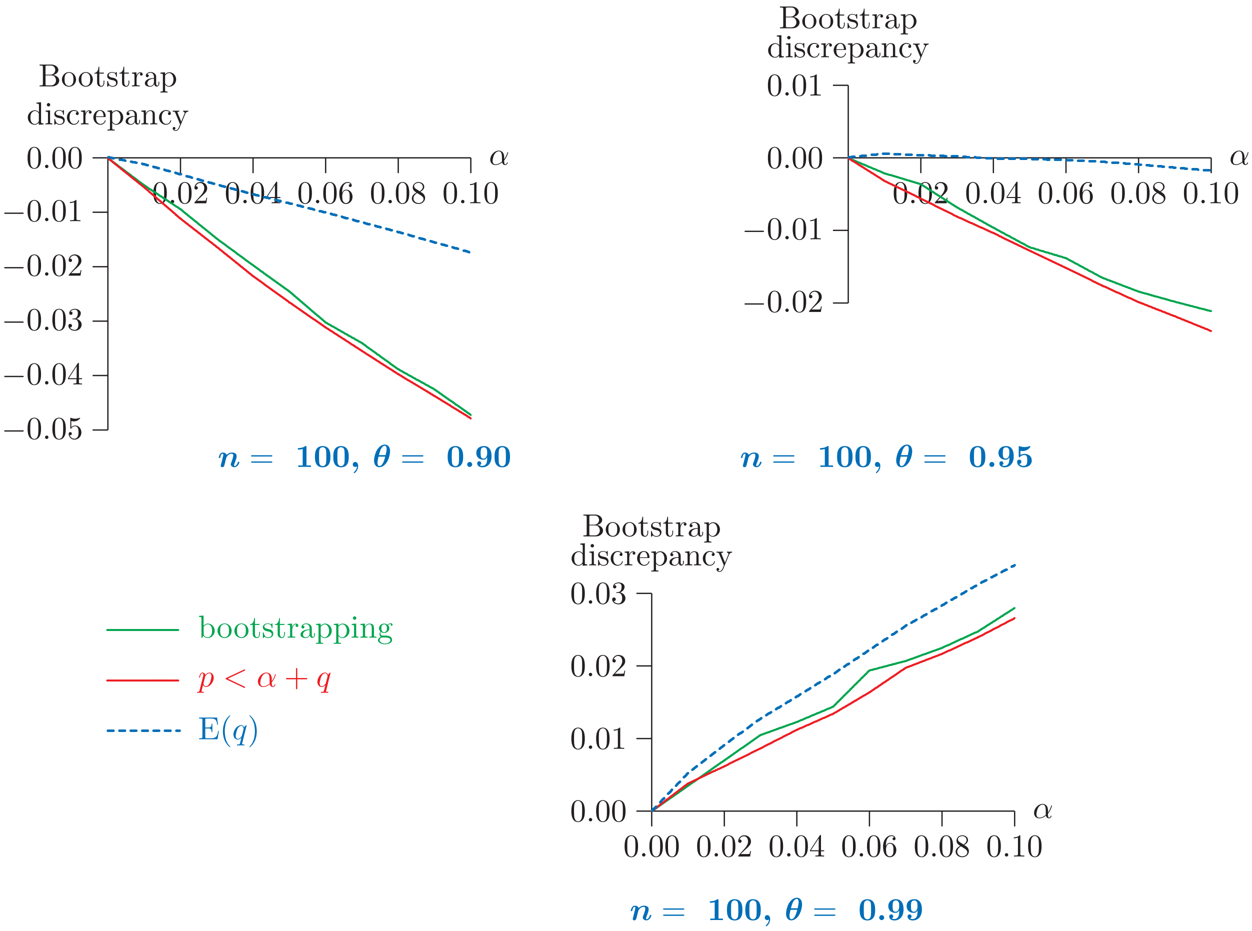
The most straightforward estimate of the rejection probability (RP) of the bootstrap test at significance level α is just the proportion of the repetitions for which $p < \alpha + q$. The bootstrap discrepancy is then estimated by the error in rejection probability (ERP), that is, the difference between the RP and α. Another estimate is somewhat simpler to compute, and gives almost identical results. For it, we do not transform τ_c and $Q(\alpha,\hat{\theta})$, but rather use the table of values of $Q(\alpha,\theta)$ to interpolate the value of $Q(\alpha,\hat{\theta})$. The bootstrap discrepancy is estimated by the proportion of repetitions with $\tau_c < Q(\alpha,\hat{\theta})$, minus α. It is of interest to see how close two approximations to the bootstrap discrepancy come to the estimate obtained in this way. Both of these can be readily computed using the set of joint realisations of p and q. The first is the estimated expectation of q, which is just the average of the realised q, with no reference to the associated p. The second is an estimate of the expectation of q conditional on $p = \alpha$, that is,

$$\int_{-\alpha}^{1-\alpha} x \, \mathrm{d}F(x \,|\, \alpha),$$

rather than the exact expression (13). This conditional expectation can readily be estimated with a kernel estimator.

In Figure 4 are depicted plots of the bootstrap discrepancy as a function of the nominal level α for values between 0.01 and 0.10. The three panels show results for three different true DGPs, with $\theta = 0.90$, 0.95, and 0.99, with sample size $n = 100$. The NLS procedure was used for the estimation of θ. Three simulation-based estimates are given. The first two were computed using 99,999 repetitions of the experiment described above, the first the proportion of repetitions with $p < \alpha + q$, the second the expectation of q. The expectation conditional on $p = \alpha$ is so close to the first estimate that it would not be distinguishable from it in the graph. The last estimate was computed after 10,000 repetitions of a full-blown bootstrap test, with 399 bootstrap repetitions.

It can be seen that the unconditional expectation of q is not a very good estimate of the bootstrap discrepancy. In all cases, it overestimates the RP. Of the other two estimates, the one based on the realisations of p and q is probably superior from the theoretical point of view, since the one based on full-blown bootstrapping, besides being based on fewer repetitions, gives the bootstrap discrepancy for a test *with 399 bootstrap repetitions*, while the other estimates the theoretical bootstrap discrepancy, corresponding to an infinite



$\boldsymbol{n =}$ **100,** $\boldsymbol{\theta =}$ **0.90**

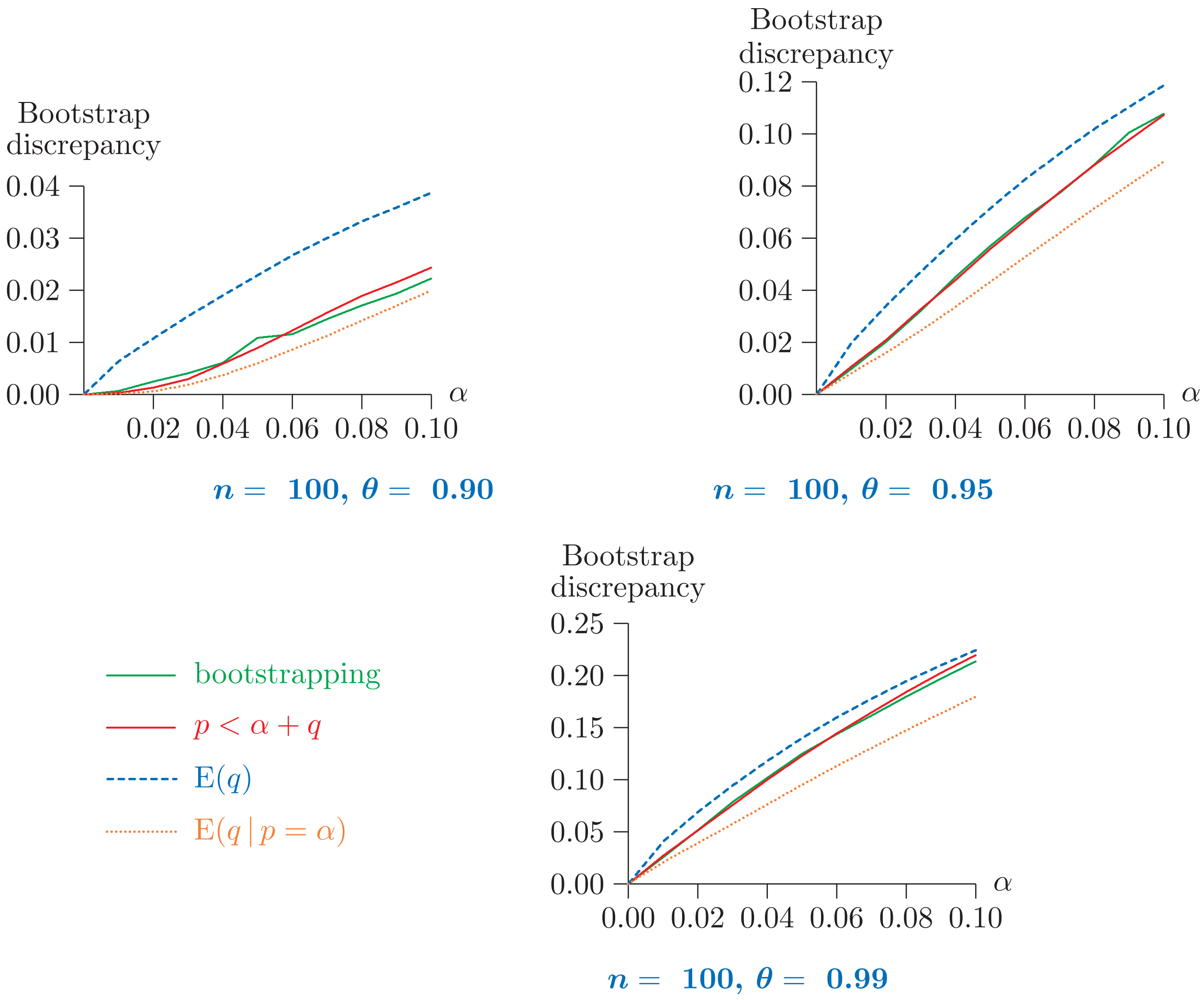
$\boldsymbol{n =}$ **100,** $\boldsymbol{\theta =}$ **0.95**

$\boldsymbol{n =}$ **100,** $\boldsymbol{\theta =}$ **0.99**

Figure 4: Bootstrap discrepancy; NLS estimation

number of bootstrap repetitions. An interesting inversion of the sign of the ERP can be seen, with negative ERP for both $\theta = 0.90$ and $\theta = 0.95$, but positive for $\theta = 0.99$. This last phenomenon is expected, since the asymptotic ADF test overrejects grossly for θ close to -1. However, even for $\theta = 0.95$, the ERP is negative. Note also that the bootstrap discrepancy is nothing like as large as the ERP of the asymptotic test, and, even for $\theta = 0.99$, is just over 1% for a nominal level of 5%.

In Figure 5, results like those in Figure 4 are shown when θ is estimated using the GZW2 estimator. A fourth curve is plotted, giving the estimate based on the expectation of q conditional on $p = \alpha$. It is no longer indistinguishable from the estimate based on the frequency of the event $p < \alpha + q$. This latter estimate, on the other hand, is very close to the one based on actual bootstrapping. Overall, the picture is very different from what we see with the NLS estimator for θ. The overrejection of the asymptotic test reappears for all three values of θ considered, and, although it is less severe, it is still much too great for $\theta = 0.95$ and $\theta = 0.99$ for the test to be of any practical use. Again, the unconditional expectation of q overestimates the RP. Evidently, bootstrap performance is much degraded by the use of the less efficient estimator of θ. The results in Figure 5 are much more similar to those in Richard (2007b) than are those of Figure 4.



$\boldsymbol{n =}$ **100,** $\boldsymbol{\theta =}$ **0.90**

$\boldsymbol{n =}$ **100,** $\boldsymbol{\theta =}$ **0.95**

$\boldsymbol{n =}$ **100,** $\boldsymbol{\theta =}$ **0.99**

Figure 5: Bootstrap discrepancy; GZW2 estimation

6. Bootstrap Performance

Any procedure that gives an estimate of the rejection probability of a bootstrap test, or of the CDF of the bootstrap P value, allows one to compute a corrected P value. This is just the estimated RP for a bootstrap test at nominal level equal to the uncorrected bootstrap P value. In principle, the analysis of the previous section gives the CDF of the bootstrap P value, and so it is interesting to see if we can devise a way to exploit this, and compare it with two other techniques sometimes used to obtain a corrected bootstrap P value, namely the double bootstrap, as originally proposed by Beran (1988), and the fast double bootstrap proposed by Davidson and MacKinnon (2007).

An estimate of the bootstrap RP or the bootstrap discrepancy is specific to the DGP that generates the data. Thus what is in fact done by all techniques that aim to correct a bootstrap P value is to *bootstrap* the estimate of the bootstrap RP, in the sense that the bootstrap DGP itself is used to estimate the bootstrap discrepancy. This can be seen for the ordinary double bootstrap as follows.

The conventional way to estimate the RP of a bootstrap test by simulation is to follow the procedure used to generate the curves labelled “bootstrapping” in Figures 4 and 5. For a test based on a statistic τ computed from a sample of size n generated by a DGP μ, the procedure is to generate M samples of size n from μ, where, for reasonable accuracy, M must be large. For each replication, indexed by $m = 1, \ldots, M$, a realisation τ_m of the statistic τ is computed from the simulated sample, along with a realisation $\hat{\mu}_m$ of the bootstrap DGP μ^*. Then B bootstrap samples are generated using $\hat{\mu}_m$, and bootstrap statistics τ^*_{mj}, $j = 1, \ldots, B$ are computed. The realized bootstrap P value for replication m is then

$$p^*_m \equiv \frac{1}{B} \sum_{j=1}^{B} \mathrm{I}(\tau^*_{mj} < \tau_m), \tag{16}$$

where we assume that the rejection region is to the left. The estimate of the RP of the bootstrap test at nominal level α is then the proportion of the p^*_m that are less than α. The whole procedure requires the computation of $M(B+1)$ statistics and of M bootstrap DGPs.

The first step of the double bootstrap is to compute the usual bootstrap P value, p^*_1 say, using B_1 bootstrap samples generated from a bootstrap DGP μ^*. Now one wants an estimate of the actual RP of a bootstrap test at nominal level p^*_1. This estimated RP is the double bootstrap P value, p^{**}_2. Thus we set $\mu = \mu^*$, $M = B_1$, and $B = B_2$ in the algorithm described in the previous paragraph. The computation of p^*_1 has already provided us with B_1 statistics τ^*_j, $j = 1, \ldots, B_1$, corresponding to the τ_m of the algorithm. For each of these, we compute the (double) bootstrap DGP μ^{**}_j realised jointly with τ^*_j. Then μ^{**}_j is used to generate B_2 second-level statistics, which we denote by τ^{**}_{jl}, $l = 1, \ldots, B_2$; these correspond to the τ^*_{mj} of the algorithm. The second-level bootstrap P value is then computed as

$$p^{**}_j = \frac{1}{B_2} \sum_{l=1}^{B_2} \mathrm{I}(\tau^{**}_{jl} < \tau^*_j); \tag{17}$$

compare (16). The estimate of the bootstrap RP at nominal level p^*_1 is then the proportion of the p^{**}_j that are less than p^*_1:

$$p^{**}_2 = \frac{1}{B_1} \sum_{j=1}^{B_1} \mathrm{I}\big(p^{**}_j \le p^*_1\big). \tag{18}$$

The inequality in (18) is not strict, because there may well be cases for which $p^{**}_j = p^*_1$. For this reason, it is desirable that $B_2 \neq B_1$. The whole procedure requires the computation of $B_1(B_2+1)+1$ statistics and B_1+1 bootstrap DGPs.

The so-called fast double bootstrap (FDB) of Davidson and MacKinnon (2007) is much less computationally demanding than the double bootstrap, but it is based on an estimate of the bootstrap RP that is theoretically justified only if the statistic τ and the bootstrap DGP μ^* are asymptotically independent. The algorithm for computing this estimate of the bootstrap RP is as follows. For $m = 1, \ldots, M$, the DGP μ is used to draw realisations τ_m and $\hat{\mu}_m$. Then $\hat{\mu}_m$ is used to draw a *single* bootstrap statistic τ^*_m. The τ^*_m are therefore IID realisations of the random variable, τ^* say, which is generated for DGP μ by first drawing a sample of size n, and then using the bootstrap DGP corresponding to this sample to generate the statistic τ^*. The estimate of the bootstrap RP is the proportion of the τ_m that are less than $Q^*(\alpha)$, the α quantile of the τ^*_m. The estimate of the RP is

$$\frac{1}{M}\sum_{m=1}^{M} \mathrm{I}\big(\tau_m < Q^*(\alpha)\big), \tag{19}$$

As a function of α, the above expression is an estimate of the CDF of the bootstrap P value. It requires the computation of $2M$ statistics and M bootstrap DGPs.

Like the double bootstrap, the FDB begins by computing the usual bootstrap P value p^*_1. In order to obtain the estimate of the RP of the bootstrap test at nominal level p^*_1, we use the above algorithm with $M = B$ and $\mu = \mu^*$. For each of the B samples drawn from μ^*, we obtain the ordinary bootstrap statistic τ^*_j, $j = 1, \ldots, B$, and the double bootstrap DGP μ^{**}_j, exactly as with the double bootstrap. One statistic τ^{**}_j is then generated by μ^{**}_j. The p^*_1 quantile of the τ^{**}_j, say $Q^{**}(p^*_1)$ is then computed. Of course, for finite B, there is a range of values that can be considered to be the relevant quantile, and we must choose one of them somewhat arbitrarily. The FDB P value is then

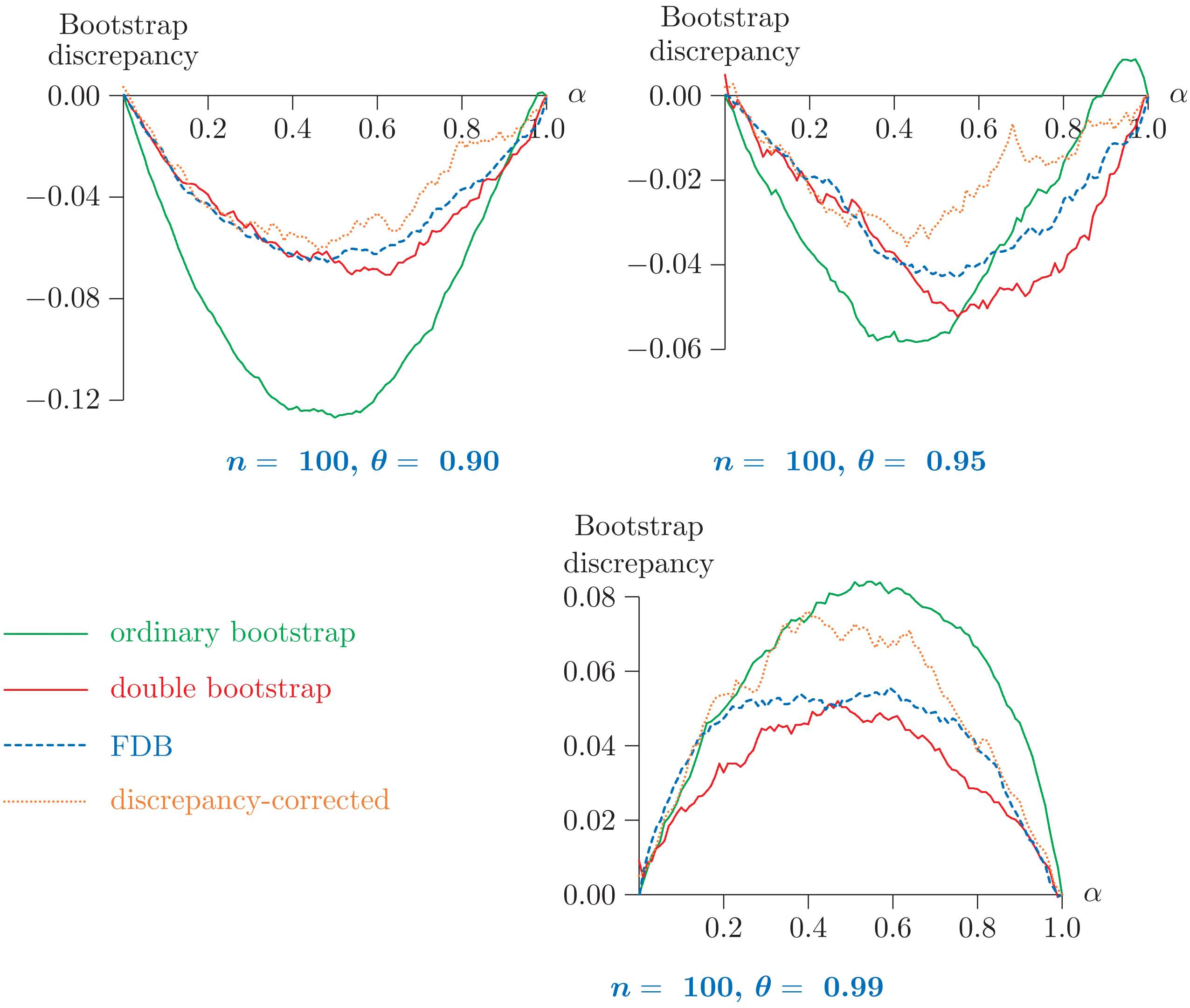
$$p^*_{\text{FDB}} = \frac{1}{B}\sum_{j=1}^{B} \mathrm{I}\big(\tau_j < Q^{**}(p^*_1)\big).$$

To obtain it, we must compute $2B + 1$ statistics and $B + 1$ bootstrap DGPs.

What makes the technique of the previous section for estimating the bootstrap discrepancy computationally intensive is the need to set up the tables giving $Q(\alpha, \theta)$ for a variety of values of α and θ. For a fixed α, of course, we need only vary θ, and this is the state of affairs when we wish to correct a bootstrap P value: we set $\alpha = p^*_1$. The fact that $Q(\alpha, \theta)$ is a rather smooth function of θ suggests that it may not be necessary to compute its value for more than a few different values of θ, and then rely on interpolation.

The discrepancy-corrected bootstrap is computed by the following algorithm. The bootstrap DGP μ^*, characterised by the estimate $\hat{\theta}$, is used to generate B bootstrap statistics τ^*_j, $j = 1, \ldots, B$, from which the first-level bootstrap P value p^*_1 is computed as usual. For each j, the parameter θ^*_j that characterises the double bootstrap DGP μ^{**}_j is computed and saved. Then the *same* random numbers as were used to generate τ^*_j are reused r times with r different values of θ, θ_k, $k = 1, \ldots, r$, in the neighbourhood of $\hat{\theta}$, to generate statistics τ^*_{jk} with τ^*_{jk} generated by the DGP with parameter θ_k. The τ^*_{jk} then allow one to estimate the p^*_1 quantile of the distribution of τ for the DGPs characterised by the θ_k, and the τ^*_j that for $\hat{\theta}$. The next step is to find by interpolation the value of $Q(p^*_1, \theta^*_j)$ for each bootstrap repetition j. The estimate of the RP of the bootstrap test is then the proportion of the τ^*_j less than $Q(p^*_1, \theta^*_j)$. This algorithm is just the one presented in the previous section applied to the bootstrap DGP μ^*. The estimated RP is the discrepancy-corrected bootstrap P value, p^*_{DCB}. It requires the computation of $(r+1)B+1$ statistics and $B+1$ bootstrap DGPs. In practice, of course, it is desirable to choose as small a value of r as is compatible with reliable inference.

In Figure 6 are shown P value discrepancy curves, as defined in Davidson and MacKinnon (1998), for four bootstrap tests, the conventional (parametric) bootstrap, the double bootstrap, the fast double bootstrap, and the discrepancy-corrected bootstrap. In these curves, the bootstrap discrepancy is plotted as a function of the nominal level α for $0 \leq \alpha \leq 1$. Although it is unnecessary for testing purposes to consider the bootstrap discrepancy for levels any greater than around 0.1, displaying the full plot allows us to see to what extent the distribution of the bootstrap P value differs from the uniform distribution U(0,1).



$n =$ 100, $\theta =$ 0.90

$n =$ 100, $\theta =$ 0.95

$n =$ 100, $\theta =$ 0.99

Figure 6: P value discrepancy plots

For the discrepancy-corrected bootstrap, the number r of DGPs used in the simulation was set equal to 4. Two of the values of θ were $\hat{\theta} + 0.02$ and $\hat{\theta} + 0.04$. The third was halfway between $\hat{\theta}$ and -1; the fourth was -1 itself.

7. Concluding Remarks

The focus of this paper is distinctly theoretical, although, quite unconventionally, no use is made of any asymptotic concepts. Asymptotic theory has so far not succeeded in giving a fully satisfactory account of the properties of bootstrap tests in finite samples; indeed the bootstrap often seems to give more reliable inference than asymptotic theory would suggest. Here, although no analytical expressions are given for the finite-sample distributions of the test statistics considered, it is seen how, in the particular case studied, inexpensive simulations can estimate the distributions of the random variables that determine the bootstrap discrepancy. It is seen that the most important factor making for bootstrap reliability is the reliability of the estimator(s) that determine the bootstrap DGP. By using a reliable estimator of the MA parameter, one can achieve inference with very little size distortion even when the parameter is close to -1.

The discrepancy-corrected bootstrap that gives highly reliable inference in this specific case would be much more computationally intensive in cases in which more than one parameter is needed to specify the bootstrap DGP. Nonetheless, it points in a direction that merits a good deal of further study aimed at elucidating the behaviour of the bootstrap and at improving the reliability of bootstrap inference.

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