Journal of the Korean
Statistical Society
Vol. 24, No. 2, 1995

On the Performance of Iterated Wild Bootstrap Interval Estimation of the Mean Response †

Woochul Kim[1] and Duk-Hyun Ko[1]

ABSTRACT

We consider the iterated bootstrap method in regression model with heterogeneous error variances. The iterated wild bootstrap confidence interval of the mean response is considered. It is shown that the iterated wild bootstrap confidence interval has coverage error of order n^{-1} whereas percentile method interval has an error of order $n^{-1/2}$. The simulation results reveal that the iterated bootstrap method calibrates the coverage error of percentile method interval successfully even for the small sample size.

KEYWORDS: Iterated bootstrap, Wild bootstrap, Heterogeneous error, Mean response, Edgeworth expansion.

1. INTRODUCTION

The iterated bootstrap method has been known as a powerful method in interval estimation. It can be used to estimate the errors which arise from a single usage of the bootstrap and to correct for them. So, in interval estimation,

†This research was supported by a grant from Korea Research Foundation 1993.

[1]Department of Computer Science and Statistics, Seoul National University, Seoul, 151-742, Korea.

it reduces the coverage error incurred by the usual percentile method interval. In i.i.d. case, many authors have shown that the iterated bootstrap calibrates the confidence coefficients driven by the percentile method very successfully. In general, Hall and Martin (1988) showed that the iterated bootstrap method reduces the coverage error by the factor n^{-1} in two-sided case and by the factor $n^{-1/2}$ in one-sided case.

In this paper, we consider the performance of iterated bootstrap in independent but not identically distributed case, especially in regression model. Consider the linear regression model with heterogeneous error variances:

$$Y_i = \beta_0 + \beta_1 x_{1i} + \cdots + \beta_p x_{pi} + \epsilon_i, \quad i = 1, \ldots, n,$$

where $\beta = (\beta_0, \ldots, \beta_p)^t$ is an unknown regression parameter and ϵ_i is an error term with mean 0 and variance σ_i^2 for each i. In this model, our main concern is in the interval estimation of the mean response y_0, $y_0 = \ell_0^t \beta$ for some fixed $\ell_0 = (1, x_{10}, \ldots, x_{p0})^t$. In this setting, the ordinary bootstrap method is also applicable, see Liu (1988) page 1707, but the ordinary bootstrap can't reflect the heteroscedasticity of the error part. So, we use the Wu's resampling method, so called *wild bootstrap*, to reflect the heteroscedasticity of error parts.

It is shown that, in this case, the iterated wild bootstrap also reduces the coverage error by the factor $n^{-1/2}$ in one-sided case, as in the i.i.d. case iterated bootstrap. The result can be driven by using Edgeworth expansion and Cornish-Fisher inversion. To assess the small sample performance, some simulation study has been carried. In the simulation study, we adopt the saddlepoint approximation method to reduce the computing time due to the nested resampling in iterated bootstrap.

Iterated bootstrap method was introduced by Hall (1986) and Beran (1987) in interval estimation context. More unified approach can be found in Hall and Martin (1988), see also Hall (1992). The wild bootstrap was suggested by Wu (1986) in regression model with non-homogeneous errors. Some asymptotic results on wild bootstrap can be found in Liu (1988) and Mammen (1993). Davison and Hinkley (1988) suggested the use of Daniel's saddlepoint approximation method to replace Monte Carlo resampling in bootstrap distribution approximation.

Section 2 describes the iterated wild bootstrap confidence interval for the mean response., In Section 3, the coverage property of the iterated wild bootstrap is examined. Section 4 provides the results of the simulation study to get the insight of the small sample performance of the proposed procedure.

2. THE ITERATED WILD BOOTSTRAP PROCEDURE

2.1 Wild Bootstrap

Assume the the data $\mathcal{X} = \{(x_{1i}, \ldots, x_{pi}, y_i), \quad i = 1, \ldots, n\}$ are generated by the model :

$$y_i = \beta_0 + \beta_1 x_{1i} + \cdots + \beta_p x_{pi} + \epsilon_i,$$

where β_i's are unknown parameters and ϵ_i's are independent random variables with mean 0 and variances σ_i^2. Let $\hat{\beta}$, $\hat{y}_0$ denote the least square estimates of β, y_0 from $\mathcal{X}$, respectively, where y_0 is the mean response at $(x_{10}, \ldots, x_{p0})$.

Define the residuals $\hat{\epsilon}_i$ as follows :

$$\hat{\epsilon}_i = y_i - \hat{\beta}_0 - \sum_{j=1}^{p} x_{ji}\hat{\beta}_j.$$

Conditional on data $\mathcal{X}$, wild bootstrap samples of error parts $\mathcal{E}^* = \{\hat{\epsilon}_i^*, \quad i = 1, \ldots, n\}$ are defined as follows :

$$\hat{\epsilon}_i^* = Z_i \cdot \hat{\epsilon}_i, \tag{2.1}$$

where the random variables Z_i's satisfy the following moment conditions;

$$E(Z_i) = 0, E(Z_i^2) = 1, E(Z_i^3) = 1.$$

Then we get the wild bootstrap samples of the responses as follows;

$$y_i^* = \hat{\beta}_0 + \sum_{j=1}^{p} x_{ji}\hat{\beta}_j\hat{\epsilon}_i^*, \quad i = 1, \ldots, n,$$

and $\mathcal{X}^* = \{(x_{1i}, \ldots, x_{pi}, y_i^*), \quad i = 1, \ldots, n\}$. Applying least square method to the sample $\mathcal{X}^*$, we can compute the bootstrap versions $\hat{\beta}^*, \hat{y}_0^*$.

In this setting, a percentile method interval which is based on wild bootstrap resampling, with nominal coverage α can be constructed as follows. Let $\hat{u}_\beta$ be the solution of the following equation

$$P\{\hat{y}_0^* \le \hat{u}_\beta | \mathcal{X}\} = \beta, \qquad 0 < \beta < 1,$$

and take $I_\alpha = (-\infty, \hat{u}_\alpha)$ as an one-sided confidence interval for y_0. In Section 3, it is shown that this percentile method interval, I_α, produces a coverage error in of order $n^{-1/2}$ as n gets larger.

2.2 Iterated Bootstrap

Although the wild bootstrap interval I_α has correct coverage asymptotically, the coverage error in finite sample may be significant. So, some calibration method to adjust the coverage error might be helpful. For this purpose, we use the iterated bootstrap method to estimate the true coverage

$$\pi(\alpha) = P\{y_0 \in I_\alpha\}$$

of the percentile method interval I_α. Let $\hat{\pi}(\alpha)$ be the estimate of $\pi(\alpha)$, then we can find the solution $\hat{\alpha}$ of the equation

$$\hat{\pi}(\hat{\alpha}) = \alpha. \tag{2.2}$$

Then, take $I_{\hat{\alpha}}$ as our final iterated bootstrap interval.

The bootstrap iteration idea for estimating $\hat{\pi}(\alpha)$ in equation (2.2) is as follows : With the notations in previous section, define $\hat{\hat{\epsilon}}$ and $\hat{\epsilon}^{**}$ by

$$\begin{aligned} \hat{\hat{\epsilon}}_i &= y_i^* - x_i'\hat{\beta}, \\ \hat{\epsilon}^{**} &= Z_i \cdot \hat{\hat{\epsilon}}_i, \quad y_i^{**} = x_i'\hat{\beta} + \hat{\epsilon}_i^{**}, \end{aligned}$$

where $x_i = (1, x_{1i}, \ldots, x_{pi})'$ and $\mathcal{X}^{**} = \{(x_i', y_i^{**}), \quad i = 1, \ldots, n\}$. Applying least squares method to re-resample $\mathcal{X}^{**}$, we obtain the second level bootstrap estimator $\hat{y}_0^{**}$. Let $\hat{u}_\beta^*$ be the solution of the equation

$$P\{\hat{y}_0^{**} \le \hat{u}_\beta^* | \mathcal{X}^*\} = \beta, \quad 0 < \beta < 1$$

and take $I_\alpha^* = (-\infty, \hat{u}_\alpha^*)$. Then we estimate $\pi(\alpha)$ by

$$\hat{\pi}(\alpha) = P(\hat{y}_0 \in I_\alpha^* | \mathcal{X}). \tag{2.3}$$

From equation (2.2) and (2.3) we can obtain $\hat{\alpha}$. So our final iterated bootstrap confidence interval is $I_{\hat{\alpha}}$. The detailed implementation method can be found in Hall and Martin (1988) and Hall (1992). The final interval $I_{\hat{\alpha}}$ has the coverage error of order n^{-1} as shown in Section 3.

2.3 Saddlepoint Approximation

In iterated bootstrap to estimate $\hat{\pi}(\alpha)$ in (2.3), usual Monte Carlo approximation method needs nested resampling to estimate

$$P(\hat{y}_0^{**} \le \hat{y}_0 | \mathcal{X}). \tag{2.4}$$

So, the saddlepoint approximation method may be used to reduce the computing time in estimation of (2.4). The saddlepoint approximation of (2.4) is given by

$$P(\hat{y}_0^{**} \le \hat{y}_0 | \mathcal{X}) \approx \Phi(\xi) + \phi(\xi)\Big\{\frac{1}{\xi} - \frac{1}{\eta}\Big\},$$

where

$$\xi = sgn(\lambda) \cdot [2n(\lambda\hat{y}_0 - K^*(\lambda))], \quad \eta = \lambda \cdot [nK^{*\prime\prime}(\lambda)]^{1/2}$$

and λ is a solution of

$$K^{*\prime}(\lambda) = \hat{y}_0.$$

Here, $nK^*(t)$ is the cumulant generating function of $\hat{y}^{**}$ evaluated at nt.

For simplicity of numerical computation, we can use the following approximation formula of $K^*(t)$, as in Wang (1990),

$$K^*(t) \approx \frac{n\kappa_2}{2}t^2 + \Big\{\frac{n^2\kappa_3}{6}t^3 + \frac{n^3\kappa_4}{24}t^4\Big\}\exp\Big[-t^2 \;/\; (8n\kappa_3)\Big],$$

where κ_j denotes the j-th cumulant of $\hat{y}_0^{**}$.

3. COVERAGE ACCURACY OF THE ITERATED WILD BOOTSTRAP PROCEDURE

In this section, we briefly sketch how the magnitude of the error in bootstrap approximation can be derived by the Edgeworth expansion. Detailed rigorous argument in i.i.d.-case can be found in Chapter 3 of Hall (1992).

First, consider the Edgeworth expansion of the bootstrap distribution of $\hat{y}_0$ and $\hat{y}_0^*$. The least squares estimator $\hat{y}_0$ can be expressed in the form of $\frac{1}{n}\sum w_i Y_i$, where $w = (w_1, \ldots, w_n) = n \cdot \ell_0'(X'X)^{-1}X'$. Let $\mu_i = E(w_i Y_i)$, $\tau_i^2 = Var(w_i Y_i)$ and $\tau^2 = \frac{1}{n}\sum \tau_i^2$. Denote $\sqrt{n}(\hat{y}_0 - y_0)/\tau$, $\sqrt{n}(\hat{y}_0 - y_0)/\hat{\tau}$ by S_n and T_n, respectively, and its bootstrap versions are denoted by $S_n^* = \sqrt{n}(\hat{y}_0^* - \hat{y}_0)/\hat{\tau}$, $T_n^* = \sqrt{n}(\hat{y}_0^* - \hat{y}_0)/\hat{\tau}^*$. Then the following conditions guarantee the Edgeworth expansion of the distribution of $\hat{y}_0$ and $\hat{y}_0^*$:

(C1) $E\epsilon_i^{s+\delta} \leq K < \infty$ for $s \geq 4$ and all j, in addition, ϵ_j's satisfy Cramér condition:

$$\limsup_{|\eta| \to \infty} |Ee^{i\eta\epsilon_j}| < 1$$

and assume $cn < \sigma_1^2 + \cdots + \sigma_n^2 < Cn$.

(C2) The design matrix X is of full rank, and

$$\limsup_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \| x_i \|^s < \infty \quad \text{for } s \geq 4,$$

where x_i is the i-th row vector of design matrix X.

(C3) Let λ_n = smallest eigenvalue of $X'X$ and $M_n = \max\{\| x_i \|, i = 1, \ldots, n\}$. Then,

$$\liminf_{n \to \infty} \lambda_n / n > 0, \quad M_n = O(n^\nu) \text{ for some } \nu \in [0, 1/2).$$

(C4) Z_j's in (2.1) satisfy Cramér condition:

$$\limsup_{|\eta|\to\infty} |Ee^{i\eta Z_1}| < 1$$

and $EZ_1 = 0$, $EZ_1^2 = 1$, $EZ_1^3 = 1$.

Under the conditions (C1) through (C3), it is well known that the following expansions hold:

$$P(S \le x) = \Phi(x) + n^{-1/2} p_1(x)\phi(x) + O(n^{-1}), \tag{3.1}$$

$$P(T \le x) = \Phi(x) + n^{-1/2} q_1(x)\phi(x) + O(n^{-1}), \tag{3.2}$$

where $p_1(x) = n^{-1/2}\bar{\mu}_{3,n}/6\tau^3(1-x^2)$ and $q_1(x) = n^{-1/2}\bar{\mu}_{3,n}/6\tau^3(2x^2+1)$ and $\bar{\mu}_{3,n} = \frac{1}{n}\sum E(w_iY_i - \mu_i)^3$ and $\Phi(x), \phi(x)$ denote the standard normal distribution function and density function, respectively. Moreover, we can obtain the following Edgeworth expansion of the bootstrap distributions.

Theorem 1. Under the conditions (C1)–(C4) the following expansions hold.

$$P(S^* \le x) = \Phi(x) + n^{-1/2}\hat{p}_1(x)\phi(x) + O_p(n^{-1}), \tag{3.3}$$

$$P(T^* \le x) = \Phi(x) + n^{-1/2}\hat{q}_1(x)\phi(x) + O_p(n^{-1}), \tag{3.4}$$

where $\hat{p}_1(x)$ and $\hat{q}_1(x)$ are polynomials with population moments in $p_1(x)$ and $q_1(x)$ have been replaced by sample moments.

Proof. We only show the validity of the Edgeworth expansion for non-studentized case, with $s = 4$ in (C1). As Liu (1988) pointed out, the main difficulty lies in establishing

$$\sup_{\epsilon\le\eta\le M}\Big|\prod_{j=1}^{n} E_Z \exp(i\eta(Y_j - x_j'\hat{\beta})Z_j)\Big| = o(n^{-1/2}) \quad \text{a.s.}$$

Following Liu(1988)'s argument on page 1705-1706, it suffices to have k_n of the $|Y_j - x_j'\hat{\beta}|$'s exceed some positive δ_0 for sufficiently large n with $k_n/\log n \to \infty$ a.s.. This can be achieved by showing that , for sufficiently large n,

$$\max_{1\le i\le n} \mid Y_i - x_i'\hat{\beta} \mid < 2\sqrt{n} \;/\; \log n \quad \text{a.s.}$$

Note that

$$\begin{aligned}
& P(\max_{1\le i\le n} \mid Y_i - x_i'\hat{\beta} \mid > 2\sqrt{n}\log n) \\
\le\ & P(\max_{1\le i\le n} \mid Y_i - x_i'\beta \mid + \max_{i\le i\le n} \mid x_i'(\hat{\beta}-\beta) \mid > 2\sqrt{n}/\log n) \\
\le\ & P(\max_{1\le i\le n} \mid Y_i - x_i'\beta \mid > \sqrt{n}/\log n) + P(\max_{1\le i\le n} \mid x_i'(\hat{\beta}-\beta) \mid > \sqrt{n}/\log n) \\
=\ & O(n^{-1-\gamma}) \text{ for some } \gamma > 0.
\end{aligned}$$

The last identity follows from Markov and Bonferroni inequality with the moment conditions (C1), (C2) and (C3). So, by Borel-Cantelli lemma, we have, for sufficiently large n,

$$\max_{1\le i\le n} \mid Y_i - x_i'\hat{\beta} \mid < 2\sqrt{n}/\log n \quad \text{a.s.}$$

From Theorem 1 and the fact the $\hat{p}_1 - p_1$, $\hat{q}_1 - q_1$ are both $O_p(n^{-1/2})$, we have

$$P(S^* \le x) - P(S \le x) = O_p(n^{-1}), \tag{3.5}$$

$$P(T^* \le x) - P(T \le x) = O_p(n^{-1}). \tag{3.6}$$

Therefore we have, from (3.5) and (3.6),

$$\begin{aligned}
P(\hat{y}_0^* \le x) - P(\hat{y}_0 \le x) &= \Phi(x/\hat{\tau}) + n^{-1/2}\hat{p}_1(x/\hat{\tau})\phi(x/\hat{\tau}) \\
&\quad -\{\Phi(x/\tau) + n^{-1/2}p_1(x/\tau)\phi(x/\tau)\} + O_p(n^{-1})
\end{aligned}$$

$$= \Phi(x/\hat{\tau}) - \Phi(x/\tau) + O_p(n^{-1})$$
$$= O_p(n^{-1/2}).$$

Thus the percentile method wild bootstrap estimates of quantiles are first order correct.

Finally, we briefly establish the coverage error of iterated bootstrap. Let $\hat{u}_\beta$ be the solution of $P(\hat{y}_0^* \leq \hat{u}_\beta | \mathcal{X}) = \beta$. Then, from (3.3) and (3.4), we have

$$\hat{u}_\beta = \hat{y}_0 + n^{-1/2}\hat{\tau}_n\{z_\beta + n^{-1/2}\hat{p}_{11}(z_\beta) + O_p(n^{-1})\}$$

and

$$\hat{u}_\beta^* = \hat{y}_0^* + n^{-1/2}\hat{\tau}_n^*\{z_\beta + n^{-1/2}\hat{p}_{11}^*(z_\beta) + O_p(n^{-1})\}.$$

Let t and $\hat{t}$ satisfy that $P(y_0 \leq \hat{u}_t) = \alpha$ and $P(\hat{y}_0 \leq \hat{u}_{\hat{t}} | \mathcal{X}) = \alpha$ respectively. Then,

$$t = \alpha + n^{-1/2}\pi_{11}(z_\alpha)\phi(z_\alpha) + O(n^{-1})$$

and

$$\hat{t} = \alpha + n^{-1/2}\hat{\pi}_{11}(z_\alpha)\phi(z_\alpha) + O_p(n^{-1}).$$

Hence, $\hat{t} - t = O_p(n^{-1})$. So $\hat{u}_{\hat{t}} - \hat{u}_t = O_p(n^{-1})$. From this, we obtain

$$P\{y_0 \in I_{\hat{\alpha}}\} = P\{y_0 \leq \hat{u}_{\hat{t}}\}$$
$$= P\{y_0 \leq \hat{u}_t\} + O(n^{-1})$$
$$= \alpha + O(n^{-1}).$$

4. RESULTS OF THE SIMULATION STUDY

We use now simulation to examine the small sample performance of iterated wild bootstrap interval. We consider simple linear regression model, $y_i = \alpha + \beta x_i + \epsilon_i, i = 1, \ldots, n$ for $n = 10, 20$ with x_i's are uniform grid on $[0, 1]$ and the interval estimation of the mean response $y_0 = \alpha + \beta x_0$, for selected values of x_0. Simulation study uses the following four error distributions:

M1 : $\epsilon_i \sim 0.5(1 + 2 \cdot (i - 1)/(n - 1))N(0.5, 0.7^2) + 0.5N(-0.5, 0.7^2), \quad i = 1, \ldots, n,$

M2 : $\epsilon_i \sim N(0, 1 + x_i), \quad i = 1, \ldots, n,$

M3 : $\epsilon_i \sim N(0, |x_i - \text{med}(x_i)|), \quad i = 1, \ldots, n,$

M4 : $\epsilon_i \sim N(0, x_i/2), \quad i = 1, \ldots, n.$

The error distribution M1 was considered by Mammen (1993) to compare the ordinary bootstrap and the wild bootstrap variance estimator, and M2 was considered by Wu (1986). M3 was suggested by Efron(1986) as an alternative to M2. We have run 500 simulations to estimate the coverage of iterated bootstrap and percentile method interval with 199 bootstrap resampling. Table 1. provides the estimated coverage probabilities.

The simulation results reveal that the iterated bootstrap method calibrates the coverage error of percentile method interval successfully while the calibration for the model M3 is not so great.

In this simulation, we have used the two point distribution for Z_i in (2.1). Note that the two point distribution does not satisfy the condition (C4), but it is easy to use in implementation. This is the reason why we have used it instead of a continuous distribution satisfying the condition (C4). Furthermore, some limited simulation with a continuous distribution have shown similar results to those in Table 1.

Table 1. Estimated Coverage of Bootstrap 90 % Confidence Interval.

model	n	method	x_0 0.1	0.3	0.5	0.7	0.9
M1	$n = 10$	WB	0.82	0.83	0.82	0.77	0.73
		IWB	0.86	0.90	0.88	0.81	0.78
	$n = 20$	WB	0.86	0.87	0.84	0.83	0.83
		IWB	0.90	0.90	0.90	0.87	0.86
M2	$n = 10$	WB	0.84	0.84	0.81	0.77	0.74
		IWB	0.88	0.88	0.85	0.82	0.79
	$n = 20$	WB	0.87	0.87	0.86	0.86	0.85
		IWB	0.90	0.90	0.90	0.87	0.89
M3	$n = 10$	WB	0.73	0.74	0.80	0.76	0.72
		IWB	0.76	0.78	0.86	0.81	0.76
	$n = 20$	WB	0.82	0.83	0.85	0.83	0.81
		IWB	0.86	0.87	0.90	0.88	0.84
M4	$n = 10$	WB	0.85	0.87	0.84	0.81	0.78
		IWB	0.88	0.90	0.88	0.85	0.82
	$n = 20$	WB	0.89	0.87	0.86	0.84	0.86
		IWB	0.90	0.90	0.89	0.88	0.90

REFERENCES

(1) Beran, R. (1987). Prepivoting to Reduce Level Error Confidence Sets. *Biometrika*, **74**, 457–468.

(2) Davison, A.C. and Hinkley, D.V. (1988). Saddlepoint Approximations in Resampling Methods. *Biometrika*, **75**, 417–431.

(3) Efron, B. (1986). Discussion on "Jackknife, Bootstrap and Other Resampling Methods in Regression Analysis". *The Annals of Statistics*, 1301–1304.

(4) Hall, P. (1986). On the Bootstrap and Confidence Intervals. *The Annals of Statistics*, **14**, 1431–1451.

(5) Hall, P. (1992). *The Bootstrap and Edgeworth Expansions*. Springer-Verlag, New York.

(6) Hall, P. and Martin, M.A. (1988). On Bootstrap Resampling and Iteration. *Biometrika*, **75**, 661–672.

(7) Liu, R.Y. (1988). Bootstrap Procedures under Some Non-i.i.d. Models. *The Annals of Statistics*, **16**, 1696–1708.

(8) Mammen, E. (1993). Bootstrap and Wild Bootstrap for High Dimensional Linear Models. *The Annals of Statistics*, **21**, 255–285.

(9) Wang, S. (1990). Saddlepoint Approximations in Resampling Analysis. *Annals of the Institute of Statistical Mathematics*, **42**, 115–131.

(10) Wu, C.F.J. (1986). Jackknife, Bootstrap and Other Resampling Methods in Regression Analysis (with Discussion). *The Annals of Statistics*, **14**, 1261–1350.