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On Bootstrap Methods in Orthogonal Regression Model

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ABSTRAK

Kertas ini membincangkan kaedah butstrap tak berparameter bagi menentukan ralat piawai anggaran parameter model regresi ortogon. Kaedah butstrap *persentil, persentil pincang dibetulkan, persentil pincang dibetulkan secara pantas* (BCA) dan BCA *terlelar* digunakan bagi membina selang keyakinan bagi parameter model tersebut. Daripada kajian simulasi yang dijalankan didapati selang keyakinan berdasarkan kaedah BCA *terlelar* mememuhi ciri-ciri selang keayakinan yang dikehendaki.

ABSTRACT

This paper discusses the nonparametric bootstrap method for evaluating the standard errors of the parameter estimates of orthogonal regression. The *percentile, bias-corrected, the bias-corrected and accelerated* (BCA), and the *calibrated or iterated* BCA method were considered for confidence intervals for the parameters of the model. Based on simulation studies, it was found that the iterated BCA method produced a more reliable confidence interval than the other methods.

Keywords: bootstrap method, orthogonal regression, bootstrap confidence intervals

INTRODUCTION

Consider a pair of variables (ξ,η) satisfying a linear relationship $\eta = \alpha + \beta\xi$, with α and β to be estimated; (ξ,η) cannot be observed directly. Instead, (ξ,η) are both observed with errors, i.e., we observe the pair (x_i, y_i) where

$$x_i = \xi_i + \delta_i$$
$$y_i = \eta_i + \varepsilon_i \qquad (1)$$

with errors δ_i and ε_i, respectively. The $\{\xi_i\}$ are (fixed) mathematical variables. The model (1) is known as a *linear functional relationship* (LFR). We shall consider the special case in which the variance ratio $\lambda = V(\varepsilon_i)/V(\delta_i) = 1$. With this specification, the LFR in (1) is better known as the *orthogonal regression* model.

Two approaches to the estimation of the parameters have been discussed in the literature. In the *maximum likelihood estimation* (MLE) (Kendall and Stuart 1973: Chapter 29; Fuller 1987) it is assumed that the observations (x_i, y_i) are independent $N(\xi_i, \sigma^2)$ and $N(\alpha+\beta\xi_i, \sigma^2)$ variates, respectively, for i=1,...,n. A more general formulation for estimating the parameters in (1) is the *generalized least squares estimation* (GLSE) (Sprent 1966). In the GLSE approach no assumptions are made about the distributions of the observations. The GLSE approach chooses the estimators of α and β which minimize

$$\sum_{i=1}^{n}(y_i-\alpha-\beta x_i)^2/(1+\beta^2)$$

Both the MLE and GLSE estimations yield identical estimators of α and β, i.e.,

$$\hat{\beta}=\frac{(S_{yy}-S_{xx})+\sqrt{(S_{yy}-S_{xx})^2+4S_{xy}^2}}{2S_{xy}} \qquad (2)\,(i)$$

$$\hat{\alpha}=\bar{y}-\hat{\beta}\bar{x} \qquad (2)\,(ii)$$

where

$$\bar{x}=n^{-1}\Sigma x_i \quad ,\bar{y}=n^{-1}\Sigma y_i$$

$$S_{xx}=\Sigma(x_i-\bar{x})^2, S_{yy}=\Sigma(y_i-\bar{y})^2, S_{xy}=\Sigma(x_i-\bar{x})(y_i-\bar{y}),$$

Patefield (1977) derives the asymptotic variance-covariance matrix of the maximum likelihood estimators of α and β. When σ^2 is unknown, a consistent estimator of the variance-covariance matrix is

$$(1+\hat{\beta})\tilde{\sigma}^2\hat{\beta}/nS_{xy}\begin{bmatrix}\bar{x}(1+\hat{\tau})+S_{xy}/\hat{\beta}-\bar{x}(1+\hat{\tau}) \\ -\bar{x}(1+\hat{\tau}) \qquad (1+\hat{\tau})\end{bmatrix} \qquad (3)$$

where

$$\hat{\tau}=\frac{\tilde{\sigma}^2\hat{\beta}}{(\lambda+\hat{\beta}^2)S_{xy}} \qquad \text{and} \qquad \tilde{\sigma}^2=\frac{2n\hat{\sigma}^2}{(n-2)}$$

is the consistent estimator of σ^2 and $\hat{\sigma}^2$ is the maximum likelihood estimator of σ^2.

Based on the normality assumptions Kendall and Stuart (1973) constructed a $100(1-\gamma)\%$ confidence interval for β. The confidence limits for β are given by

$$\tan^{-1}\beta \pm \frac{1}{2}\sin^{-1}\left\{2t_{n-2,\gamma/2}\left[\frac{(S_{xx}S_{yy}-S_{xy}^2}{(n-2)\left[\left(S_{yy}-S_{xx}\right)^2+4S_{xy}^2\right]}\right]\right\} \qquad (4)$$

where $t_{n-2,\gamma/2}$ is the (1-γ / 2) percentile point of the t distribution with n-2 degrees of freedom.

Our interest is to examine an alternative approach to the parametric confidence interval in (4) which does not rely on the normality assumption. This paper discusses, via a simulation study, the use of the nonparametric bootstrap method to assess the standard error and confidence intervals for the parameters of the model. The use of the nonparametric bootstrap method is justified since the estimators in (2) (i)-(ii) can be considered as being derived from a general formulation which makes no normality assumptions about the observations.

BOOTSTRAPPING THE ORTHOGONAL REGRESSION

Let the model (1) be written in the form

$$\mathbf{z_i} = \begin{pmatrix} x_i \\ y_i \end{pmatrix} = \begin{pmatrix} \xi_i \\ \eta_i \end{pmatrix} + \begin{pmatrix} \delta_i \\ \varepsilon_i \end{pmatrix} = \zeta_i + \mathbf{u_i}$$

where

$$\eta_i = \alpha + \beta\xi_i.$$

Let F denote the common distribution function of the z_i and the parameter vector $\theta = (\alpha, \beta)^T$. As shown in the previous section, existing methods for estimating the statistical accuracy of the estimators are largely asymptotic, and may not apply in finite samples. The bootstrap method, however, may overcome this difficulty as it automatically produces accuracy of the estimates and it can be applied in a wide range of situations.

BOOTSTRAP STANDARD ERRORS

The bootstrap method advocated by Efron (1979) works by sampling from the empirical distribution function of F, denoted by F_n, and then estimating the parameter $\theta(F)$ by $\theta(F_n)$. The sampling distribution of $\theta(F)$ is estimated by simulating that of $\theta(F_n)$. This is done by repeatedly drawing 'resamples' from the original sample 'with replacement' and for each resample calculating a value of $\theta(F_n)$.

Suppose we are interested in obtaining a bootstrap distribution of $\hat{\theta}=\left(\hat{\alpha},\hat{\beta}\right)^{T}$ where $\hat{\alpha}$ and $\hat{\beta}$ are given by (2)(i)-(ii), respectively. We may proceed by calculating Monte Carlo approximations based on the complete observation vector z_i. The bootstrap distribution of $\hat{\theta}=\left(\hat{\alpha},\hat{\beta}\right)^{T}$ may be approximated by drawing B samples of size n from

F_n: mass 1/n at $z_i=\begin{pmatrix}x_i\\ y_i\end{pmatrix}$ i=1,..., n, each time creating pseudo-data set $z_i^*=\begin{pmatrix}x_i^*\\ y_1^*\end{pmatrix}$ from which $\hat{\theta}^*=\left(\hat{\alpha}^*,\hat{\beta}^*\right)^{T}$ is calculated from

$$\hat{\beta}^{*b}=\frac{\left(S_{yy}^{*b}-S_{xx}^{*b}\right)+\sqrt{\left(S_{yy}^{*b}-S_{xx}^{*b}\right)^2+4S_{xy}^{*b2}}}{2S_{xy}^{*b}},b=1,\mathrm{K}\ ,B \qquad (2)(i)$$

$$\hat{\alpha}^{*b}=\bar{y}^{*b}-\beta^{*b}\bar{x}^{*b} \qquad (2)(ii)$$

where

$$\bar{x}^{*b}=n^{-1}\sum x_i^{*b}\quad ,\ \bar{y}^{*b}=n^{-1}\sum y_i^{*b}$$

and

$$S_{xx}^{*b}=\sum\left(x_i^{*b}-\bar{x}^{*b}\right)^2\ ,S_{yy}^{*b}=\sum\left(y_i^{*b}-\bar{y}^{*b}\right)^2,S_{xy}^{*b}=\sum\left(x_i^{*b}-\bar{x}^{*b}\right)\left(y_i^{*b}-\bar{y}^{*b}\right).$$

After drawing B bootstrap samples, we use the resulting bootstrap estimates $\hat{\theta}^*=\left(\hat{\alpha}^*,\hat{\beta}^*\right)^{T}$ to calculate the standard errors of the estimates $\hat{\theta}=\left(\hat{\alpha},\hat{\beta}\right)^{T}$, i.e.

$$\text{s.e.}\left(\hat{\theta}\right)=\left[\frac{\sum\left(\hat{\theta}^{*b}-\bar{\hat{\theta}}\right)^2}{(B-1)}\right]^{1/2}\quad\text{where}\ \bar{\hat{\theta}}=B^{-1}\sum\hat{\theta}^{*b}$$

NONPARAMETRIC BOOTSTRAP CONFIDENCE INTERVALS

In a series of papers, Efron (1979, 1982, 1987) and Efron and Tibshirani (1993) have developed procedures for constructing approximate confidence intervals for a statistic of interest. The procedures rely on estimating the sampling distribution of a statistic or an approximate pivot. We shall consider four popular methods, namely the percentile, the bias-corrected (BC) percentile, the bias-corrected and accelerated (BCA), and the iterated BCA methods.

The percentile method takes the interval 100γ and $100(1-\gamma)$ percentiles of the bootstrap distribution of $\hat{\theta}^* = \left(\hat{\alpha}^*, \hat{\beta}^*\right)^T$, $\hat{G}(s)$. If

$$\hat{G}(s) = \Pr^*\left\{\hat{\theta}^* < s\right\}$$

where Pr* indicates probability computed according to the bootstrap distribution of $\hat{\theta}^* = \left(\hat{\alpha}^*, \hat{\beta}^*\right)^T$, then $100(1-2\gamma)\%$ approximate interval for $\theta=(\alpha,\beta)^T$ is

$$\left[\hat{G}^{-1}(\gamma), \hat{G}^{-1}(1-\gamma)\right] \tag{5}$$

The bias-corrected (BC) method is given by

$$\left[\hat{G}^{-1}\left(z^{(\gamma)} + 2z_0\right), \hat{G}^{-1}\left(z^{(1-\gamma)} + 2z_0\right)\right] \tag{6}$$

where z_0 is the bias correction factor and both z and z_0 are standard normal distribution functions. If $z_0=0$, then the BC method reduces to the percentile method. The disadvantage of both the percentile and the BC methods is that they have less satisfactory coverage properties.

An improved version of the percentile and the BC methods is the *bias-corrected and accelerated* (BCA) method. The BCA has better coverage properties because it is *second-order accurate*. This means that for a central $(1-2\gamma)$ confidence interval $(\hat{\theta}_L, \hat{\theta}_U)$ its errors in matching the probability α of not covering the true value of θ from above $\left(\text{i.e., } \Pr\left\{\theta > \hat{\theta}_U\right\} = \alpha\right)$ or from below $\left(\text{i.e., } \Pr\left\{\theta > \hat{\theta}_L\right\} = \alpha\right)$ go to zero at rate $1/n$, for a sample of size n. The percentile and the BC methods are only *first-order accurate* because their errors in matching α go to zero at a slower rate, i.e., $1/\sqrt{n}$ (Efron and Tibshirani 1993: 187). The BCA intervals are *transformation respecting*, meaning that the BCA endpoints transform correctly if a parameter of interest θ is changed to some function of θ.

In the BCA method the percentiles of the bootstrap distribution are also used to form the endpoints of the intervals. However, the percentiles used are now determined by the bias-correction and acceleration factors. Let a denote the acceleration factor, then the BCA interval with $(1-2\gamma)$ coverage is given by

$$\left[\hat{\theta}^*(\gamma_1), \hat{\theta}^*(\gamma_2)\right] \tag{7}$$

where

$$\gamma_1 = \phi^{-1}\left\{z_0 + \left(z_0 + z^{(\gamma)}\right)/\left(1 - a\left(z_0 + z^{(\gamma)}\right)\right)\right\}$$

$$\gamma_{21} = \phi^{-1}\left\{z_0 + \left(z_0 + z^{(1-\gamma)}\right)/\left(1 - a\left(z_0 = z^{(1-\gamma)}\right)\right)\right\}$$

$$z_{0=}\ \phi^{-1}\left\{\left(no.\ of\ \hat{\theta}^* s < \hat{\theta}\right)/B\right\}$$

$$a = \sum_{i=1}^{n}\left(\hat{\theta}_{(.)} - \hat{\theta}_{-i}\right)^3 / 6\left\{\sum_{i=1}^{n}\left(\hat{\theta}_{(.)} - \hat{\theta}_{-i}\right)^2\right\}^{3/2}, \hat{\theta}_{(.)} = n^{-1}\sum\theta_{-i}$$

where ϕ (.) is the standard normal cumulative distribution function and $\hat{\theta}_{-i}$ is the estimate with the i-th observation deleted.

As pointed out by Efron and Tibshirani (1993), the actual coverage of a bootstrap confidence procedure is rarely equal to the desired (nominal) coverage and is often substantially different. One way to achieve the coverage is by use of *calibration*. The idea of calibration of the bootstrap was first discussed by Hall (1986, 1987) and Loh (1987, 1991). Booth and Hall (1993) discussed the *calibrated* confidence interval which is also known as the *iterated* confidence interval in the context of function errors-in-variables model.

The iterated or calibrated confidence interval can be constructed as follows; Compute λ-level confidence points

$$\left[\hat{\theta}^*_{\lambda}(b), \hat{\theta}^*_{(1-\lambda)}(b)\right] \quad , b = 1, \text{K} \ , B \tag{8}$$

for a grid of values of λ. For example, these might be the normal confidence points

$$\left[\hat{\theta}^*(b) - z_{(1-\lambda)} s.e\left(\hat{\theta}^*\right) \qquad {}_{(1-\lambda)} s.e\left(\hat{\theta}^*\right)\right] \quad , b = 1, \text{K} \ , B$$

For each λ compute

$$\hat{P}(\lambda) = \left\{no.\ of\ \hat{\theta} \le \hat{\vartheta}^*_{\lambda}(b)\right\},\ B$$

and

$$\hat{P}(1-\lambda) = \left\{no.\ of\ \hat{\theta} \ge \hat{\theta}^*_{1-\lambda}(b)\right\}/B$$

Find the value of γ that satisfies

$$\hat{P}(\lambda) = \hat{P}(1-\lambda) = \alpha/2$$

The calibration process can be applied to any bootstrap method. In this paper we consider the calibration on the BCA method. With the calibrated BCA method the resulting confidence interval has the desired properties, i.e., it is second-order accurate, transformation-respecting and also has the correct nominal coverage.

EXAMPLE

The data are from Miller (1980) and have been analysed by Kelly (1984) using errors-in-variables model. They consist of simultaneous pairs of measurements of serum kanamycin levels in blood samples drawn from 20 babies. A heelstick method on umbilical catherer was used to measure the levels. It was reasoned that the assumption $\gamma = 1$ was correct, A scatterplot of these twenty pairs of observations is illustrated in *Fig. 1.*

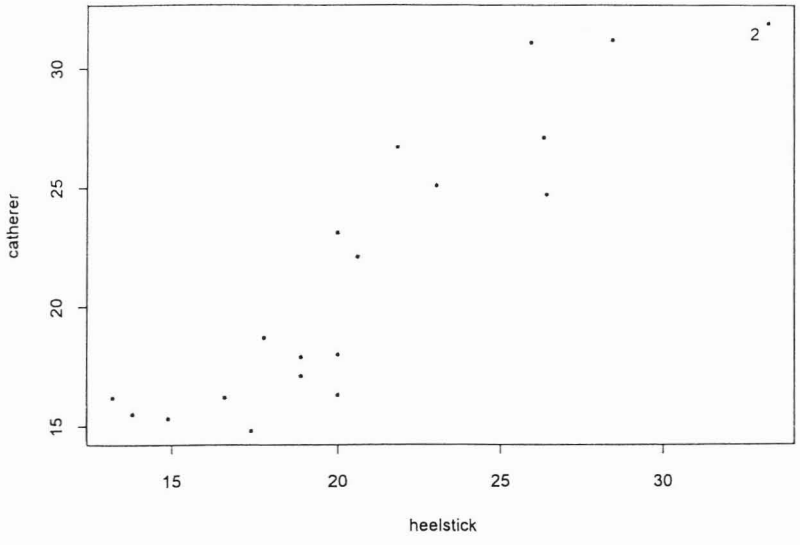

Fig. 1. Serum kanamycin levels (catherer vs heelstick)

The estimates based on (2)(i)-(ii) were

$$\hat{\alpha} = -1.16, \qquad \hat{\beta} = 1.07$$

The consistent estimate of σ^2 is $\tilde{\sigma}^2$=1.53. The standard error of the estimated slope and the corresponding 90% confidence interval based on the exact normal (asymptotic) theory and the bootstrap methods are presented in Table 1. In bootstrap methods we used B = 1000.

Table 1 displays summary statistics pertaining to the bootstrap analyses. The bootstrap standard error is relatively close to that of the normal theory. Two properties associated with all the confidence intervals are their lengths and shapes, respectively (Efron 1987)."Shape" measures the asymmetry of the interval about the point estimate. An interval is said to be symmetrical if shape = 1. Shape > 1 indicates asymmetry with greater distance from the upper limit to the point estimate than from the point estimate to the lower limit. The bias-corrected interval is shorter than the other intervals and the iterated BCA produces the longest confidence interval among those considered. All the confidence intervals, except the iterated BCA, indicate some degree of asymmetry with greater distances from the upper limits to $\hat{\beta}$ than from $\hat{\beta}$ to the lower limits.

TABLE 1

Standard errors of $\hat{\beta}$ and 90% confidence interval for β

Standard error of $\hat{\beta}$	
Exact (normal-theory)	0.160
Bootstrap (B=1000)	0.182

90% Confidence Interval for β

	Lower	Upper	Length	Shape
Exact (Normal-theory)	0.811	1.418	0.607	1.347
Percentile	0.797	1.420	0.623	1.281
BC	0.855	1.438	0.583	1.713
BCA	0.871	1.493	0.622	2.130
Iterated BCA	0.710	1.493	0.783	1.178

Tables 2-4 illustrate the exact (normal-theory), the percentile, the BC, the BCA, and the iterated BCA confidence intervals for the slope parameter. The exact confidence interval is given by (4) and the bootstrap intervals are given by (5)-(8), respectively. Tabulated characteristics for confidence intervals are average values of lower and upper endpoints, lengths, shape, and also estimated coverages of the intervals (with nominal coverage 90%).

It is clear from Tables 2-4 that in most cases the percentile, the BC, and the BCA intervals suffer from moderate undercoverage when the underlying population is non-normal. The exact confidence intervals also suffer from moderate undercoverage even in the case of normal population. The strength of the iterated BCA method is that it yields confidence intervals that have coverage equal to the desired nominal 90% coverage. However, the iterated BCA intervals tend to show some degree of asymmetry and are slightly longer than the other intervals.

TABLE 2
Exact and bootstrap confidence intervals, n=20

Error-distr.	Method	Lower	Upper	Length	Shape	Coverage
Normal	Exact	0.914	1.108	0.194	1.102	0.85
	Percentile	0.907	1.097	0.189	1.167	0.90
	BC	0.903	1.090	0.187	1.034	0.90
	BCA	0.888	1.094	0.207	1.116	0.91
	Iter. BCA	0.891	1.130	0.239	1.214	0.90
D-exp.	Exact	0.918	1.112	0.194	1.102	0.92
	Percentile	0.918	1.101	0.127	1.127	0.87
	BC	0.916	1.098	0.182	1.109	0.84
	BCA	0.919	1.100	0.181	1.169	0.84
	Iter. BCA	0.902	1.136	0.234	1.197	0.90
t(3)	Exact	0.862	1.227	0.364	1.197	0.87
	Percentile	0.853	1.213	0.360	1.202	0.87
	BC	0.859	1.210	0.355	1.163	0.85
	BCA	0.853	1.210	0.357	1.216	0.88
	Iter. BCA	0.817	1.320	0.502	1.486	0.90

CONCLUSION

The existing methods for evaluating the statistical accuracy of estimates of the parameters of orthogonal regression model are largely asymptotic and may not apply in finite samples. The nonparametric bootstrap method has facilitated the evaluations of standard errors and confidence intervals for the parameters of the model. A limited simulation study presented in this paper shows that the iterated BCA method, in particular, provides a reliable method for constructing a nonparametric confidence interval. The method produces a confidence interval that has the most desirable properties, i.e., it is second-order accurate, transformation-respecting, and has a correct nominal coverage.

TABLE 3
Exact and bootstrap confidence intervals, n=30

Error-distr.	Method	Lower	Upper	Length	Shape	Coverage
Normal	Exact	0.942	1.043	0.101	1.052	0.87
	Percentile	0.952	1.048	0.096	0.988	0.89
	BC	0.951	1.047	0.096	0.973	0.91
	BCA	0.944	1.049	0.104	1.051	0.91
	Iter. BCA	0.935	1.067	0.132	1.123	0.90
D-exp.	Exact	0.951	1.052	0.102	1.052	0.90
	Percentile	0.952	1.051	0.099	1.028	0.89
	BC	0.948	1.048	0.100	0.951	0.85
	BCA	0.941	1.051	0.110	1.025	0.85
	Iter. BCA	0.937	1.065	0.128	1.068	0.90
t(3)	Exact	0.951	1.051	0.186	1.097	0.89
	Percentile	0.911	1.095	0.183	1.031	0.84
	BC	0.912	1.096	0.183	1.061	0.84
	BCA	0.900	1.099	0.200	1.138	0.86
	Iter. BCA	0.889	1.130	0.241	1.118	0.90

TABLE 4
Exact and bootstrap confidence intervals, n=50

Error-distr.	Method	Lower	Upper	Length	Shape	Coverage
Normal	Exact	0.978	1.025	0.047	1.024	0.84
	Percentile	0.979	1.023	0.044	0.960	0.86
	BC	0.979	1.023	0.044	0.010	0.83
	BCA	0.968	1.024	0.063	1.050	0.83
	Iter. BCA	0.970	1.028	0.058	1.061	0.90
D-exp.	Exact	0.978	1.024	0.046	1.023	0.94
	Percentile	0.979	1.022	0.043	1.142	0.88
	BC	0.976	1.019	0.044	0.877	0.86
	BCA	0.928	1.020	0.092	1.886	0.85
	Iter. BCA	0.974	1.032	0.057	1.186	0.90
t(3)	Exact	0.958	1.040	0.082	1.042	0.88
	Percentile	0.959	1.035	0.076	1.000	0.87
	BC	0.959	1.035	0.076	1.022	0.87
	BCA	0.951	1.037	0.085	1.114	0.90
	Iter. BCA	0.949	1.050	0.101	1.085	0.09

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REFERENCES

BOOTH, J.G. and P. HALL. 1993. Bootstrap confidence regions for functional relationships in errors-in-variables models. *Annals of Statistics* **21**: 1780-1791.

EFRON, B. 1979. Bootstrap methods: Another look at the jackknife. *Annals of Statistics* **7**: 1-26.

EFRON, B. 1982. *The Jackknife, the Bootstrap and Other Resampling Plans* . Phil: SIAM.

EFRON, B. 1987. Better bootstrap confidence intervals. *Journal of the American Statistical Association* **82**: 171-200.

EFRON, B. and R.J. TIBSHIRANI. *An Introduction to the Bootstrap*. New York: Chapman and Hall.

FULLER, W.A. 1987. *Measurement Error Models*. New York: Wiley.

HALL, P. 1986. On the bootstrap and confidence intervals. *Annals of Statistics* **14**: 1431-1452.

HALL, P. 1987. On the bootstrap and likelihood-based confidence intervals. *Biometrika* **74**: 481-493.

KELLY, G.E. 1984. The influence function in the errors in variables problems. *Annals of Statistics* **12**: 87-100.

KENDALL, M.G. and A. STUART. 1973. *The Advanced Theory of Statistics*. London: Griffin.

LOH, W.-Y. 1987. Calibrating confidence coefficients. *Journal of American Statistical Association* **82**: 155-162.

LOH, W.-Y. 1994. Bootstrap calibration for confidence construction and selection. *Statistica Sinica* **82**: 155-162.

MILLER, R.G. Jr. 1980. Kanamycin levels in premature babies. *Biostatistics Casebook*, **III**: 127-142. Technical Report No. 57, Division of Biostatistics, Stanford University.

PATEFIELD, W.M. 1977. On the information matrix in the linear functional relationship problem. *Applied Statistics* **26**: 69-70.

SPRENT, P. 1966. A generalised least squares approach to linear functional relations. *Journal of the Royal Statistical Society* B **28**: 278-297.