SAMPLE SIZE CORRECTIONS FOR THE MAXIMUM PARTIAL LIKELIHOOD ESTIMATOR

F. R. B. Cruz, E. A. Colosimo
Department of Statistics
Federal University of Minas Gerais
31270-901 - Belo Horizonte - MG, Brazil
{fcruz,enricoc}@est.ufmg.br

J. MacGregor Smith
Department of Mechanical & Industrial Engineering
University of Massachusetts
Amherst, MA 01003, USA
E-mail: jmsmith@ecs.umass.edu

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ABSTRACT

In this paper, resampling methods, namely the jackknife and the bootstrap, are considered for bias evaluation and correction of maximum partial likelihood estimators. A complete set of Monte Carlo simulations compare the proposed approaches with formulae recently proposed for bias correction to order n^{-1}. The results indicate a competitive performance for these methods.

1. INTRODUCTION

The proportional hazards model (PHM) proposed by Cox (1) is probably one of the most important statistical methods for the analysis of censored data because of its flexibility for exploring the association of covariates with failure rates. Over the past recent years, the PHM has been applied for several practical situations ranging from medical studies to the analysis of economical data on employment and unemployment cycle duration. The most popular form of the Cox regression model makes use of the exponential form of the hazard function:

$$\lambda(t) = \lambda_0(t) \exp(\boldsymbol{\beta}^{\mathrm{T}}\mathbf{x}), \tag{1.1}$$

in which $\lambda_0(t)$ is a baseline hazard function (an unknown non-negative function of time), $\boldsymbol{\beta}$ is a $p \times 1$ vector of unknown parameters (to be estimated), and $\mathbf{x} = (x_1, x_2, \ldots, x_p)^{\mathrm{T}}$ is a covariate vector.

The estimation of coefficients $\boldsymbol{\beta}$ in Eq. (1.1) is based on the partial likelihood function (2) which is biased, typically of order n^{-1}, where n is the sample size. Due to its semiparametric nature, maximum partial likelihood estimators (MPLE's) are very sensitive to small and medium sample sizes and high proportions of censored observations. Unfortunately, in many instances in which the PHM is of use, the sample size is too small. For instance, in a phase II clinical trial with 20 patients, a 20% censoring will lead to only around 16 patients. Thus, in small or moderate-sized samples such as the situation above, the bias can be rather large and their evaluation and correction would be a boost for the applications.

In fact, the bias evaluation and correction for the maximum likelihood estimates have received much attention in the literature. The basic methodology has been applied to the one-parameter family (3), nonlinear regression models with normal errors (4, 5), binary response models (6), logistic discrimination problems (7), generalized linear models (8), generalized linear models with dispersion covariates (9), generalized log-gamma regression models (10), nonlinear exponential family regression models (11), multiplicative heteroscedastic regression models (12), ARMA models (13), von Mises regression models (14), one-parameter PHM (15), and p-parameter PHM (16).

The objective of this paper is to present two resampling approaches, the jackknife and the bootstrap, for second-order bias evaluation and correction of MPLE's, and to compare them with the analytical approach established by Montenegro et al. (16), extending their computational experiments. The paper is organized as follows. Section 2 presents the bias correction methods. Monte Carlo simulations were performed and the results are shown and discussed in Section 3. Section 4 presents numerical examples and Section 5 closes the paper with final remarks.

2. BIAS CORRECTIONS

Let $l = l(\boldsymbol{\beta})$ be the partial log-likelihood function, given the sample of n individuals, in which $k \leq n$ failures occur in times $t_1 \leq t_2 \leq \cdots \leq t_k$. In the absence of ties this function is written for model (1.1) as

$$l = \sum_{i=1}^{n} \delta_i \left[\boldsymbol{\beta}^{\mathrm{T}} \mathbf{x}_i - \log \left(\sum_{j \in R_{(t_i)}} \exp(\boldsymbol{\beta}^{\mathrm{T}} \mathbf{x}_j) \right) \right], \tag{2.1}$$

in which $R_{(t_i)} = \{k : \ t_k \geq t_i\}$ is the risk set at time t_i, δ_i is the failure indicator ($\delta_i = 1$, for failures, and $\delta_i = 0$, for censored observations), and $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{ip})^{\mathrm{T}}$ corresponds to the covariate row vector for the i-th individual. The MPLE of $\boldsymbol{\beta}$ (biased) is obtained by maximizing Eq. (2.1) and the interest is to correct the bias of this estimate.

2.1. ANALYTICAL CORRECTION

In order to obtain the n^{-1} bias of $\hat{\beta}_a$, $B(\hat{\beta}_a)$, Cox and Snell's (17) formula can be used in a simplified version as

$$B(\hat{\beta}_a) = \frac{1}{2} \sum{}' \kappa^{ar} \kappa^{st} \kappa_{rst}, \tag{2.2}$$

in which $\kappa_{rs} = E(\partial^2 l / \partial\beta_r \partial\beta_s)$, $\kappa_{rst} = E(\partial^3 l / \partial\beta_r \partial\beta_s \partial\beta_t)$, $\kappa_{rs,t} = E\Big((\partial^2 l / \partial\beta_r \partial\beta_s)(\partial l / \partial\beta_t)\Big)$, $\kappa_{rs}^{(t)} = \partial\kappa_{rs} / \partial\beta_t$, κ^{rs} is the inverse of matrix κ_{rs}, and $\sum'$ denotes a summation over all the combinations of parameters $\beta_1, \ldots, \beta_p$. Expression (2.2) was simplified based on the fact that $\kappa_{rs}^{(t)} = \kappa_{rst}$, since expected and observed cumulants are identical conditionally on the history of failures and censoring (15).

After some algebra, it can be shown that the $p \times 1$ bias vector $B(\hat{\boldsymbol{\beta}})$ reduces to

$$B(\hat{\boldsymbol{\beta}}) = (X^{\mathrm{T}} W X)^{-1} X^{\mathrm{T}} W \xi, \tag{2.3}$$

in which $(X^{\mathrm{T}} W X)$ is the Fisher information matrix for $\boldsymbol{\beta}$ and X is an $n \times p$ matrix of fixed regressors with full column rank. Additionally, $W = \Delta - \Delta^{(2)}$, $\Delta = \sum_{i=1}^{n} \Delta_i$, $\Delta_i =$

$\text{diag}\Big\{\delta_i\gamma_{ji}\exp(\boldsymbol{\beta}^{\mathrm{T}}\mathbf{x}_j)/s_i\Big\}$, $\gamma_{ji}=1$, if $t_j\geq t_i$, and $\gamma_{ij}=0$, if $t_j<t_i$, $s_i=\sum_{j=1}^n\gamma_{ji}\exp(\boldsymbol{\beta}^{\mathrm{T}}\mathbf{x}_j)$, $\Delta^{(2)}=\sum_{i=1}^n\Delta_iE\Delta_i$, $E=\mathbf{1}\mathbf{1}^{\mathrm{T}}$, $\mathbf{1}$ is a $n\times 1$ vector of ones, and ξ is an $n\times 1$ vector defined as $\xi=\frac{1}{2}W^{-1}\Big(\overline{\Delta}+2M-\Delta Z_d-2\overset{\bullet}{\Delta}\Big)\mathbf{1}$. Here, $\overline{\Delta}=\sum_{i=1}^n t_i\Delta_i$, $t_i=\mathbf{1}^{\mathrm{T}}Z_d\Delta_i\mathbf{1}$, $Z_d=\text{diag}\{Z\}$, $Z=X(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}$, $M=\sum_{i=1}^n\Delta_iZ\Delta_i$, $\overset{\bullet}{\Delta}=\sum_{i=1}^n v_i\Delta_i$, and $v_i=\mathbf{1}^{\mathrm{T}}\Delta_iZ\Delta_i\mathbf{1}$. The interested reader may find all the details in the paper of Montenegro et al. (16).

In the right-hand side of Eq. (2.3), which is of order n^{-1}, an estimate of the parameter $\boldsymbol{\beta}$ can be inserted in order to define the corrected MPLE

$$\tilde{\boldsymbol{\beta}}_{\mathrm{C}}=\hat{\boldsymbol{\beta}}-B(\hat{\boldsymbol{\beta}}). \tag{2.4}$$

The bias-corrected estimate $\tilde{\boldsymbol{\beta}}_{\mathrm{C}}$ is expected to have better sampling properties than the uncorrected one.

2.2. RESAMPLING CORRECTIONS

One of the most popular resampling correction methods is the jackknife (18), which is described as follows. Suppose that $\boldsymbol{\beta}$ is an unknown parameter vector of a distribution function $F_{\boldsymbol{\beta}}$ and that $T=T_1,T_2,\ldots,T_n$ is a sample of n *i.i.d* observations from that distribution. Suppose also that a reasonably good but biased estimation method is available and denote by $\hat{\boldsymbol{\beta}}$ such an estimator. Indicate by $\hat{\boldsymbol{\beta}}_{(i)}$ the biased estimate of $\boldsymbol{\beta}$ obtained by removing the i-th observation from sample T and define the new estimate $\tilde{\boldsymbol{\beta}}_i=n\hat{\boldsymbol{\beta}}-(n-1)\hat{\boldsymbol{\beta}}_{(i)}=\hat{\boldsymbol{\beta}}-(n-1)(\hat{\boldsymbol{\beta}}_{(i)}-\hat{\boldsymbol{\beta}})$, for $i=1,\ldots n$. The bias-corrected jackknife estimate of $\boldsymbol{\beta}$ is then the average of $\tilde{\boldsymbol{\beta}}_i$, as shown

$$\tilde{\boldsymbol{\beta}}_{\mathrm{J}}=n\hat{\boldsymbol{\beta}}-(n-1)\hat{\boldsymbol{\beta}}_{(\bullet)}=\hat{\boldsymbol{\beta}}-(n-1)(\hat{\boldsymbol{\beta}}_{(\bullet)}-\hat{\boldsymbol{\beta}}), \tag{2.5}$$

in which $(n-1)(\hat{\boldsymbol{\beta}}_{(\bullet)}-\hat{\boldsymbol{\beta}})$ is the jackknife estimate of bias and $\hat{\boldsymbol{\beta}}_{(\bullet)}=\sum_{i=1}^n\hat{\boldsymbol{\beta}}_{(i)}/n$. The jackknife estimates the term of order n^{-1} of the bias.

Another popular resampling correction is the bootstrap (19). The (nonparametric) bootstrap procedure may be described as follows. Let the parameter of interest be written as the functional $\boldsymbol{\beta}=t(F)$ of the distribution function F and let $\hat{\boldsymbol{\beta}}=t(\hat{F})$ be its 'plug-in' estimate, where $\hat{F}$ is the empirical distribution function of the data $t = (t_1, \ldots, t_n)$. The bias of $\hat{\boldsymbol{\beta}}$ is defined as

$$\text{bias}_F = \mathrm{E}_F(\hat{\boldsymbol{\beta}}) - \boldsymbol{\beta} = \mathrm{E}_F(\hat{\boldsymbol{\beta}}) - t(F),$$

in which $\mathrm{E}_F(\hat{\boldsymbol{\beta}})$ is the expectation of $\hat{\boldsymbol{\beta}}$.

In order to estimate bias_F, it is necessary to draw a random sample of size n with replacement $t^* = (t_1^*, \ldots, t_n^*)$ from the original data $(t_1, \ldots, t_n)$, called the bootstrap sample from the empirical distribution function $\hat{F}$. The bootstrap estimate of the bias is then defined as

$$\text{bias}_{\hat{F}} = \mathrm{E}_{\hat{F}}(\hat{\boldsymbol{\beta}}^*) - t(\hat{F}),$$

in which $\mathrm{E}_{\hat{F}}(\hat{\boldsymbol{\beta}}^*)$ is the expectation of $\hat{\boldsymbol{\beta}}$ based on the empirical distribution function of the bootstrap sample.

The bootstrap estimate of the bias may be approximated by a Monte Carlo simulation procedure by choosing, from the empirical distribution $\hat{F}$, B independent bootstrap samples $t^{*1}, t^{*2}, \ldots, t^{*B}$. Then, the bootstrap replications $\hat{\boldsymbol{\beta}}^*_{(b)}$ are evaluated and the expectation $\mathrm{E}_{\hat{F}}(\hat{\boldsymbol{\beta}}^*)$ is approximated by $\hat{\boldsymbol{\beta}}^*_{(\bullet)} = \sum_{b=1}^{B} \hat{\boldsymbol{\beta}}^*_{(b)}/B$. The bootstrap estimate of the bias of order n^{-1} based on the B replications is then given by

$$\text{bias}_B = \hat{\boldsymbol{\beta}}^*_{(\bullet)} - \hat{\boldsymbol{\beta}}.$$

Thus, the (nonparametric) bootstrap bias-corrected estimate of β is

$$\tilde{\boldsymbol{\beta}}_B = 2\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}^*_{(\bullet)}. \tag{2.6}$$

3. MONTE CARLO SIMULATIONS

The estimators were implemented in Fortran and are available upon request. Monte Carlo simulations were done to compare the performance of the usual MPLE's and their corrected versions given by Eq. (2.4), (2.5), and (2.6). The simulation study was performed on a PC, 400 MHz, 64 MB RAM, operating system Windows NT 4.0, and using the *Compaq*

Visual Fortran Professional Edition 6.5.0. The simulation study was based on a Weibull regression model with three explanatory variables. For each experiment, maximum partial likelihood estimates $\hat{\boldsymbol{\beta}}$, jackknife corrected estimates $\tilde{\boldsymbol{\beta}}_{\mathrm{J}}$, bootstrap corrected estimates $\tilde{\boldsymbol{\beta}}_{\mathrm{B}}$, and analytical corrected estimates $\tilde{\boldsymbol{\beta}}_{\mathrm{C}}$ were computed.

Two independent sets of n independent random variables $T^{\mathrm{T}} = (T_1, \ldots, T_n)$ and $U^{\mathrm{T}} = (U_1, \ldots, U_n)$ were generated for each repetition and the lifetime $\min(T_i, U_i)$ and δ_i were recorded. T_i is a vector of realizations of a three-parameter Weibull$\big(\rho, \exp(\boldsymbol{\beta}^{\mathrm{T}}\mathbf{x}_i)\big)$ and $U_i \sim \mathcal{U}(0, \theta)$ corresponds to the random censoring mechanism. The set of covariate values $\mathbf{x}_i$ was maintained the same in all repetitions. The covariates used were independent Bernoulli with $p = 0.5$, gamma with scale and shape parameters equal to 1.0, and standard normal, *i.e.*, $x_{i1} \sim \mathcal{B}(0.5)$, $x_{i2} \sim \mathcal{G}(1, 1)$, and $x_{i3} \sim \mathcal{N}(0, 1)$.

The parameters $\boldsymbol{\beta} = (\beta_1, \beta_2, \beta_3)$ were set equal to $(1.0, 1.0, 1.0)$ and 10,000 replications were run for each simulation. The bootstrap estimates were computed using $N = 200$ bootstrap replications as suggested by Efron and Tibshirani (19). Slightly larger and smaller values for N have been tried but the results (not shown) were essentially the same. The simulations were performed for several combinations varying the parameter ρ (0.2, 0.5, 1.0, and 2.0), the proportion of censoring in the sample, F (0%, 20%, and 40%), and the sample sizes, n (10, 20, and 30). The nominal proportion of censoring, $P(U_i < T_i)$, was obtained by controlling the value of the parameter θ in the uniform distribution.

Figure 1 displays the average estimates as a function of the parameters ρ, F, and n, for the set of covariates aforementioned. The bias can be quite pronounced for small sample size and high proportion of censoring. There is a substantial bias reduction using the analytical and bootstrap corrected estimators when compared with the standard MPLE's. The jackknife bias reduction does not work properly, mainly in very small sample sizes, and tends to underestimate $\boldsymbol{\beta}$.

Other conclusions that can be drawn from Figure 1 are:

(1) the standard MPLE's always overestimate the true parameters;

(2) as expected, the bias increases as F increases and n decreases;

(3) the bias is really large for $n = 10$;

(4) in general, as a function of n, the boostrap and the analytical methods provide zig-zig pattern estimates (underestimates followed by overestimates) that tend to the correct values as n increases and that are mostly in opposite sides;

(5) $\mathcal{B}(0.5)$ is the less biased covariate and $\mathcal{N}(0,1)$ is the most biased covariate.

Figure 2 displays the average of the root of the mean square errors (RMSE's) as function of the parameters ρ, F, and n. As expected, in general, the RMSE increases as ρ decreases, as F increases, and as n decreases. No variance inflation is observed whatsoever for all correction methods but for the jackknife in comparison to the standard MPLE's. In most of the cases, the analytical method provides the lowest RMSE followed closely by the bootstrap method.

Another set of covariates, $x_{i1} \sim \mathcal{N}(0,1)$, $x_{i2} \sim \mathcal{N}(0,2)$, and $x_{i3} \sim \mathcal{N}(0,3)$, was examined and the results (not shown) lead to similar conclusions.

4. NUMERICAL EXAMPLES

EXAMPLE 1

The data are from Glasser (20) and it also appears in Lawless (21). The response variable y is the logarithm of survival time (in days) for patients with primary lung tumors. There are 16 patients and six of them are censored. Two covariates are represented in the data set: x_1 is the patient's age and x_2 is a performance status rating (divided by 10). The main goal of the study is to evaluate the importance of these covariates.

Table 1 displays the estimates for parameter β_1 and β_2, associated with covariates x_1 and x_2, as well as the respective standard error and 95% confidence intervals. The confidence intervals for the jackknife and bootstrap methods are built in terms of their empirical percentiles (19). For all four methods, the disagreement among the point estimates for $\boldsymbol{\beta}$ is noticeable. According to the results presented in Section 3, the analytical and bootstrap estimates are the most reliable. All methods however agreed that no covariate has a significant

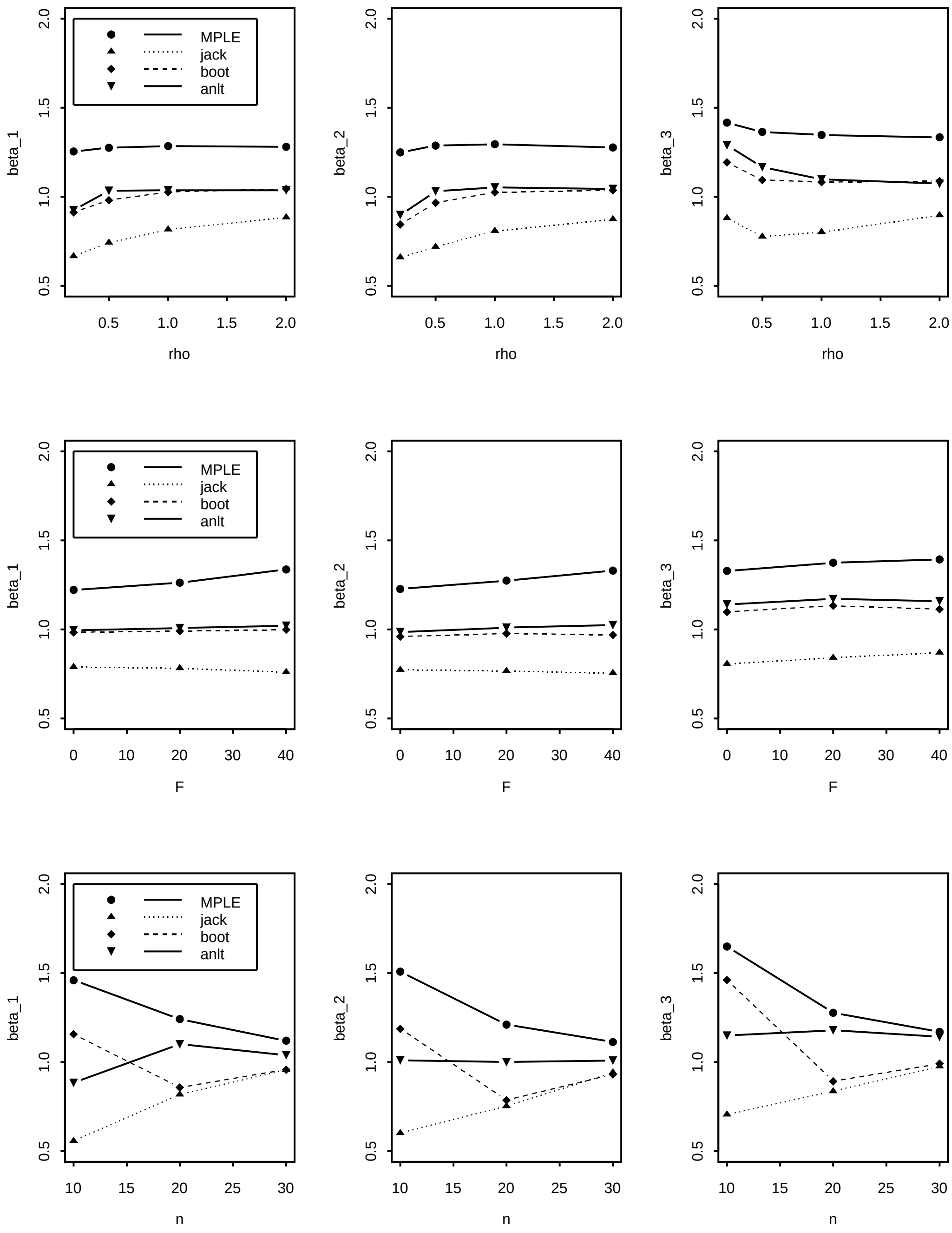

Figure 1: Average Estimates, Covariates $x_1 \sim \mathcal{B}(0.5)$, $x_2 \sim \mathcal{G}(1, 1)$, $x_3 \sim \mathcal{N}(0, 1)$

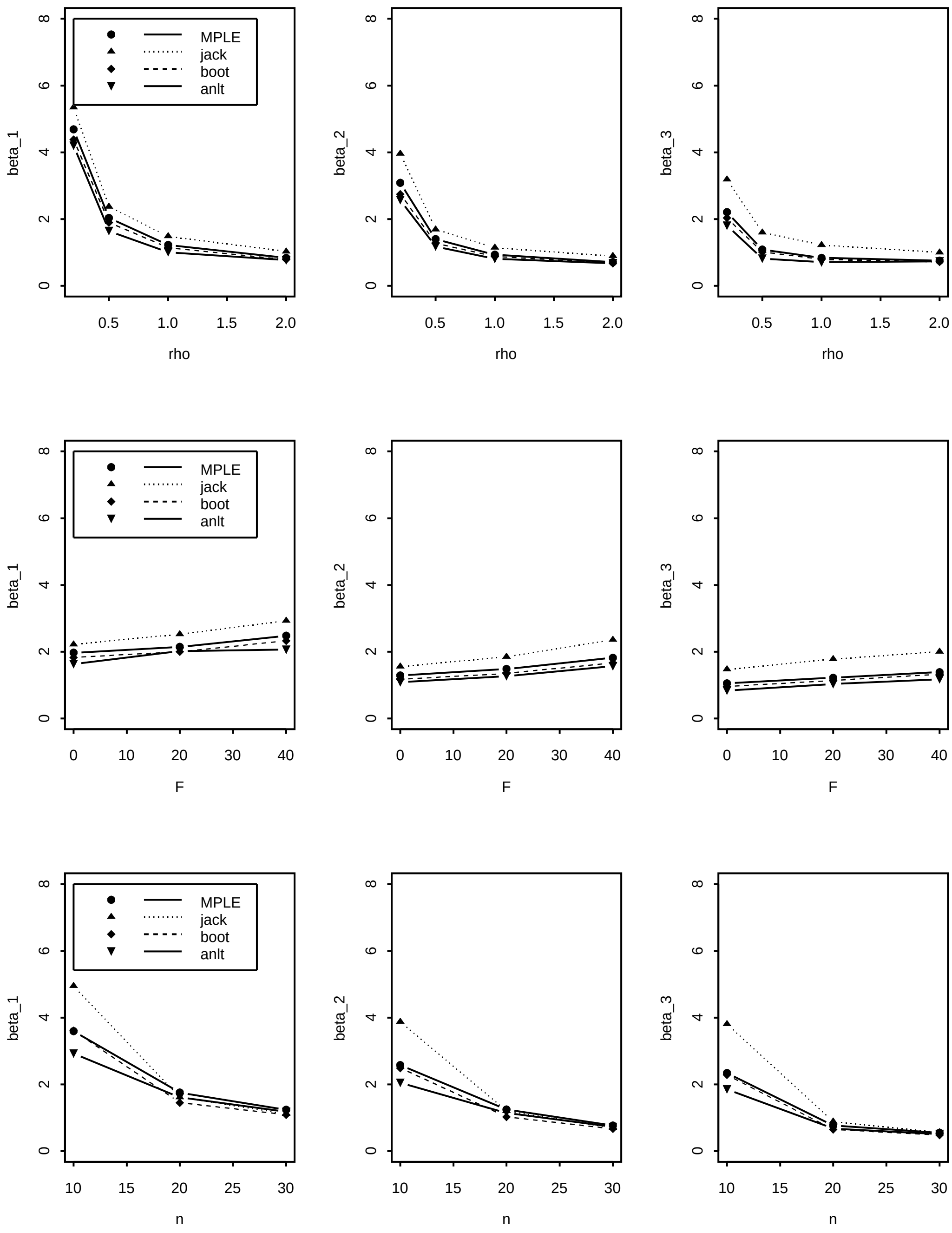

Figure 2: Average RMSE, Covariates $x_1 \sim \mathcal{B}(0.5)$, $x_2 \sim \mathcal{G}(1,1)$, $x_3 \sim \mathcal{N}(0,1)$

Table 1: Point and 95% Confidence Interval Estimates for Example 1

		MPLE	jackknife	bootstrap	analytical
β_1	Estimate	-0.00178	-0.02931	-0.02081	-0.00300
	S.E.	0.04182	–	–	0.04182
	95% CI	(-0.08374;0.08018)	(-0.57841;0.18377)	(-0.15490;0.08403)	(-0.08496;0.07896)
β_2	Estimate	-0.20714	-0.00050	-0.10780	-0.20437
	S.E.	0.16170	–	–	0.16170
	95% CI	(-0.52408;0.10980)	(-1.04667;3.33462)	(-0.45034;0.56988)	(-0.52131;0.11257)

effect on the response.

EXAMPLE 2

The data are adapted from Lee (22). Thirty melanoma patients (stages 2-4) were studied to compare the immunotherapies BCG (*Bacillus Calmette-Guérin*) and *Corynebacterium parvum* for the ability to prolong remission and survival time. The response variable y is the remission time (in months) and there are 14 censored observations. Three covariates for each patient are represented in the data set: x_1 is age, x_2 is gender, x_3 is the treatment received. The main goal of the study is to compare treatments controlling for the other covariates.

Table 2 displays the estimates for parameter β_1, β_2, and β_3, associated with covariates x_1, x_2, and x_3, as well as the respective standard error and 95% confidence intervals. For this example, the covariates do not seem to have a significant effect on the response. Excluding the jackknife, all other methods produced fairly similar point estimates as well as confidence intervals.

EXAMPLE 3

The data are from Lee (22, p. 257) that represents survival times from thirty patients with acute myelocytic leukemia (AML). Two covariates for each patient are represented in the data set: x_1 is age (1 if patient's age is greater or equal to 50 and 0 otherwise), x_2 is

Table 2: Point and 95% Confidence Interval Estimates for Example 2

		MPLE	jackknife	bootstrap	analytical
β_1	Estimate	0.01254	0.01377	0.01316	0.01392
	S.E.	0.01338	-	-	0.01338
	95% CI	(-0.01367;0.03876)	(-0.11045;0.10733)	(-0.02432;0.04744)	(-0.01229;0.04014)
β_2	Estimate	-0.64544	-0.62788	-0.57372	-0.62895
	S.E.	0.54847	-	-	0.54847
	95% CI	(-1.72045;0.42957)	(-4.14489;6.42742)	(-1.83691;0.78039)	(-1.70396;0.44606)
β_3	Estimate	-0.33029	-0.28872	-0.32634	-0.35898
	S.E.	0.53819	-	-	0.53819
	95% CI	(-1.38515;0.72457)	(-4.21905;5.34097)	(-1.82504;0.74485)	(-1.41383;0.69588)

1 if cellularity of marrow clot section is 100% and 0 otherwise. There are seven censored observations.

Table 3 displays the estimates for parameters β_1 and β_2, associated with covariates x_1 and x_2, as well as the respective standard error and 95% confidence intervals. In this case, the data set confirms the association between survival time and age by the standard MPLE and by the analytical correction. The resampling methods however do not show the covariate as important.

5. SUMMARY AND FINAL REMARKS

The main purpose of this paper was to provide two resampling approaches, the jackknife and the bootstrap, for second-order bias evaluation and correction of maximum partial likelihood estimators (MPLE's). The performance of the bootstrap resampling method was compared to the analytical correction method recently developed by Montenegro et al. (16). The comparisons were made by means of Monte Carlo simulations over a wide range of experiments. The results indicated that the resampling techniques are quite appealing and present a competitive performance. They are also an attractive alternative for bias reduction,

Table 3: Point and 95% Confidence Interval Estimates for Example 3

		MPLE	jackknife	bootstrap	analytical
β_1	Estimate	1.01320	0.89681	0.85911	0.98159
	S.E.	0.45740	-	-	0.45740
	95% CI	(0.11670;1.90971)	(-3.83705;4.66528)	(-0.34925;1.70364)	(0.08508;1.87810)
β_2	Estimate	0.35026	0.40541	0.37895	0.32667
	S.E.	0.43917	-	-	0.43918
	95% CI	(-0.51052;1.21105)	(-2.46925;6.77925)	(-0.36532;1.25731)	(-0.53412;1.18745)

avoiding the sophisticated mathematics commonly present in analytical methods. Future directions for research in the area include the performance evaluation of multi-level resampling techniques (23) applied to the MPLE's.

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