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by

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# CORRECTED MAXIMUM LIKELIHOOD ESTIMATION IN A CLASS OF SYMMETRIC NONLINEAR REGRESSION MODELS<sup>1</sup>

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#### Abstract

In this paper we derive general formulae for second-order biases of maximum likelihood estimates in a class of symmetric nonlinear regression models. This class of models is commonly used for the analysis of data containing extreme or outlying observations in samples from a supposedly normal distribution. The formulae of the biases can be computed by means of an ordinary linear regression. They generalize some previous results by Cook, Tsai and Wei (1986), Cordeiro and Vasconcellos (1997) and Cordeiro, Vasconcellos and Santos (1998). We derive simple closed-form expressions for these biases in special models. Simulation results are presented assessing the performance of the bias corrected estimates which indicate that they have smaller biases than the corresponding unadjusted estimates.

Keywords: Bias correction; Maximum likelihood estimate; Nonlinear regression; Symmetric distribution; t distribution.

### 1 Introduction

It is well known that the normal model is not always a good model for representing data containing extreme or outlying observations and there is presently a widespread awareness of the danger posed by the occurence of outliers. To overcome these problems, new statistical models that are not so easily affected by outlying observations have been developed. The symmetric family of distributions provides a useful extension of the normal distribution for statistical modeling of data sets involving errors with longer—than—normal tails. Symmetric distributions are appearing with increasing frequency in the statistical literature to model several types of data containing more outlying observations than can be expected based on a normal distribution. Specifically, a symmetric distribution with flat tails or with tails that decrease to zero more slowly than those of the normal distribution provides a useful model for achieving robust statistical inference in the analysis of such types of data. For these models, the inference remains trustworthy even if a certain amount of data is contaminated.

The random variable y is said to have a symmetric distribution with location parameter  $\mu \in \mathbb{R}$  and scale parameter  $\phi > 0$  if its density function is of the form

$$\pi(y;\mu,\phi) = \frac{1}{\phi}h\left(\left(\frac{y-\mu}{\phi}\right)^2\right), \quad y \in \mathbb{R},$$
 (1)

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for some function h (which is independent of y,  $\mu$  and  $\phi$ ), such that h(u)>0, for u>0 and  $\int_0^\infty u^{-1/2}h(u)\mathrm{d}u=1$ . In this paper, any particular symmetric distribution will be denoted by  $S(\mu,\phi^2)$ . The characteristic function  $\psi(t)=\mathrm{E}(e^{ity})$  is given by  $\psi(t)=e^{it\mu}\varphi(t^2\phi^2)$ ,  $t\in\mathbb{R}$ , for some function  $\varphi$ , with  $\varphi(x)\in\mathbb{R}$ , for x>0. Provided that they exist,  $\mathrm{E}(y)=\mu$  and  $\mathrm{Var}(y)=k\phi^2$ , where k>0 is a constant given by  $k=-2\varphi'(0)$ , where  $\varphi'(0)=\mathrm{d}\varphi(u)/\mathrm{d}u|_{u=0}$ . Thus, the parameter  $\phi$  is a kind of dispersion parameter. If the distribution  $S(\mu,\phi^2)$  has r moments, then  $x^{-(r+1)/2}h(x)$  is integrable (Kelker, 1970). The probability density function of  $z=(y-\mu)/\phi$  is  $\pi(v;0,1)=h(v^2)$ ,  $v\in\mathbb{R}$ , which does not involve the parameters  $\mu$  and  $\phi$ , i.e.  $z\sim S(0,1)$ . It is the standardized form of the symmetric distributions.

The symmetric family of location-scale densities (1) retains the structure of the normal distribution, while eliminating the specific form of the normal density. Densities in this family are mainly distinguished by their tail length and some of them may have sharper or flatter tails than the normal form, although the main interest focuses on flat-tailed distributions. The class of symmetric distributions defined in (1) has been considered by several authors (Kelker, 1970; Chu, 1973; Cambanis, Huang and Simons, 1981). The properties of these distributions have been explored by Muirhead (1980, 1982), Berkane and Bentler (1986), Rao (1990) and Fang, Kotz and Ng (1990). It is easy to find many properties of  $S(\mu,\phi^2)$  parallel to those of  $N(\mu,\phi^2)$ . A review of different areas in which symmetric distributions are applied is given by Chmielewski (1981).

The modern area of research in symmetric distributions starts perhaps with the engineering applications considered by Blake and Thomas (1968) and McGraw and Wagner (1968). Cambanis, Huang and Simons (1981) presented a systematic treatment for symmetric distributions and Chmielewski (1981) gave a detailed survey of these distributions with applications to different areas. The special cases of (1) listed bellow have a wide range of practical applications in various fields such as engineering, biology, medicine and economics, among others.

- (i) Normal:  $h(u) = (2\pi)^{-1/2} \exp(-u/2)$ ;
- (ii) Cauchy:  $h(u) = {\pi(1+u)}^{-1}$ ;
- (iii) Student's t:  $h(u) = \nu^{\nu/2} B(1/2, \nu/2)^{-1} (\nu + u)^{-\frac{\nu+1}{2}}, \nu > 0$ , where  $B(\cdot, \cdot)$  is the beta function;
- (iv) Generalized Student's t:  $h(u) = s^{r/2}B(1/2, r/2)^{-1}(s+u)^{-\frac{r+1}{2}}, s, r > 0$ . It includes Student's t  $(s=r=\nu)$  and Cauchy distribution (s=r=1);
- (v) Type I logistic:  $h(u) = ce^{-u}(1+e^{-u})^{-2}$ , where  $c \approx 1.484300029$  is the normalizing constant which follows from  $\int_0^\infty u^{-1/2}h(u)\mathrm{d}u = 1$ ;
- (vi) Type II logistic:  $h(u) = e^{-u^{1/2}} (1 + e^{-u^{1/2}})^{-2}$ ;
- (vii) Generalized logistic:  $h(u) = cB(m,m)^{-1} \{e^{-c\sqrt{u}}(1+e^{-c\sqrt{u}})^{-2}\}^m$ , m>0, c>0. The type II logistic density corresponds to the case m=1, c=1;
- (viii) Kotz distribution:

$$h(u) = \frac{r^{(2m-1)/2}}{\Gamma(\frac{2m-1}{2})} u^{m-1} \exp(-ru), \ r > 0, \ m \ge 1,$$

(Kotz, 1975), where  $\Gamma(\cdot)$  is the gamma function. If m=1 this distribution reduces to the normal distribution with mean  $\mu$  and variance  $\phi^2/(2r)$ ;

### (ix) Generalized Kotz distribution:

$$h(u) = \frac{sr^{(2m-1)/(2s)}}{\Gamma(\frac{2m-1}{2s})} u^{m-1} \exp(-ru^s), \ r, s > 0, \ m \ge 1.$$

For s=1, it reduces to Kotz distribution and for m=s=1 and r=1/2, it becomes the  $N(\mu,\phi^2)$  distribution. When m=1, r=1/2 and s=1/(1+k), it coincides with the power exponential distribution defined below in case (xii);

### (x) Contaminated normal:

$$h(u) = (1 - \varepsilon) \frac{1}{\sqrt{2\pi}} \exp(-u/2) + \varepsilon \frac{1}{\sqrt{2\pi}\sigma} \exp\{-u/(2\sigma^2)\}, \quad \sigma > 0, \quad 0 \le \varepsilon \le 1;$$

- (xi) Double exponential:  $h(u) = \exp(-\sqrt{u})/2$ ;
- (xii) Power exponential:

$$h(u) = c(r) \exp\left\{-\frac{1}{2} u^{1/(1+r)}\right\}, \ -1 < r \le 1,$$

where  $c(r)^{-1} = \Gamma(1 + \frac{1+r}{2})2^{1+(1+r)/2}$  (Box and Tiao, 1973);

### (xiii) Extended power family:

$$h(u) = K(c,\lambda) \exp\left\{-\frac{1}{2}c\rho_{\lambda}\left(1+\frac{u}{c-1}\right)\right\},\,$$

where  $K(c,\lambda)$  is the normalizing constant,  $c>1,\,\lambda\geq 0$  and

$$\rho_{\lambda}(v) = \begin{cases} \frac{v^{\lambda} - 1}{\lambda}, & \text{if } \lambda > 0, \\ \lim_{\lambda \to 0} \frac{v^{\lambda} - 1}{\lambda} = \log v, & \text{if } \lambda = 0. \end{cases}$$

(Albert, Delampady and Polasek, 1991).

The 13 distributions listed above provide a rich source of alternative models for analysing univariate data containing outlying observations. However, some regularity conditions needed for the validity of our results do not hold for the Kotz, generalized Kotz and double exponential distributions. Moreover, we have not developed our results for the contaminated normal and extended power distributions. Therefore, in what follows, we restric our attention to the following distributions: normal, Cauchy, Student's t, generalized Student's t, type I logistic, type II logistic, generalized logistic and power exponential.

The subject matter of this paper is the symmetric nonlinear regression model

$$y_i \sim S(\mu_i, \phi^2), \quad i = 1, ..., n,$$
 (2)

where  $y_1,\ldots,y_n$  are assumed to be independent and each  $y_i$  has a symmetric distribution (1) with location parameter  $\mu_i$  ( $\mu_i \in \mathbb{R}$ ) and scale parameter  $\phi > 0$  which is common to all observations. In order to introduce a regression structure in the class of models (2), we assume that  $\mu_i = f(x_i; \beta)$ , where  $x_i$  is an  $m \times 1$  vector of known explanatory variables associated with the i-th observable response  $y_i$  and  $\beta \in \Omega_\beta \subset \mathbb{R}^p$  is a  $p \times 1$  vector of unknown regression parameters. We further assume that  $\Omega_\beta$  is

compact with interior points and f is an injective and twice continuously differentiable function with respect to  $\beta$  at these interior points. Then, inference about  $\beta$  and  $\phi$  can be performed by likelihood methods analogously to those for the normal nonlinear model. A very convenient way for obtaining the maximum likelihood estimates (MLEs)  $\hat{\beta}$  and  $\hat{\phi}$  of  $\beta$  and  $\phi$  is given by an iteratively reweighted least squares algorithm presented in Section 2.

The computation of second-order biases is perhaps one of the most important of all approximations arising from the theory of estimation by maximum likelihood in nonlinear regression models. The obvious difficulty with nonlinear estimates is that they cannot be expressed as explicit functions of the data. Over the last ten years, there have been many advances with respect to bias calculation of nonlinear MLEs whose second-order biases can be larger than the corresponding standard errors of the estimates when the sample size n or the total Fisher information is small. In these cases, bias corrections can be important and the availability of formulae for calculating the biases is useful. Numerous applications for second-order bias corrections of MLEs are available in the literature. We refer the reader to the papers by Cook et al. (1986), Young and Bakir (1987), Cordeiro and McCullagh (1991), Paula (1992), Cordeiro and Klein (1994), Paula and Cordeiro (1995), Cordeiro and Vasconcellos (1997) and Cordeiro, Vasconcellos and Santos (1998). Except for the paper by Young and Bakir, all other papers deal with matrix formulae that are useful for applied researchers to compute bias corrections in some classes of nonlinear regression models. These formulae can be used to obtain bias-corrected estimates by subtracting the second-order biases from the MLEs. Despite these results, there is still skepticism from some researchers about the usefulness of second-order bias reduction. We address this issue by Monte Carlo simulation to show that bias-corrected estimates of the parameters in symmetric nonlinear regression models outperform traditional MLEs.

The main goal of this paper is to derive general formulae for the second-order biases of the MLEs  $\hat{\beta}$  and  $\hat{\phi}$  in model (2). The plan of this paper is as follows. Section 2 presents a simple matrix formula for computing the  $n^{-1}$  bias of  $\hat{\beta}$ . The formula can be of direct practical use since the bias of  $\hat{\beta}$  is easily obtained as a vector of regression coefficients in an ordinary linear regression conveniently defined. In Section 3, we apply this formula to derive the  $n^{-1}$  bias of  $\hat{\beta}$  for some special models. In Section 4, we obtain a bias correction for the MLE of  $\phi$ . We emphasize that the biases of  $\hat{\beta}$  and  $\hat{\phi}$  presented here include as special cases some results due to Cook, Tsai and Wei (1986), Cordeiro and Vasconcellos (1997) and Cordeiro, Vasconcellos and Santos (1998). Finally, in Section 5, some Monte Carlo simulation results from model (2) are given on the finite-sample performance of their bias-corrected MLEs. The simulations indicate that bias-corrected estimates have smaller biases than the corresponding unadjusted estimates.

## 2 Bias of the Estimate $\hat{\beta}$

The purpose of this section is to use Cox and Snell's (1968) formula (20) for the  $n^{-1}$  bias of the MLE in order to obtain the second-order bias of  $\hat{\beta}$ . In Section 4, we focus on the bias of  $\hat{\phi}$ . Let  $l=l(\beta,\phi)$  be the total log-likelihood function, given the sample  $y_1,\ldots,y_n$ , for the parameters  $\beta$  and  $\phi$  in model (2). We are interested in jointly estimation by maximum likelihood of the parameters  $\beta$  and  $\phi$  and in correcting the biases of these estimates. We have

$$l(\beta, \phi) = -n \log \phi + \sum_{i=1}^{n} \log h(z_i^2),$$
 (3)

where

$$z_i = (y_i - \mu_i)/\phi$$

is the standardized i-th observation.

The function l is assumed to be regular (Cox and Hinkley, 1974; Chapter 9) with respect to all  $\beta$  and  $\phi$  derivatives up to third order. Furthermore, the  $n \times p$  matrix of derivatives of  $\mu = (\mu_1, \dots, \mu_n)^{\top}$  with respect to  $\beta$ , denoted by  $D = D(\beta) = \partial \mu/\partial \beta$ , is assumed to be of full rank, i.e. rank (D) = p for all  $\beta$ . Inference about  $\beta$  and  $\phi$  can be performed by likelihood methods analogous to those for the normal model. Regularity conditions are also stated in Serfling (1980, p. 144). We must assume that the MLEs  $\hat{\beta}$  and  $\hat{\phi}$  converge to their true parameter values as  $n \to \infty$  and that their joint asymptotic distribution is multivariate normal with the usual covariance matrix to the correct order.

We now introduce the notation for moments of the log-likelihood derivatives:  $\kappa_{rs}=E(\partial^2 l/\partial\beta_r\beta_s)$ ,  $\kappa_{r,s}=E(\partial l/\partial\beta_r\partial l/\partial\beta_s)$ ,  $\kappa_{rst}=E(\partial^3 l/\partial\beta_r\partial\beta_s\partial\beta_t)$ . Not all the  $\kappa's$  are functionally independent. For example,  $\kappa_{rs}=-\kappa_{r,s}$  is the typical element of the information matrix for  $\beta$ . Note that  $\kappa_{rs,t}$  is the covariance between the first derivative of l with respect to  $\beta_t$  and the mixed second derivative of l with respect to  $\beta_r$  and  $\beta_s$ . Furthermore, we define the derivatives of the moments as  $\kappa_{rs}^{(t)}=\partial\kappa_{rs}/\partial\beta_t$ . All  $\kappa's$  and their derivatives are assumed to be of order O(n). Also, the following notation is adopted:  $d_{ir}=\partial\mu_i/\partial\beta_r$  and  $g_{irs}=\partial^2\mu_i/\partial\beta_r\partial\beta_s$  for the first and second partial derivatives of  $\mu_i$  with respect to the elements of  $\beta$ .

Now define  $\alpha_{r,s} = E\{t^{(r)}(z)z^s\}$  for r,s=0,1,2,3, where  $t(z) = \log h(z^2)$  and  $t^{(r)}(z) = \mathrm{d}^r t(z)/\mathrm{d}z^r$ . Differentiating (3) and taking expectations, we obtain

$$\begin{split} \kappa_{r,s} &= -\frac{\alpha_{2,0}}{\phi^2} \sum_{i=1}^n \ d_{ir} d_{is}, \quad \kappa_{r,\phi} = 0, \quad \kappa_{\phi,\phi} = \frac{n}{\phi^2} (1 - \alpha_{2,2}), \quad \kappa_{rt}^{(u)} = \frac{\alpha_{2,0}}{\phi^2} \sum_{i=1}^n \ (d_{ir} g_{itu} + d_{it} g_{iru}), \\ \kappa_{rst} &= \frac{\alpha_{2,0}}{\phi^2} \sum_{i=1}^n \ (d_{ir} g_{ist} + d_{is} g_{irt} + d_{it} g_{irs}), \quad \kappa_{rs\phi} = -\frac{\alpha_{3,1} + 2\alpha_{2,0}}{\phi^3} \sum_{i=1}^n \ d_{ir} d_{is}, \quad \kappa_{r\phi\phi} = 0, \\ \kappa_{\phi\phi\phi} &= -\frac{n}{\phi^3} (\alpha_{3,3} + 6\alpha_{2,2} - 4). \end{split}$$

In view of the global orthogonality between  $\beta$  and  $\phi$  ( $\kappa_{r,\phi}=0$ ), the joint information matrix for these parameters is block-diagonal, i.e.  $K=\mathrm{diag}\{K_{\beta},\kappa_{\phi,\phi}\}$ , where  $K_{\beta}=-(\alpha_{2,0}/\phi^2)D^{\top}D$  is the information matrix for  $\beta$ . The Fisher scoring method can be used to estimate  $\beta$  and  $\phi$  simultaneously by iteratively solving the equations

$$\begin{split} \beta^{(m+1)} &= \beta^{(m)} - \frac{1}{\alpha_{2,0}} (D^{(m)^\top} D^{(m)})^{-1} D^{(m)^\top} \zeta^{(m)}, \\ \phi^{(m+1)} &= \phi^{(m)} + \frac{1}{\phi^{(m)} (1 - \alpha_{2,2})} \left\{ \frac{1}{n} (y - \mu^{(m)})^\top W^{(m)} (y - \mu^{(m)}) - \phi^{(m)^2} \right\}, \end{split}$$

where  $\zeta^{(m)}=W^{(m)}(y-\mu^{(m)})$  with  $W=\mathrm{diag}\{w_1,\ldots,w_n\}$  and  $w_i=-z_i^{-1}\mathrm{d}\log h(z_i^2)/\mathrm{d}z_i$ .

Let  $B(\widehat{\beta}_a)$  be the  $n^{-1}$  bias of  $\widehat{\beta}_a$ . The use of Cox and Snell's formula to obtain  $B(\widehat{\beta}_a)$  is greatly simplified, since  $\beta$  and  $\phi$  are globally orthogonal. We obtain

$$B(\widehat{\beta}_a) = \sum_{r,t,u} {'} \kappa^{ar} \kappa^{tu} \left( \frac{1}{2} \kappa_{rtu} + \kappa_{rt,u} \right) + \sum_r {'} \kappa^{ar} \kappa^{\phi\phi} \left( \frac{1}{2} \kappa_{r\phi\phi} + \kappa_{r\phi,\phi} \right),$$

where  $-\kappa^{r_{\theta}}$  and  $-\kappa^{\phi\phi}$  are the corresponding elements of the inverse of the joint information matrix K and  $\sum'$  denotes the summation over all combinations of the parameters  $\beta_1,\ldots,\beta_p$ . Since  $\kappa_{rtu}/2+\kappa_{rt,u}=\kappa_{rt}^{(u)}-\kappa_{rtu}/2$  and  $\kappa_{r\phi\phi}/2+\kappa_{r\phi,\phi}=\kappa_{r\phi}^{(\phi)}-\kappa_{r\phi\phi}/2=0$ , it follows that

$$B(\widehat{\beta}_a) = \sum_{r,t,u} {'\kappa^{ar}\kappa^{tu}} \left(\frac{\alpha_{2,0}}{2\phi^2}\right) \sum_{i=1}^n \left(d_{ir}g_{itu} + d_{it}g_{iru} - d_{iu}g_{irt}\right).$$

By rearranging the summation terms we have

$$B(\widehat{\beta}_a) = \left(\frac{\alpha_{2,0}}{2\phi^2}\right) \sum_{i=1}^n \sum_r \kappa^{ar} d_{ir} \sum_{t,u} \kappa^{tu} g_{itu}.$$

Let  $d_i^{\top}(1 \times p)$  and  $g_i^{\top}(1 \times p^2)$  be vectors containing the first and second partial derivatives of  $\mu_i$  with respect to the  $\beta's$ . We can write the above equation in matrix notation as

$$B(\widehat{\beta}_a) = \frac{\alpha_{2,0}}{2\phi^2} \sum_{i=1}^n \ \rho_a^\mathsf{T} K_\beta^{-1} d_i g_i^\mathsf{T} \mathrm{vec}(K_\beta^{-1}),$$

where  $\rho_a^{\rm T}$  is the a-th row of the  $p \times p$  identity matrix and  ${\rm vec}(.)$  is the operator which transforms a matrix into a vetor by stacking the columns of the matrix one underneath the other. It is straightforward to check that

$$B(\widehat{\beta}_a) = \frac{\alpha_{2,0}}{2\phi^2} \rho_a^{\mathsf{T}} K_{\beta}^{-1} D^{\mathsf{T}} G \text{vec}(K_{\beta}^{-1}),$$

where  $D=\partial\mu/\partial\beta=(d_1,\ldots,d_n)^{\rm T}$  and  $G=\partial^2\mu/\partial\beta^{\rm T}\partial\beta=(g_1,\ldots,g_n)^{\rm T}$  denote  $n\times p$  and  $n\times p^2$  matrices of the first and second partial derivatives of  $\mu$  with respect to the  $\beta's$ , respectively. The  $n^{-1}$  bias vector  $B(\widehat{\beta})$  of  $\widehat{\beta}$  can then be written as

$$B(\widehat{\beta}) = \left(D^{\mathsf{T}}D\right)^{-1}D^{\mathsf{T}}d,\tag{4}$$

where d is an  $n \times 1$  vector defined as  $d = (\phi^2/(2\alpha_{2,0}))G\text{vec}\{(D^TD)^{-1}\}.$ 

A number of remarks are worth making with respect to expression (4). The bias vector  $B(\widehat{\beta})$  can be obtained from the simple least-squares regression of d on the columns of D. Clearly, the bias  $B(\widehat{\beta})$  depends on the symmetric distribution of the data only through the quantity  $\alpha_{2,0}$  and it can be large when  $\alpha_{2,0}$  and n are both small. Further, the bias of  $\widehat{\beta}$  increases with the dispersion parameter  $\phi$ . For some symmetric distributions, the values of  $\alpha_{2,0}$  are given in Table 1. For normal models,  $\alpha_{2,0}=-1$  and equation (4) coincide with the result due to Cook, Tsai and Wei (1986, Equation (3)). For t models,  $\alpha_{2,0}=-(\nu+1)/(\nu+3)$  and equation (4) reduces to Cordeiro, Vasconcellos and Santos's (1998) formulae (2)-(3). For linear models, G=0 and then  $B(\widehat{\beta})=0$ , as expected.

Equation (4) is easy to be handled algebraically for any type of nonlinear regression, since it involves only simple operations on matrices and vectors. It will compute  $B(\widehat{\beta})$  algebraically with minimal effort if it is used in conjunction with a computer algebra system such as MATHEMATICA (Wolfram, 1996) or MAPLE (Abell and Braselton, 1994). For special models with closed-form inverse matrix  $(D^TD)^{-1}$ , it is possible to obtain closed-form expressions for  $B(\widehat{\beta})$ . In order to obtain  $B(\widehat{\beta})$  numerically, the quantities D and G in the right-hand side of equation (4) have to be evaluated at the point  $(\widehat{\beta}^T, \widehat{\phi})$ . The bias vector  $B(\widehat{\beta})$  is equal to the least squares estimate in the linear regression of  $\widehat{d}$  on  $\widehat{D}$ . The bias-corrected estimate is simply defined as  $\widehat{\beta}_c = \widehat{\beta} - \widehat{B}(\widehat{\beta})$ , where  $\widehat{B}(\cdot)$  denotes the value of  $B(\cdot)$  at  $(\widehat{\beta}^T, \widehat{\phi})$ .

### 3 Special Regression Models

We now consider a few special models which produce some simplification in equation (4). Other important special models can also be easily handled because of the simplicity of this equation which only requires simple operations on matrices and vectors. First, consider a one parameter nonlinear regression model whose regression function depends on a single parameter  $\beta$ . Equation (4) yields

$$B(\widehat{\beta}) = \frac{\phi^2}{\alpha_{2,0}} \frac{s_2}{s_1^2},\tag{5}$$

where  $s_1 = \sum_{i=1}^n (\mathrm{d}f_i/\mathrm{d}\beta)^2$  and  $s_2 = \sum_{i=1}^n (\mathrm{d}f_i/\mathrm{d}\beta)(\mathrm{d}^2f_i/\mathrm{d}\beta^2)$ . Now,  $s_1$  and  $s_2$  evaluated at  $\widehat{\beta}$  and  $\phi$  replaced by  $\widehat{\phi}$  yield  $\widehat{B}(\widehat{\beta})$  and the corrected estimate is  $\widetilde{\beta} = \widehat{\beta} - \widehat{B}(\widehat{\beta})$ .

As a second application we consider a partially nonlinear regression model defined by

$$\mu = Z\alpha + \eta g(\gamma),\tag{6}$$

where Z is a known full rank  $n\times (p-2)$  matrix,  $g(\gamma)$  denotes an  $n\times 1$  vector and  $\beta^{\top}=(\alpha^{\top},\eta,\gamma)$ , where  $\alpha^{\top}=(\alpha_1,\ldots,\alpha_{p-2})$  and  $\eta$  and  $\gamma$  are scalar parameters. This class of models is commonly used in the statistical literature. For example,  $\mu=\alpha_1z_1+\alpha_2z_2+\eta\exp(\gamma_2x)$  (Gallant, 1975),  $\mu=\alpha-\eta\log(x_1+\gamma x_2)$  (Darby and Ellis, 1976; Stone, 1980). Other types of models of the form (6) are discussed by Ratkowsky (1983, Chapter 5). The  $n\times p$  matrix D reduces to the form  $D=(Z,g(\gamma),\eta\mathrm{d}g(\gamma)/\mathrm{d}\gamma)$  and we obtain from (4), after some algebra,

$$B(\widehat{\beta}) = -\eta^{-1} \operatorname{Cov}(\widehat{\eta}, \widehat{\gamma}) \tau_p - \frac{\eta}{2} \operatorname{Var}(\widehat{\gamma}) \delta_p, \tag{7}$$

where  $\tau_p$  is a  $p \times 1$  vector with a one in the last position and zeros elsewhere,  $\delta_p = (D^{\mathsf{T}}D)^{-1}D^{\mathsf{T}}\mathrm{d}^2g(\gamma)/\mathrm{d}\gamma^2$  is simply the set of coefficients from the ordinary regression of  $\mathrm{d}^2g(\gamma)/\mathrm{d}\gamma^2$  on D, and  $\mathrm{Var}(\widehat{\gamma})$  and  $\mathrm{Cov}(\widehat{\eta},\widehat{\gamma})$  are the large-sample second moments obtained from the appropriate elements of the asymptotic covariace matrix  $\mathrm{Cov}(\widehat{\beta}) = K_{\beta}^{-1} = (-\phi^2/\alpha_{2,0})(D^{\mathsf{T}}D)^{-1}$ . It is clear from (7) that  $B(\widehat{\beta})$  does not depend on the linear parameters  $\alpha$  and that it is proportional to  $\phi^2/\alpha_{2,0}$ . Moreover, the biases of  $\widehat{\alpha}$  and  $\widehat{\eta}$  are both proportional to the value of  $\eta$ .

We conclude this section with a nonlinear regression model, known as the Michaelis-Menton model, which is very useful for estimating growth curves, where it is common for the response to approach an asymptote as the stimulus increases. The Michaelis-Menton model (McCullagh and Nelder, 1989, p.16) provides an hyperbolic form for  $\mu_i$  against  $x_i$  given by

$$\mu_i = \frac{\eta x_i}{\gamma + x_i},\tag{8}$$

where the curve has an asymptote at  $\mu=\eta$ . We can express the  $n^{-1}$  biases of  $\widehat{\eta}$  and  $\widehat{\gamma}$  in terms of the quantities

$$s_r = \sum_{i=1}^n \frac{x_i^2}{(\gamma + x_i)^r},$$

for  $r=2,\ldots,5$ . We find

$$B(\hat{\eta}) = \frac{\phi^2}{\alpha_{2,0}} \frac{s_2(s_4^2 - s_3 s_5)}{\eta(s_2 s_4 - s_3^2)^2}$$

and

$$B(\widehat{\gamma}) = \frac{\phi^2}{\alpha_{2,0}} \frac{\{s_3(2s_2s_4 - s_3^2) - s_2^2s_5\}}{\eta^2(s_2s_4 - s_3^2)^2}.$$

The biases of  $\hat{\eta}$  and  $\hat{\gamma}$  involve both  $\eta$  and  $\gamma$  and are proportional to  $\phi^2/(\eta \alpha_{2,0})$  and to  $\phi^2/(\eta^2 \alpha_{2,0})$ , respectively. Thus, they tend to be large when the regression parameter  $\eta$  is small.

# 4 Biases of Estimates $\hat{\phi}$ and $\hat{\phi}^2$

Here we turn to the derivation of the  $n^{-1}$  biases  $B(\widehat{\phi})$  and  $B(\widehat{\phi}^2)$  of  $\widehat{\phi}$  and  $\widehat{\phi}^2$ , respectively. To calcule  $B(\widehat{\phi})$  from Cox and Snell's (1968) formula, we have to take into account the following sums due to the orthogonality of  $\beta$  and  $\phi$ 

$$B(\widehat{\phi}) = -\frac{1}{2} \kappa^{\phi\phi} \sum_{t,u} \kappa^{tu} \kappa_{\phi t u} + (\kappa^{\phi\phi})^2 (\kappa^{(\phi)}_{\phi\phi} - \frac{1}{2} \kappa_{\phi\phi\phi}). \tag{9}$$

On inserting the expression for the cumulant  $\kappa_{\phi tu}$  given in Section 2, the first sum in (9),  $B_1(\hat{\phi})$  say, follows after some calculation as

$$B_1(\widehat{\phi}) = \frac{p\phi}{2n} \frac{(\alpha_{3,1} + 2\alpha_{2,0})}{\alpha_{2,0}(\alpha_{2,2} - 1)}.$$

The second sum,  $B_2(\widehat{\phi})$  say, comes immediately from  $\kappa^{\phi\phi}$ ,  $\kappa^{(\phi)}_{\phi\phi}$  and  $\kappa_{\phi\phi\phi}$  as

$$B_2(\widehat{\phi}) = \frac{\phi}{2n} \left\{ \frac{\alpha_{3,3} + 2\alpha_{2,2}}{(\alpha_{2,2} - 1)^2} \right\}.$$

Finally, we obtain the  $n^{-1}$  bias of  $\widehat{\phi}$  by adding  $B_1(\widehat{\phi})$  and  $B_2(\widehat{\phi})$ :

$$B(\widehat{\phi}) = \frac{\phi}{2n(\alpha_{2,2} - 1)} \left\{ p\left(\frac{\alpha_{3,1}}{\alpha_{2,0}} + 2\right) + \frac{\alpha_{3,3} + 2\alpha_{2,2}}{(\alpha_{2,2} - 1)} \right\}. \tag{10}$$

Equation (10) gives the  $n^{-1}$  bias  $B(\widehat{\phi})$  of the MLE  $\widehat{\phi}$  in the class of symmetric nonlinear regression models (2). The bias  $B(\widehat{\phi})$  depends on the symmetric distribution only through the quantities  $\alpha_{2,0}$ ,  $\alpha_{2,2}$ ,  $\alpha_{3,1}$  and  $\alpha_{3,3}$ . As equation (10) makes clear, this bias is always a linear function of the dimension p of  $\beta$ . In Table 1 we give these quantities for some symmetric models discussed in Section 1. Note that  $B(\widehat{\phi})$  depends directly on the nonlinear structure of the model regression only through the rank p of D.

We define the corrected MLE  $\hat{\phi}_c$  of  $\phi$  by  $\hat{\phi}_c = \hat{\phi} - \hat{B}(\hat{\phi})$  where  $\hat{B}(\hat{\phi})$  is the value of  $B(\hat{\phi})$  in equation (10) at  $\hat{\phi}$ . We give below the  $n^{-1}$  biases of  $\hat{\phi}$  obtained from (10) for some symmetric models:

- (i) Normal:  $B(\widehat{\phi}) = -\phi(1+2p)/(4n)$ , which is in agreement with Cordeiro and Vasconcellos's (1997) expression (14);
- (ii) Cauchy:  $B(\widehat{\phi}) = \phi(1-p)/n$ ;

(iii) Student's t:

$$B(\widehat{\phi}) = -\frac{\phi(\nu+2)(\nu+3)}{4n\nu(\nu+5)} \left(2p + \frac{\nu-7}{\nu+2}\right),$$

which is identical to Cordeiro, Vasconcellos and Santos' (1998) expression (7);

(iv) Generalized Student's t:

$$B(\widehat{\phi}) = -\phi \frac{(r+2)(r+3)}{4nr(r+5)} \left(2p + \frac{r-7}{r+2}\right);$$

- (v) Type I logistic:  $B(\hat{\phi}) \approx -\phi(0.47547p + 0.24972)/n$ ;
- (vi) Type II logistic:  $B(\hat{\phi}) \approx -\phi(0.52445p + 0.05257)/n$ ;
- (vii) Generalized logistic:

$$B(\widehat{\phi}) = -\frac{\phi(2m+1)}{2n(m+1)(2m^2\psi'(m+1)+2m+1)} \left\{ (2m+1)p + \frac{2m^2(2m+1)\psi'(m+1)}{(2m^2\psi'(m+1)+2m+1)} \right\}.$$

In this case, the bias correction is a complicated function of m requiring the evaluation of polygamma functions. In order to simplify the evaluation of the bias correction, we give simple approximations for large m and small m. For large m, we have

$$B(\widehat{\phi}) = -\frac{\phi}{n} \left[ \left( \frac{1}{2} + \frac{1}{12m^2} - \frac{1}{8m^3} \right) p + \left( \frac{1}{4} - \frac{3}{8m} + \frac{5}{8m^2} - \frac{25}{96m^3} \right) \right] + O(m^{-4}),$$

and for small values of m

$$\begin{split} B(\widehat{\phi}) &= -\frac{\phi}{n} \left[ \left( \frac{1}{2} + \frac{m}{2} - \left( \frac{\pi^2}{6} + \frac{1}{2} \right) m^2 + \left( \frac{1}{2} + 2\zeta(3) + \frac{\pi^2}{6} \right) m^3 \right) p \\ &- \frac{\pi^2}{6} m^2 + \left( 2\zeta(3) + \frac{5}{6} \pi^2 \right) m^3 \right] + O(m^4), \end{split}$$

where  $\zeta$  is the Riemann zeta-function, i.e.,  $\zeta(\alpha) = \sum_{i=1}^n i^{-(\alpha+1)}$ .

(viii) Power exponential:  $B(\widehat{\phi}) = -\phi(1-r+2p)/(4n)$ , for -1 < r < -1/2.

We now give a simple formula for the  $n^{-1}$  bias of the MLE of the variance parameter  $\phi^2$ . This formula can be easily obtained by expanding  $G(\phi) = \phi^2$  in Taylor series together with the bias of  $\widehat{\phi}$  given in (10). From

 $B(\widehat{\phi}^2) = 2\phi B(\widehat{\phi}) + \operatorname{Var}(\widehat{\phi}) + O(n^{-2})$ 

we obtain to order  $n^{-1}$ 

$$B(\widehat{\phi}^2) = 2\phi B(\widehat{\phi}) - \frac{\phi^2}{n(\alpha_2 - 1)}.$$
 (11)

The  $n^{-1}$  bias of the MLE of the variance  $\mathrm{Var}(y)=k\phi^2$  follows easily from equation (11) when one replaces  $\phi^2$  by  $\widehat{\phi}^2$ . The estimate  $\widehat{\phi}_c^2=\widehat{\phi}^2-\widehat{B}(\widehat{\phi}^2)$  is expected to have better sampling properties than the uncorrected estimate  $\widehat{\phi}^2$ . Applications of equation (11) cover many important cases including the following distributions, where we give the values of k: normal (k=1), Student's t  $(k=\nu/(\nu-2))$ , generalized Student's t (k=s/(r-2)), type I logistic (k=0.79569), type II logistic  $(k=\pi^2/3)$ , generalized logistic  $(k=2\psi'(m)/c)$  and power exponential  $(k=2^{1+r}\{\Gamma(3(1+r)/2)/\Gamma((1+r)/2)\})$ . For the normal distribution, equation (11) yields  $B(\widehat{\phi}^2)=-p\phi^2/n$ , as expected.

Table 1: Values of  $\alpha_{2,0}$ ,  $\alpha_{2,2}$ ,  $\alpha_{3,1}$  and  $\alpha_{3,3}$  for some symmetric distributions\*

Model	$\alpha_{2,0}$	$\alpha_{2,2}$	$\alpha_{3,1}$	$\begin{array}{c} \alpha_{3,3} \\ 0 \\ -1/2 \\ \frac{6(3\nu-5)}{(\nu+3)(\nu+5)} \end{array}$	
Normal	-1	-1	0		
Cauchy	-1/2	1/2	1/2		
Student t	$\frac{-(\nu+1)}{(\nu+3)}$	$\frac{(3-\nu)}{(\nu+3)}$	$\frac{6(\nu+1)}{(\nu+3)(\nu+5)}$		
Generalized Student $t$	$\frac{-r(r+1)}{s(r+3)}$	$\frac{(3-r)}{(r+3)}$	$\frac{6r(r+1)}{s(r+3)(r+5)}$	$\frac{6(3r-5)}{(r+3)(r+5)}$	
Type I logistic	-1.47724	-2.01378	-1.27916	-0.50888	
Type II logistic	-1/3	-0.42996	1/6	0.64493	
Generalized logistic	$-\frac{c^2m^2}{(2m+1)}$	$\frac{2(1-m^2\psi'(m))}{(2m+1)}$	$\frac{c^2m^2}{(2m+1)(m+1)}$	$\frac{6(m^2\psi'(m)-1)}{(2m+1)(m+1)}$	
Power exponential	$\frac{-\Gamma((3-r)/2)}{2^{r-1}(1+r)^2\Gamma((r+1)/2)}$	<u>r-1</u> r+1	$\frac{r\Gamma((3-r)/2)}{2^{r-2}(1+r)^3\Gamma((r+1)/2)}$	$\frac{2r(1-r)}{(1+r)^2}$	

<sup>\*</sup>  $\Gamma(x)$  is the gamma function and  $\psi(x) = d \log \Gamma(x)/dx$  is the digamma function. For the power exponential distribution, r < -1/3.

### 5 Simulation Results

We consider the nonlinear regression model  $\mu_i = x_i \{1 - \eta e^{(-\gamma/x_i)}\}$  for which the biases of  $\hat{\eta}$  and  $\hat{\gamma}$  come easily from (4) as

$$B(\widehat{\eta}) = \frac{\phi^2}{2\alpha_{2,0}} \frac{(s_0^2 s_2 - s_{-1} s_1 s_2)}{\eta(s_0 s_2 - s_1^2)^2}$$

and

$$B(\widehat{\gamma}) = \frac{\phi^2}{2\alpha_{2,0}} \frac{(3s_0s_1s_2 - 2s_1^3 - s_{-1}s_2^2)}{\eta^2(s_0s_2 - s_1^2)^2},$$

where

$$s_r = \sum_{i=1}^n x_i^r e^{(-2\gamma/x_i)}$$

for r = -1, 0, 1 and 2.

This section presents Monte Carlo simulation results comparing the performance of the MLEs  $\widehat{\eta}$ ,  $\widehat{\gamma}$  and  $\widehat{\phi}$  and their bias corrected counterparts  $\widehat{\eta}_c$ ,  $\widehat{\gamma}_c$  and  $\widehat{\phi}_c$  in five symmetric nonlinear models with the same systematic component given above but with the response generated from the normal, Cauchy, Student t ( $\nu=2$  and  $\nu=5$ ) and type II logistic distributions. The Cauchy model was generated from the equation  $y=\mu+\phi v_1/v_2$ , where  $v_1$  and  $v_2$  are independent unit normal random variables. The t model with  $\nu$  degrees of freedom was generated as the distribution of  $y=\mu+\phi v(\chi^2_\nu/\nu)^{-1/2}$ , the two random variables v (a unit normal variable), and  $\chi^2_\nu$  (a chi-squared random variable with  $\nu$  degrees of

freedom) being mutually independent. The type II logistic distribution was obtained as the distribution of  $y = \mu + \phi \log\{u/(1-u)\}$ , where u is a standard uniform (0,1) random variable.

For the simulations we have set  $\eta=3$ ,  $\gamma=2$  and  $\phi=2$  for the cases n=30 and n=40. The covariates values  $x_i's$  were obtained as random draws from a uniform U(2,4) distribution and their values were held fixed throughout the study with equal samples sizes. For each model, we generated 10,000 vectors y of observations. For each replication, we fitted the model in GLIM using Cordeiro and Paula's (1989) offset algorithm in order to compute the MLEs  $\widehat{\eta}$ ,  $\widehat{\gamma}$  and  $\widehat{\phi}$ , their biases  $\widehat{B}(\widehat{\eta})$ ,  $\widehat{B}(\widehat{\gamma})$  and  $\widehat{B}(\widehat{\phi})$ , and the corrected estimates  $\widehat{\eta}_c = \widehat{\eta} - \widehat{B}(\widehat{\eta})$ ,  $\widehat{\gamma}_c = \widehat{\gamma} - \widehat{B}(\widehat{\gamma})$  and  $\widehat{\phi}_c = \widehat{\phi} - \widehat{B}(\widehat{\phi})$ , evaluating the biases (given by formulae in this section and (10)) at the estimates  $(\widehat{\eta},\widehat{\gamma})$  and  $\widehat{\phi}$ . Further, we computed the sample means of the estimates  $\widehat{\eta}$ ,  $\widehat{\gamma}$ ,  $\widehat{\phi}$ ,  $\widehat{\eta}_c$ ,  $\widehat{\gamma}_c$  and  $\widehat{\phi}_c$  from all 10,000 replications. The figures are given in Table 2 for n=30 and in Table 3 for n=40 with the respective standard errors in brackets.

For all five models, the bias correction tends to shrink the uncorrected estimates of the parameters  $\eta$  and  $\gamma$ , whereas for the parameter  $\phi$  the bias correction tends to increase the values of the uncorrected estimates. The bias correction in all cases reported in these tables bring the estimates closer to their true values, thus correctly signalizing the direction of the such biases. This suggest that the second-order bias of MLEs should not be ignored in samples of small to moderate size since they can be nonnegligible. As expected, the bias correction has less impact as n increases. Also, the mean squared errors of the corrected estimates are smaller than those of the uncorrected estimates, although in a few cases the standard errors of the corrected estimates were slightly greater than those of the uncorrected estimates with the accuracy of four decimal places. Therefore, the bias correction yields a second-order reduction in the mean squared errors of the modified estimates.

Table 2: Uncorrected and corrected estimates, five symmetric nonlinear models and n = 30.

			True Values			
	$\eta = 3$		$\gamma=2$		$\phi = 2$	
Estimate	$\widehat{\eta}$	$\widehat{\eta}_c$	$\widehat{\gamma}$	$\widehat{\gamma}_c$	$\hat{\phi}$	$\phi_c$
Normal	3.43	3.11	2.13	2.05	1.90	1.97
	(0.02)	(0.02)	(0.03)	(0.02)	(0.00)	(0.00)
Cauchy	3.91	3.34	2.23	2.08	1.88	1.94
	(0.04)	(0.04)	(0.05)	(0.04)	(0.02)	(0.02)
Student $t$ , $\nu = 2$	3.70	3.16	2.26	2.13	1.81	1.89
	(0.03)	(0.03)	(0.04)	(0.04)	(0.02)	(0.02)
Student $t$ , $\nu = 5$	3.57	3.14	2.17	2.09	1.83	1.91
	(0.02)	(0.02)	(0.03)	(0.03)	(0.01)	(0.01)
Type II logistic	3.97	3.28	2.31	2.12	1.75	1.89
	(0.04)	(0.03)	(0.05)	(0.04)	(0.01)	(0.01)

Table 3: Uncorrected and corrected estimates, five symmetric nonlinear models and n = 40.

Hode	S allu /L	TU.					
			True Values			espirit i	
	$\eta = 3$		$\gamma = 2$		$\phi = 2$		
Estimate	$\widehat{\eta}$	$\widehat{\eta}_c$	$\widehat{\gamma}$	$\widehat{\gamma}_c$	$\hat{\phi}$	$\phi_c$	
Normal	3.29	3.13	2.09	2.06	1.93	1.98	
	(0.02)	(0.02)	(0.03)	(0.02)	(0.00)	(0.00)	
Cauchy	3.48	3.26	2.17	2.10	1.87	1.92	
	(0.03)	(0.03)	(0.04)	(0.03)	(0.02)	(0.01)	
Student $t$ , $\nu = 2$	3.35	3.20	2.19	2.12	1.86	1.94	
	(0.03)	(0.03)	(0.03)	(0.03)	(0.01)	(0.01)	
Student $t$ , $\nu = 5$	3.31	3.18	2.15	2.11	1.84	1.93	
	(0.02)	(0.01)	(0.02)	(0.02)	(0.00)	(0.00)	
Type II logistic	3.62	3.33	2.28	2.14	1.88	1.95	
	(0.03)	(0.03)	(0.04)	(0.04)	(0.01)	(0.01)	

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- The complete list of "Relatórios do Departamento de Estatística", IME-USP, will be sent upon request.

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