Statistica Sinica **8**(1998), 467-476

MARGINAL CURVATURES FOR FUNCTIONS OF PARAMETERS IN NONLINEAR REGRESSION

Gunseog Kang and John O. Rawlings

Soongsil University, Korea and North Carolina State University

Abstract: The marginal curvature by Clarke (1987) for individual parameters in nonlinear models not only improves the inference on each parameter but also has been found useful in experimental design for nonlinear models. In this article we develop the marginal curvature for functions of parameters. We show that, for a given reparametrization, the marginal curvatures for the transformed parameters can be computed without determining the inverse transformation. Furthermore, the marginal curvature for a function of parameters depends only on the marginal curvatures of the original parameters and on the derivatives of the function with respect to the parameters involved in that function.

We also present a more efficient computing algorithm of Clarke's marginal curvature measure. The resulting expression enables us to compare Clarke's measure with other available measures.

Key words and phrases: Experimental design, linear approximation, parameter-effects curvature, parameter transformation.

1. Introduction

Consider the univariate nonlinear regression model

$$y_u = \eta(\mathbf{x}_u, \boldsymbol{\theta}) + \varepsilon_u, \quad u = 1, \ldots, n,$$

where the model function $\eta_u = \eta(\mathbf{x}_u, \boldsymbol{\theta})$ depends on a vector $\mathbf{x}_u$ of design variables and on the unknown parameter vector $\boldsymbol{\theta}$. The errors ε_u are uncorrelated random variables, normally distributed with mean zero and constant variance σ^2.

The least squares estimate $\hat{\boldsymbol{\theta}}$ of $\boldsymbol{\theta}$ is obtained iteratively by using the locally linear approximation to the model function about the current value of $\boldsymbol{\theta}$. Also inferences on $\hat{\boldsymbol{\theta}}$ are usually based on the linear approximation. Although the error of this approximation becomes negligible in large samples, the accuracy of the approximation is dependent upon the degree of nonlinearity of the model in practical problems.

Beale (1960) and Bates and Watts (1980) defined two "global" measures of nonlinearity, intrinsic curvature which is independent of the parametrization and parameter-effects curvature which is dependent on the parametrization. In practice intrinsic curvature is relatively small whereas parameter-effects curvature is large (Bates and Watts (1980), and Ratkowsky (1983)) and large parameter-effects curvature can be an indicator of poor linear approximation.

Cook and Witmer (1985), on the other hand, gave a couple of examples where the exact and the linear approximation confidence regions have a reasonable agreement even though the parameter-effects curvatures are large. Also Clarke (1987) gave a few examples which show that large overall parameter-effects curvature does not necessarily imply the poor performance of all the confidence intervals based on the linear approximation. Apparently with these observations, Clarke (1987) defined the marginal curvature for individual parameters in nonlinear models, and Cook and Goldberg (1986) generalized the Bates and Watts' measure for arbitrary subsets of parameters.

While it is known that the experimental design also affects nonlinearity of the model, previous work has focused on finding reparametrizations of the model which would reduce the parameter-effects curvature and thereby improve the linear approximation (Bates and Watts (1981), Hougaard (1982), Kass (1984)) rather than finding a design which reduces the parameter-effects curvature for the original parametrization. However, reparametrization techniques are difficult to be pursued in practice and even, in multiparameter problems, "best" parametrizations may not exist (Kass (1984)). Also the transformed parameter set may no longer be interpretable within the context of the problem.

It was noted recently that curvature measures are related with an optimal design criterion (Hamilton and Watts (1985)) and particularly Clarke's marginal curvature can be a useful measure in finding "optimal" designs for a nonlinear model (Dassel and Rawlings (1990a, 1990b)). Since it is common to design experiments for precise estimation of functions of the model parameters as well as for precise estimation of the model parameters themselves, it is necessary to develop the marginal curvature for functions of parameters. It is possible, of course, to compute marginal curvatures for a reparametrization by rewriting the model in terms of the new parameters and recalculating all the necessary derivatives. Our results show that this tedious work can be avoided.

Section 2 contains the main results of this paper. First we present a different expression, using a matrix, for Clarke's measure, which provides an efficient computing method. This expression also enables us to compare Clarke's measure with other available measures (Section 2.2). In Section 2.3, we develop the marginal curvature for functions of parameters. We give an example in Section 3 and concluding remarks in Section 4. The Appendix contains details of the necessary algebra.

2. Main Results

2.1. Marginal curvatures in matrix form

Clarke (1987) derived a measure of marginal curvature for each parameter θ_i in nonlinear models by using a power series expansion of the profile curve of θ_i about $\theta_i - \hat{\theta}_i$. (See Clarke (1987) for the necessary assumptions.) Let $\dot{V}$ be the $n \times p$ derivative matrix of the model function with respect to $\boldsymbol{\theta}$, so $\{\dot{V}\}_{ui} = \partial\eta_u/\partial\theta_i$, and let $\hat{\sigma}^2$ be the variance estimate. Then the *marginal curvature* m_i for θ_i is defined as

$$m_i = -\frac{1}{2}(g_{ii})^{-3/2}\gamma_i\hat{\sigma}, \tag{2.1}$$

where

$$\gamma_i = \sum_{a=1}^{p}\sum_{b=1}^{p}\sum_{c=1}^{p} g_{ia}g_{ib}g_{ic}\sum_{u=1}^{n}(\frac{\partial\eta_u}{\partial\theta_a})(\frac{\partial^2\eta_u}{\partial\theta_b\partial\theta_c}) \tag{2.2}$$

and g_{ik} is the ikth element of the $p \times p$ matrix $G = (\dot{V}^{\mathrm{T}}\dot{V})^{-1}$. (Superscript $^{\mathrm{T}}$ denotes the transpose of a matrix.) Note that m_i utilizes up to second derivatives of the model function η with respect to the parameters. Clarke (1987) originally derived a confidence limit to θ_i which includes both the second-order correction term γ_i and a third-order correction term. Since the contribution of the third-order term is generally small, he called m_i the marginal curvature for θ_i.

For computational purposes, it is more convenient to identify γ_i as an element of an array. Also this enables us to compare Clarke's marginal curvature with other measures (Section 2.2). We form a three-dimensional array $\ddot{V}$ with the second derivatives of the model function with respect to $\boldsymbol{\theta}$. The $n \times p \times p$ array $\ddot{V}$ has n faces and its uth face is the $p \times p$ matrix whose ijth element is given as $\partial^2\eta_u/\partial\theta_i\partial\theta_j, \;\; i,j = 1,\ldots,p$.

Propositions 1. *Define the $p \times p \times p$ array Γ as*

$$\Gamma = [G\dot{V}^{\mathrm{T}}][G\ddot{V}G]. \tag{2.3}$$

Then γ_i defined in (2.2) *is the iith element of the ith face of Γ.*

This proposition can be easily verified. (Since Γ and $\ddot{V}$ are three-dimensional arrays, two types of matrix multiplications are involved in (2.3), one in $G\ddot{V}G$ and the other denoted by the square brackets. See the Appendix for definitions.) Computation of Γ can be further simplified by using the QR decomposition of $\dot{V}$, $\dot{V} = Q_1R_1$, where Q_1 is an $n \times p$ matrix whose columns are orthogonal to each other and R_1 is the $p \times p$ upper triangular matrix (Dongarra et al. (1979)). Since $\dot{V}^{\mathrm{T}}\dot{V} = R_1^{\mathrm{T}}R_1$, $G = R_1^{-1}R_1^{-\mathrm{T}}$ and by using the properties of the bracket multiplication described in the Appendix, we can show that Γ can be expressed as

$$\begin{aligned}\Gamma &= R_1^{-1}[R_1^{-1}Q_1^{\mathrm{T}}][R_1^{-\mathrm{T}}\ddot{V}R_1^{-1}]R_1^{-\mathrm{T}} \\ &= R_1^{-1}[R_1^{-1}][A]R_1^{-\mathrm{T}},\end{aligned} \tag{2.4}$$

where $A = [Q_1^{\mathrm{T}}][R_1^{-\mathrm{T}}\ddot{V}R_1^{-1}]$, which is the parameter-effects curvature array defined in Bates and Watts (1980).

2.2. Relation with other measures

The relationship (2.4) between the arrays Γ and A enables us to compare Clarke's marginal curvature with the Cook and Goldberg's measure. Cook and Goldberg (1986) generalized the Bates and Watts' global measure to one for arbitrary subsets of parameters. Especially, for individual parameters, they showed that the maximum parameter-effects curvature for θ_p is simply $\{A\}_{ppp}\hat{\sigma}$. (In Cook and Goldberg's derivation, the parameters are divided into two subsets and curvature is computed for the trailing subset of parameters. Hence to compute the marginal curvature of a parameter, the parameter should be the last element of $\boldsymbol{\theta}$. Also they define a "total" curvature by combining the intrinsic and the parameter-effects curvatures. Since we assume that the intrinsic curvature is negligible, Cook and Goldberg's measure in this paper refers to only the first part of their total curvature, i.e., the parameter-effects curvature.)

We now show that Clarke's measure m_i is in fact the same as the Cook and Goldberg's measure up to a constant. First note that the matrix R_1^{-1} is also an upper triangular matrix. If we denote by r^{pp} the pth diagonal element of R_1^{-1}, then it is easy to show that

$$\{\Gamma\}_{ppp} = (r^{pp})^3\{A\}_{ppp}$$

and

$$\{G\}_{pp} = (r^{pp})^2$$

Hence, for the last parameter θ_p, Clarke's marginal curvature m_p is

$$m_p = -\frac{1}{2}\{A\}_{ppp}\hat{\sigma}.$$

Since Clarke's measure is not dependent on the order of the parameters, this shows that Clarke's measure is $-\frac{1}{2}$ times that of Cook and Goldberg. While both methods provide essentially the same curvature measure as far as individual parameters are concerned, using equations (2.1) and (2.4) is more efficient in computing marginal curvatures than using Cook and Goldberg's method which evaluates the measures one at a time for each parameter. Once the array A is formed, Γ is obtained by applying a sequence of back-substitution operations since R_1 is an upper triangular matrix. Also we note that g_{ii} in (2.1) is simply the squared length of the ith row of R_1^{-1}.

For assessing the significance of m_i, Clarke (1987) suggested that curvature effects may be ignored and the linear approximation will suffice if $|m_i c| < 0.1$, or $|\{A\}_{ppp}\hat{\sigma}c| < 0.2$ for θ_p, where c is an appropriate critical value. For a single parameter, Bates and Watts' rule of assessing the significance of the curvature becomes a percentage deviation of the expectation surface from the tangent plane at a distance c from the tangent point (Bates and Watts (1980, 1988)). If we let $c = t(n-p; 0.05)$, the upper 0.05 quantile of the t distribution with $n-p$ degrees of freedom, then Clarke's rule is equivalent to accepting a deviation of no more than 10%. To accept a deviation of up to 15%, the rule may be loosened to $|m_i c| < 0.15$.

2.3. Marginal curvatures for parameter functions

Suppose we have a reparametrization of $\boldsymbol{\theta}$, $\boldsymbol{\phi} = \mathbf{h}(\boldsymbol{\theta})$. Then we can show that, using the superscript to denote each parametrization,

$$\dot{V}^{\phi} = \frac{\partial \boldsymbol{\eta}}{\partial \boldsymbol{\phi}^{\mathrm{T}}} = \dot{V}^{\theta}\dot{D} \tag{2.5}$$

$$\ddot{V}^{\phi} = \frac{\partial^2 \boldsymbol{\eta}}{\partial \boldsymbol{\phi}\partial \boldsymbol{\phi}^{\mathrm{T}}} = \dot{D}^{\mathrm{T}}\ddot{V}\dot{D} + [\dot{V}][\ddot{D}] \tag{2.6}$$

(Bates and Watts (1981)), where $\dot{D} = \partial\boldsymbol{\theta}/\partial\boldsymbol{\phi}^{\mathrm{T}}$ and $\ddot{D} = \partial^2\boldsymbol{\theta}/\partial\boldsymbol{\phi}\partial\boldsymbol{\phi}^{\mathrm{T}}$. Hence one may compute the marginal curvature for each element of $\boldsymbol{\phi}$ by replacing $\dot{V}$ and $\ddot{V}$ in equation (2.3) by $\dot{V}^{\phi}$ and $\ddot{V}^{\phi}$, respectively. However, since each element of $\mathbf{h}(\boldsymbol{\theta})$ is usually a nonlinear function of $\boldsymbol{\theta}$, the second derivatives array $\ddot{D}$ of the inverse transformation is not available in practice. Also in most cases, what we are interested in is only a function of $\boldsymbol{\theta}$ (for example, the model function itself), in which case we would not want to specify a complete form of $\boldsymbol{\phi} = \mathbf{h}(\boldsymbol{\theta})$. In this section we show that first, marginal curvatures for a full reparametrization $\boldsymbol{\phi}$ can be computed easily without determining the inverse transformation, and secondly, the marginal curvature for a function of parameters is dependent only on the partial derivatives of the function with respect to the parameters involved in that function.

Let $\dot{H} = \partial\boldsymbol{\phi}/\partial\boldsymbol{\theta}^{\mathrm{T}}$, then $\dot{H}^{-1} = \dot{D}$ and

$$\begin{aligned} G^{\phi} &= ((\dot{V}^{\phi})^{\mathrm{T}}\dot{V}^{\phi})^{-1} \\ &= \dot{H}G^{\theta}\dot{H}^{\mathrm{T}} \end{aligned} \tag{2.7}$$

Proposition 2. *The array* Γ *for the parametrization* $\boldsymbol{\phi}$ *is*

$$\begin{aligned} \Gamma^{\phi} &= \Gamma_1 - \Gamma_2 \\ &= \dot{H}[\dot{H}][\Gamma^{\theta}]\dot{H}^{\mathrm{T}} - \dot{H}G^{\theta}\ddot{H}G^{\theta}\dot{H}^{\mathrm{T}}, \end{aligned} \tag{2.8}$$

where $\Gamma_1 = \dot{H}[\dot{H}][\Gamma^{\theta}]\dot{H}^{\mathrm{T}}$ *and* $\Gamma_2 = \dot{H}G^{\theta}\ddot{H}G^{\theta}\dot{H}^{\mathrm{T}}$.

(The proof is given in the Appendix.) Hence the marginal curvature m_i^{ϕ} for ϕ_i is given by

$$m_i^{\phi} = -\frac{1}{2}(g_{ii}^{\phi})^{-3/2}\gamma_i^{\phi}\hat{\sigma}, \tag{2.9}$$

where $\gamma_i^{\phi} = \{\Gamma^{\phi}\}_{iii}$. Equations (2.7) and (2.8) show that marginal curvatures for $\boldsymbol{\phi}$ are expressed in terms of the original parameters $\boldsymbol{\theta}$, so we do not have to determine the inverse transformation. Each marginal curvature m_i^{ϕ} is computed from the array Γ^{θ} of the original parameters $\boldsymbol{\theta}$, the matrix R_1 from previous computations [since $G^{\theta} = (R_1^{\mathrm{T}}R_1)^{-1}$], and the derivatives of the reparametrization functions with respect to $\boldsymbol{\theta}$.

As elementwise expressions, it can be shown that

$$\{\Gamma_1\}_{iii} = \sum_{a=1}^{p}\sum_{b=1}^{p}\sum_{c=1}^{p}\phi_i^a\phi_i^b\phi_i^c\{\Gamma^{\theta}\}_{abc}$$

and

$$\{\Gamma_2\}_{iii} = \sum_{d=1}^{p}\sum_{e=1}^{p}\sum_{f=1}^{p}\sum_{g=1}^{p}\phi_i^d\phi_i^e g_{df}g_{eg}\phi_i^{fg},$$

where $\phi_i^a = \partial\phi_i/\partial\theta_a$, $\phi_i^{ab} = \partial^2\phi_i/\partial\theta_a\partial\theta_b$. Also $g_{ii}^{\phi} = \sum_{a=1}^{p}\sum_{b=1}^{p}\phi_i^a\phi_i^b g_{ab}$. Hence we can see from equation (2.9) that, to obtain the marginal curvature of, say, $\phi_i = h_i(\boldsymbol{\theta})$, it is enough to specify the first and second derivatives of ϕ_i with respect to the original parameters involved in h_i. For other derivatives, arbitrary values can be assigned. For example, a program we have written for this computation (Kang and Rawlings (1989)) can handle q $(1 \le q \le p)$ transformations and use identity functions for the other $p - q$ transformations so that the derivatives of those functions are assigned to zero automatically within the program.

For the simple case of $\phi_i = h(\theta_i)$, only a 1–1 transformation, $\phi_i^a = 0$ for $a \neq i$. Hence, using equation (2.8), we can easily verify the relationship

$$m_i^\phi = m_i^\theta + \frac{1}{2}(\frac{\partial^2 \phi_i}{\partial \theta_i^2})(\frac{\partial \phi_i}{\partial \theta_i})^{-1}(g_{ii}^\theta)^{1/2}\hat{\sigma}$$

which is shown in Clarke (1987).

3. An Example

Consider an example from Bliss and James (1966) with the Michaelis–Menten model

$$\eta(x, \boldsymbol{\theta}) = \frac{\theta_1 x}{\theta_2 + x} \tag{3.1}$$

which relates reaction velocity (η) to substrate concentration (x) in enzyme chemistry. A data set with 6 observations was used in this example. (See Clarke (1987) for a preliminary analysis of this example.) Another popular form of model (3.1) is

$$\eta(x, \boldsymbol{\beta}) = \frac{x}{\beta_1 + \beta_2 x}. \tag{3.2}$$

That is, we have a reparametrization with $\beta_1 = \theta_2/\theta_1$, $\beta_2 = 1/\theta_1$.

Table 1. Summary of several curvatures

	$\boldsymbol{\theta}$	$\boldsymbol{\beta}$
γ_N	0.031	0.031
γ_T	0.125	0.064
m_1	0.048	0.025
m_2	0.063	0.005

Table 1 gives a summary of several curvatures for these two parametrizations. The root mean square (rms) intrinsic curvature, γ_N, is the same for both parametrizations as it should be by the definition. Since $\gamma_N \sqrt{F} = 0.081(\ll 0.2)$, where F is the upper 0.05 quantile of the F distribution with degrees of freedom 2 and 4, this curvature is considered small by the Bates and Watts' rule of assessing significance. Hence, this example satisfies the assumptions of Clarke (1987). The second term, γ_T, denotes the rms parameter-effects curvature. Since $\gamma_T^\theta \sqrt{F} = 0.331(> 0.2)$, γ_T^θ is considered a little large, which implies that linear approximation may not be adequate. This is so for θ_2 which has a marginal curvature $m_2 = 0.063$ and is significant by Clarke's rule of assessing significance. ($m_2\, t = 0.134(> 0.1)$, where t is the upper 0.05 quantile of the t distribution with 4 degrees of freedom.) However, since θ_1 has a marginal curvature of $m_1 = 0.048$

and $m_1 t = 0.103$, inference about $\hat{\theta}_1$ based on the linear approximation theory will be still valid.

The $\boldsymbol{\beta}$ parametrization reduces γ_T by half, implying that linear approximation will work well for both β_1 and β_2. The marginal curvatures m_i for $\beta_i, i = 1, 2$ were computed from equation (2.9). We could check these values by directly using model (3.2). The size of m_i agrees with that of γ_T in this parametrization.

Next suppose we want to estimate an expected value of the response at a large value of the concentration, say, at $x = 5$, which is $\phi = \eta(5, \boldsymbol{\theta}) = \frac{5\theta_1}{\theta_2+5}$. The parameter estimates are $(\hat{\theta}_1, \hat{\theta}_2) = (0.6904, 0.5965)$, so the estimated response at this point is $\hat{y}_{x=5} = 0.6181$. Since ϕ is a function of $\boldsymbol{\theta}$, we can obtain its marginal curvature from equation (2.9), which is $m^{\phi} = 0.0324$. This value is considered negligible since $0.0324t = 0.069$, less than 0.1. Hence the usual confidence interval based on linear approximation can be used to make interval estimation for η at that point, although θ_2 has a somewhat large marginal curvature. More complicated forms of parameter transformations such as the point of inflection can be studied by considering other nonlinear regression models.

4. Conclusion

In this article we have developed the marginal curvature for functions of parameters in a nonlinear model. Two important facts are noted. First, for a given reparametrization, marginal curvatures for the transformed parameters are expressed in terms of the original parameters, so it is not necessary to determine the inverse transformation. The computation involves only marginal curvatures of the original parameters $\boldsymbol{\theta}$, the matrix R_1 from previous computations, and the derivatives of the reparametrization functions with respect to $\boldsymbol{\theta}$. Second, the marginal curvature for a function of the parameters depends only on the marginal curvatures of the original parameters and on the derivatives of the function with respect to the parameters involved in that function. Hence in order to use the efficient equation (2.8) for computing the marginal curvature for a function of parameters, we can use an arbitrary set of functions for the other $p-1$ transformations.

It should be noted that Clarke's measure is meaningful only when the intrinsic curvature is small enough to ignore. The choice of design points affects not only the parameter-effects curvature but also the intrinsic curvature. Hence one should continually check intrinsic curvature when Clarke's measure is used for the experimental design.

Even though we have developed the marginal curvature for functions of parameters to be used for experimental design in nonlinear regression analysis, results of this paper can be useful also for inference about the estimates of functions of parameters as demonstrated in Section 3.

Appendix: Proof of Proposition 2

When three-dimensional arrays are involved in matrix multiplication, generally two types of multiplications are used. Let A be an $n_1 \times n_2 \times n_3$ array, M_1 an $n_4 \times n_2$ matrix, and M_2 an $n_3 \times n_5$ matrix, then $Z_1 = M_1 A M_2$ is an $n_1 \times n_4 \times n_5$ array. That is, each $n_2 \times n_3$ face of A is pre- and postmultiplied by M_1 and M_2. For an $n_0 \times n_1$ matrix B, the bracket multiplication is defined as $Z_2 = [B][A]$, where Z_2 is an $n_0 \times n_2 \times n_3$ array with $\{Z_2\}_{ijk} = \sum_{a=1}^{n_1} \{B\}_{ia}\{A\}_{ajk}$. That is, the summation is over the first index of the array (Bates and Watts (1980)). We now list a few properties of the bracket multiplication.
P1: $[B][A + A_1] = [B][A] + [B][A_1]$ where A_1 is the same type of array as A.
P2: $[CB][A] = [C][\,[B][A]\,]$ where C is an $m \times n_0$ matrix.
P3: $[B][M_1 A M_2] = M_1[B][A]M_2$.

Proof of Proposition 2. By Proposition 1, $\Gamma^\phi = [G^\phi(\dot V^\phi)^{\mathrm T}][G^\phi \ddot V^\phi G^\phi]$. Since $G^\phi = [(\dot V^\phi)^{\mathrm T}\dot V^\phi]^{-1}$ and $\dot V^\phi = \dot V \dot H^{-1}$ (omitting the superscript θ for simplicity), $G^\phi = \dot H G \dot H^{\mathrm T}$ and $G^\phi(\dot V^\phi)^{\mathrm T} = \dot H G \dot V^{\mathrm T}$. Using the expression of $\ddot V^\phi$ in (2.6),

$$\begin{aligned}\Gamma^\phi &= [\dot H G \dot V^{\mathrm T}][G^\phi(\dot D^{\mathrm T}\ddot V \dot D + [\dot V][\ddot D])G^\phi]\\ &= G^\phi[\dot H G \dot V^{\mathrm T}][\dot D^{\mathrm T}\ddot V \dot D]G^\phi - G^\phi[\dot H G \dot V^{\mathrm T}][\,-[\dot V][\ddot D]\,]G^\phi\end{aligned}$$

by P1 and P3. Let $\Gamma_1 = G^\phi[\dot H G \dot V^{\mathrm T}][\dot D^{\mathrm T}\ddot V \dot D]G^\phi$ and $\Gamma_2 = G^\phi[\dot H G \dot V^{\mathrm T}][-[\dot V][\ddot D]]G^\phi$. Then

$$\begin{aligned}\Gamma_1 &= [\dot H G \dot V^{\mathrm T}][G^\phi \dot D^{\mathrm T}\ddot V \dot D G^\phi]\\ &= [\dot H G \dot V^{\mathrm T}][\dot H G \ddot V G \dot H^{\mathrm T}]\\ &= \dot H[\dot H][\,[G\dot V^{\mathrm T}][G\ddot V G]\,]\dot H^{\mathrm T}\\ &= \dot H[\dot H][\Gamma]\dot H^{\mathrm T}\end{aligned}$$

and

$$\begin{aligned}\Gamma_2 &= -\dot H G \dot H^{\mathrm T}[\dot H G \dot V^{\mathrm T}\dot V][\ddot D]\dot H G \dot H^{\mathrm T}\\ &= -\dot H G \dot H^{\mathrm T}[\dot H][\ddot D]\dot H G \dot H^{\mathrm T}\\ &= -\dot H G[\dot H][\dot H^{\mathrm T}\ddot D \dot H]G \dot H^{\mathrm T}.\end{aligned}$$

Noting that $\dot H^{\mathrm T}\ddot D \dot H = -[\dot H^{-1}][\ddot H]$ (Bates and Watts (1981)), we have

$$\begin{aligned}\Gamma_2 &= \dot H G[\dot H][\,[\dot H^{-1}][\ddot H]\,]G \dot H^{\mathrm T}\\ &= \dot H G \ddot H G \dot H^{\mathrm T}\end{aligned}$$

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Department of Statistics, Soongsil University, 1-1 Sangdo 5 Dong, Dongjak-ku, Seoul, 156-743, Korea.

E-mail: gskang@stat.soongsil.ac.kr

Department of Statistics, North Carolina State University, Box 8203, Raleigh, NC 27695-8203, U.S.A.

(Received April 1996; accepted March 1997)