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ON PARAMETER-EFFECTS ARRAYS IN NON-LINEAR
REGRESSION MODELS

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Summary. Formulas for a new three- and four-dimensional parameter-effects arrays corresponding to transformations of parameters in non-linear regression models are given. These formulae make the construction of the confidence regions for parameters easier. An example is presented which shows that some care is necessary when a new array is computed.

Keywords: Non-linear regression model, parameter-effects arrays, confidence region

1. INTRODUCTION

A non-linear regression model can be written as

$$(1) \quad y_a = f(x_a, \Theta) + \varepsilon_a \quad a = 1, \dots, n$$

where $y = (y_1, \dots, y_n)'$ is a vector of observations, $x_a = (x_{a1}, \dots, x_{ak})$ are known constants, $\Theta = (\Theta_1, \dots, \Theta_p)'$ is a vector of unknown parameters and ε_a are independent, normally distributed random variables, $\varepsilon = (\varepsilon_1, \dots, \varepsilon_n)' \sim N_n(0, \sigma^2 \mathbf{I})$. The function f is supposed to be of a known form, nonlinear in Θ . In vector notation we have

$$(2) \quad y = \eta(\Theta) + \varepsilon$$

where $\eta(\Theta) = (\eta_1(\Theta), \dots, \eta_n(\Theta))'$ with $\eta_a(\Theta) = f(x_a, \Theta)$, $a = 1, \dots, n$.

For such a model the least squares estimates $\hat{\Theta}$ are the values of the parameters which minimize the sum of squares

$$S(\Theta) = \sum_{a=1}^n (y_a - f(x_a, \Theta))^2,$$

or in vector notation

$$S(\Theta) = \|y - \eta(\Theta)\|^2.$$

It is well known that the nonlinearity of the above model can be characterized by means of the intrinsic and parameter-effects curvatures introduced by Bates and Watts in [1]. Experience has shown that while the intrinsic curvature is negligible in almost all practical cases the parameter-effects curvature may be relatively large (see [1], [2], [3], [4]). This curvature, however, can be substantially reduced by a reparametrization. It would be tedious to compute the parameter-effects array for each new transformation of parameters. Fortunately this work can be avoided and the new array may be computed directly from the original one. On the other hand, our example shows that some care is needed to avoid mistakes.

As noted by many authors (see e.g. [4], [5]) there exist models for which the Bates-Watts approach is unsatisfactory. Therefore we introduce a four-dimensional parameter-effects array which together with the three-dimensional array explains the behaviour of models better than the Bates-Watts array alone. In addition, we present a formula for such an array after reparametrization. This formula will be useful when improved confidence regions for parameters of a model presented in [7] are constructed.

2. PARAMETER-EFFECTS ARRAY

In what follows we denote by V . and V .. the first and second derivatives of the model function $\eta(\Theta)$. Their elements are

$$V_{aj} = \frac{\partial \eta_a}{\partial \Theta_j} \Big|_{\hat{\Theta}} \quad \text{and} \quad V_{ajk} = \frac{\partial^2 \eta_a}{\partial \Theta_j \partial \Theta_k} \Big|_{\hat{\Theta}},$$

respectively. We suppose that the rank of V . is p and V . = UR is the unique orthogonal-triangular decomposition of V . (QR -decomposition for short) where the columns of the $n \times p$ matrix U form an orthogonal basis for V . and R is an upper triangular matrix with $R_{ii} > 0$, $i = 1, \dots, p$. Then the parameter-effects array for the parameter Θ at $\hat{\Theta}$ is defined as follows (see [1])

$$(3) \quad A_{..}^{\Theta} = [U'] [L' V.. L]$$

where $L = R^{-1}$ and the pre- post- and square-bracket multiplications of matrices and arrays are defined in the following way.

If E is an $m \times p$ matrix and T is an $n \times p \times q$ array, then the term of the a -th face of the $n \times m \times q$ array ET residing in the i -th row and the j -th column is

$(ET)_{ij}^a = \sum_t E_{it} T_{tj}^a$. Analogously for a $q \times s$ matrix E and an $n \times p \times q$ array T we have $(TE)_{ij}^a = \sum_t T_{it}^a E_{tj}$, $a = 1, \dots, n$, $i = 1, \dots, p$, $j = 1, \dots, s$. Finally, if E is an $s \times n$ matrix and T is an $n \times p \times q$ array then the term residing in the a -th face, the i -th row and the j -th column of the array $[E][T]$ is $([E][T])_{ij}^a = \sum_t E_{at} T_{tj}^a$, $a = 1, \dots, s$, $i = 1, \dots, p$, $j = 1, \dots, q$.

The following properties can be easily verified (see, e.g. [4], [7]).

a) $[D][ETG] = F[D][T]G$ where D , F and G are $s \times n$, $t \times p$ and $q \times k$ matrices, respectively, T is an $n \times p \times q$ array;

b) $[JE][T] = [J][[E][T]]$ where J and E are $r \times k$ and $k \times n$ matrices, respectively, and T is an $n \times p \times q$ array.

Definition 1. By an $n \times p \times q \times r$ array we understand

$$T_{...} = \begin{pmatrix} T_{...}^1 \\ \vdots \\ T_{...}^n \end{pmatrix}$$

where $T_{...}^a$, $a = 1, \dots, n$ are $p \times q \times r$ arrays.

The premultiplication $ET_{...}$, the postmultiplication $T_{...}E$ the \star -multiplication $E \star T_{...}$ and the square-bracket multiplication $[E][T_{...}]$, where E is a matrix, denote summation over the second, third, first subscripts and the superscript, respectively.

For example, if E is an $s \times r$ matrix and $T_{...}$ is an $n \times r \times p \times q$ array then the (a, i, j, k) -term of the $n \times s \times p \times q$ array $E \star T_{...}$ is $(E \star T_{...})_{ijk}^a = \sum_t E_{it} T_{tjk}^a$. Analogously, the square-bracket multiplication of an $s \times n$ matrix E by an $n \times r \times p \times q$ array $T_{...}$ results in the $s \times r \times p \times q$ array $[E][T_{...}]$ with terms $([E][T_{...}])_{ijk}^a = \sum_t E_{at} T_{tjk}^a$ and so on. The reader is recommended to consult Table 1 for better understanding of the above operations.

The following properties will be used throughout the paper:

$$\begin{aligned} [E][FT_{...}G] &= F([E][T])G, \\ [E][H \star (FTG)] &= H \star (F[E][T]G) = F(H \star ([E][T]))G, \end{aligned}$$

where T is a four-dimensional array and E , F , G , H are matrices.

Definition 2. The $p \times p \times p \times p$ array

$$(4) \quad A^\Theta = [U'] [L' \star (L' V_{...} L)]$$

where U , L are as above and $V_{...}$ is the $n \times p \times p \times p$ array of the third derivatives of the model function η with the elements $\eta_{jkl}^a = \frac{\partial^3 \eta_a}{\partial \theta_j \partial \theta_k \partial \theta_l} \Big|_{\hat{\Theta}}$ is called the four dimensional parameter-effects array.

Table 1

Rules for computation

$T - n \times p \times q$ $E - s \times p$	$ET - n \times s \times q$	$(ET)_{ij}^a = \sum_t E_{it} T_{tj}^a$
$T - n \times p \times q$ $E - q \times s$	$TE - n \times p \times s$	$(ET)_{ij}^a = \sum_t T_{it}^a E_{tj}$
$T - n \times p \times q$ $E - s \times n$	$[E][T] - s \times p \times q$	$([E][T])_{ij}^a = \sum_t E_{at} T_{tj}^a$
$T... - n \times r \times p \times q$ $E - s \times p$	$ET... - n \times r \times s \times q$	$(ET...)_{ijk}^a = \sum_t E_{jt} T_{itk}^a$
$T... - n \times r \times p \times q$ $E - q \times s$	$T...E - n \times r \times p \times s$	$(T...E)_{ijk} = \sum_t T_{ijt}^a E_{tk}$
$T... - n \times r \times p \times q$ $E - s \times r$	$E * T... - n \times s \times p \times q$	$(E * T...)_{ijk}^a = \sum_t E_{it} T_{tjk}^a$
$T... - n \times r \times p \times q$ $E - s \times n$	$[E][T...] - s \times r \times p \times q$	$([E][T...])_{ijk}^a = \sum_t E_{at} T_{tjk}^a$

3. THE BATES-WATTS ARRAY AFTER REPARAMETRIZATION

Suppose we wish to determine the parameter-effects array in a parameter β which is the result of a non-linear transformation of Θ ,

$$\beta = G(\Theta)$$

or

$$\beta_i = G_i(\Theta) \quad i = 1, \dots, p.$$

We assume that the inverse transformation is

$$\Theta = S(\beta)$$

or

$$\Theta_i = S_i(\beta) \quad i = 1, \dots, p$$

and denote by S . and G . the $p \times p$ Jacobian matrices with elements $\frac{\partial S_i}{\partial \beta_j} | \hat{\beta}$ and $\frac{\partial G_i}{\partial \Theta_j} | \hat{\Theta}$, respectively, where $\hat{\beta} = \beta(\hat{\Theta})$. The $p \times p \times p$ second derivatives arrays with elements $\frac{\partial^2 S_i}{\partial \beta_j \partial \beta_k}$ and $\frac{\partial^2 G_i}{\partial \Theta_j \partial \Theta_k}$, evaluated at $\hat{\beta} = \beta(\hat{\Theta})$ and $\hat{\Theta}$ are denoted by $S_{..}$ and $G_{..}$, respectively, where a term with subscript i, j, k resides in the i -th face, j -th row and k -th column.

In [2] Bates and Watts claim that the parameter-effect array for the new parameter is

$$(5) \quad A_{..}^{\Theta} = [L^{-1}][L'[G_{..}^{-1}][G_{..}][L].$$

The following example shows that this formula is, in general, wrong.

Example 1. The Fieller-Creasy problem. Let

$$f(x_a, \Theta) = \Theta_1 x_a + \Theta_1 \Theta_2 (1 - x_a)$$

where x_a is an indicator variable that takes the values 1 and 0 for populations 1 and 2, respectively. We assume equal sample sizes for the two populations, $n_1 = n_2 = n$, and assume that σ^2 is known and $\hat{\Theta} = (\hat{\Theta}_1, \hat{\Theta}_2)'$ with $\hat{\Theta}_1 > 0$, $\hat{\Theta}_2 > 0$.

In other words we have the model

$$\begin{aligned} y_a &= \Theta_1 & a &= 1, \dots, n, \\ y_a &= \Theta_1 \Theta_2 & a &= n+1, \dots, 2n. \end{aligned}$$

The parameter-effects array for Θ is

$$A_{..} = \begin{pmatrix} A_{..}^1 \\ A_{..}^2 \end{pmatrix}, \text{ where } A_{..}^1 = \hat{\Theta}_2 A_{..}^2, \quad A_{..}^2 = \hat{\Theta}_1^{-1} (n(1 + \hat{\Theta}_2^2))^{-1/2} \begin{pmatrix} 0 & 1 \\ 1 & -2\hat{\Theta}_2 \end{pmatrix}.$$

The matrix R from (3) is

$$R = n^{1/2} (1 + \hat{\Theta}_2^2)^{-1/2} \begin{pmatrix} 1 + \hat{\Theta}_2^2 & \hat{\Theta}_1 \hat{\Theta}_2 \\ 0 & \hat{\Theta}_1 \end{pmatrix} \quad (\text{see [4]}).$$

Consider now the transformation $\beta_1 = \Theta_2$, $\beta_2 = \Theta_1 \Theta_2$. We have $G = \begin{pmatrix} 0 & 1 \\ \hat{\Theta}_2 & \hat{\Theta}_1 \end{pmatrix}$; $S = \begin{pmatrix} -\hat{\Theta}_1 \hat{\Theta}_2^{-1} & \hat{\Theta}_2^{-1} \\ 1 & 0 \end{pmatrix}$, and $G_{..} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 1 \\ 1 & 0 \end{pmatrix}$. Using (5) we obtain that the new parameter-effects array should be

$$\hat{\Theta}_1^{-1} (1 + \hat{\Theta}_2^2)^{-1/2} n^{-1/2} \begin{pmatrix} 0 & \hat{\Theta}_2^{-1} \\ \hat{\Theta}_2^{-1} & 2 \\ 0 & 1 \\ 1 & -2\hat{\Theta}_2 \end{pmatrix}.$$

The straightforward computation leads, however, to the different result

$$(\hat{\Theta}_1^{-1} \hat{\Theta}_2^{-1} n^{-1/2}) \begin{pmatrix} (-2\hat{\Theta}_2 & -1) \\ -1 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

Theorem 1. *The parameter-effects array for the parameter β is*

$$(6) \quad A_{..}^{\beta} = [X'] [X' \bar{A}_{..} X]$$

where

$$(7) \quad \bar{A}_{..} = A_{..}^{\Theta} - L' [L^{-1} G_{..}^{-1}] [G_{..}] L,$$

$A_{..}^{\Theta}$ is the original parameter-effects array, X is the orthogonal part of the QR -decomposition of $RS_{..} = RG_{..}^{-1}$; i.e. $RG_{..}^{-1} = XK$, where K is an upper triangular matrix with elements $K_{ii} > 0$ and $L = R^{-1}$.

We omit the proof since it goes along the same lines as the proof of Theorem 2 which is given below.

4. FOUR-DIMENSIONAL PARAMETER-EFFECTS ARRAY

In what follows, given an array $T_{...}$, the array $T_{...}^{\sim}$ is defined to have the terms $(T_{...}^{\sim})_{ijk}^a = T_{ijk}^a + T_{jki}^a + T_{kij}^a$. Evidently,

$$(8) \quad Q' \star (Q' T_{...}^{\sim} Q) = (Q' \star (Q' T_{...} Q))^{\sim}$$

where Q is a matrix.

Now we prove a formula for the four-dimensional parameter-effects array in the new parameter β which is the result of a reparametrization $\beta = G(\Theta)$ given above.

Put $h(\beta) = \eta(\Theta(\beta))$ and let $\hat{\beta} = \beta(\hat{\Theta})$ be the least squares value of β . Denote the Jacobian matrix, the second and the third derivatives arrays of h , β and Θ by $B_{..}$, $G_{..}$, $S_{..}$, $B_{...}$, $G_{...}$, $S_{...}$ and $B_{...}$, $G_{...}$, $S_{...}$, respectively. Then the following theorem holds.

Theorem 2. *The four-dimensional parameter-effects array for the parameter β is*

$$(9) \quad A_{...}^{\beta} = [X'] [X' \star (X' \bar{A}_{...} X)]$$

where

$$(10) \quad \bar{A}_{...} = A_{...}^{\Theta} - L' \star (L' [L^{-1} G_{...}^{-1}] [G_{...}] L) - \left([\bar{A}_{...}] [L' [L^{-1} G_{...}^{-1}] [G_{...}] L]^{\sim} \right),$$

$A_{...}^{\Theta}$ is the original four-dimensional parameter-effects array, $G_{..}$, $G_{...}$ and $G_{...}$ are defined as above, X , L and $\bar{A}_{..}$ are as in Theorem 1.

Proof. Differentiating once, twice and three times the identities $h(\beta) = \eta(\Theta(\beta))$ and $\beta = \beta(\Theta(\beta))$ we obtain

$$(11) \quad \begin{aligned} B. &= V.S. \\ B.. &= [V.][S..] + S'V..S. \\ B... &= S' \star (S'V...S.) + ([S'V..][S..])^{\sim} + [V.][S...] \end{aligned}$$

and

$$(12) \quad \begin{aligned} I &= G.S. \quad \text{or} \quad G..^{-1} = S.. \\ 0 &= [G.][S..] + S'G..S. \quad \text{or} \quad -S..^{-1}S..S..^{-1} = [G..^{-1}][G..] \\ 0 &= S' \star (S'G...S.) + ([S'G..][S..])^{\sim} + [G.][S...] \quad \text{or} \end{aligned}$$

$$(13) \quad S..^{-1} \star (S..^{-1}S...S..^{-1}) \stackrel{(8),(12)}{=} -[G..^{-1}][G...] + \left([[G..^{-1}][G..]] [[G..^{-1}][G..]] \right)^{\sim}.$$

We recall that the first and second formulae in (11) can be found in [2].

From the QR-decompositions $V. = UR$ and $RS. = XK$ we get

$$(14) \quad \begin{aligned} X'U'V. &= X'U'UR = X'R, \quad K = X^{-1}RS. \quad \text{or} \\ K^{-1} &= S..^{-1}R^{-1}X, \quad SK^{-1} = R^{-1}X. \end{aligned}$$

Since $(UX)'(UX) = I$, UX is a matrix with orthogonal columns. It follows that $B. = V.S. = URS. = (UX)K$, which provides the QR-decomposition of B . Hence

$$(15) \quad \begin{aligned} A_{..}^{\beta} &\stackrel{\text{def.}}{=} [(UX)'] [K'^{-1} \star (K'^{-1}B..K^{-1})] \stackrel{(14),(11)}{=} \\ &[X'U'] \left[(X'R'^{-1}S'^{-1}) \star \left\{ X'R'^{-1}S'^{-1} \left(S' \star (S'V...S.) + ([S'V..][S..])^{\sim} + \right. \right. \right. \\ &\left. \left. \left. + [V.][S...] \right) S..^{-1}R^{-1}X \right\} \right] = O_1 + O_2 + O_3. \end{aligned}$$

Refining further we obtain

$$(16) \quad \begin{aligned} O_1 &= [X'U'] [(X'R^{-1}) \star (X'R'^{-1}V...R^{-1}X)] = [X'] [X' \star (X'A_{..}^{\ominus}X)] \\ O_2 &\stackrel{(8)}{=} [X'U'] \left[\left([X'R'^{-1}V..][X'R'^{-1}(S'^{-1}S..S..^{-1})R^{-1}X] \right)^{\sim} \right] \stackrel{(12)}{=} \\ &= -[X'] \left[\left([X'R'^{-1}[U][V..]R^{-1}R] [X'R'^{-1}[G..^{-1}][G..]R^{-1}X] \right)^{\sim} \right] = \end{aligned}$$

$$(17) \quad = -[X'] \left[\left([X'A_{..}^{\ominus}] [X'R'^{-1}[RG..^{-1}][G..]R^{-1}X] \right)^{\sim} \right] \stackrel{(8)}{=} [X'] [X' \star (X'Z...X)]$$

where $Z = -\left([A_{..}^{\beta}][R'^{-1}RG^{-1}][G_{..}R^{-1}]\right)^{\sim}$,

$$\begin{aligned}
 (18) \quad O_3 &= [X'U'V_{.}][X'R'^{-1}S'^{-1}] \star (X'R'^{-1}S'^{-1}S_{..}S'^{-1}R^{-1}X) \\
 &= [X'R][X'R'^{-1}] \star (X'R'^{-1}T_{..}R^{-1}X) \\
 &= [X'] \left[X' \star X' \left([R][R'^{-1} \star (R'^{-1}T_{..}R^{-1})] \right) \right] X
 \end{aligned}$$

where $T_{..} = S'^{-1} \star (S'^{-1}S_{..}S'^{-1})$.

Using (8) and (13) we obtain from (17) and (18)

$$(19) \quad O_2 + O_3 = [X'] [X' \star (X'W_{..}X)]$$

where

$$\begin{aligned}
 W_{..} &= -[RG^{-1}][R'^{-1} \star (R'^{-1}G_{..}R^{-1})] \\
 &\quad + \left([R'^{-1}[RG^{-1}][G_{..}R^{-1}][R'^{-1}[RG^{-1}][G_{..}R^{-1}]] \right. \\
 &\quad \left. - [A_{..}^{\beta}][R'^{-1}[RG^{-1}][G_{..}R^{-1}]\right)^{\sim} \\
 &= -L' \star (L'[L^{-1}G_{..}^{-1}][G_{..}L]) - ([\bar{A}_{..}][L'[L^{-1}G_{..}^{-1}][G_{..}L])^{\sim}.
 \end{aligned}$$

Finally, inserting (16) and (19) into (15) we obtain (9). □

5. CONCLUSIONS

It turns out that the error in the Bates-Watts formula stems from the fact that $M = S_{..}^{-1}L$ is not, generally, an upper triangular matrix. If this is the case, e.g. when $S_{..}^{-1}$ is an upper triangular matrix then $X = I$ and the Bates-Watts result is correct, i.e. $A_{..}^{\beta} = \bar{A}_{..}$.

It is worth mentioning that it makes no difference whether $A_{..}^{\beta}$ or $\bar{A}_{..}$ is used for computing the Bates-Watts parameter-effects curvature but they can lead to different results when the confidence regions for parameters are constructed.

As shown in [7], not only the Bates-Watts but also the four-dimensional parameter-effects array should be used in order to obtain an improved confidence region for parameters in the case when the parameter-effects curvature is moderate. If it is relatively large a suitable reparametrization is recommended. Having constructed the confidence region for the new parameter one can back-transform it to obtain the confidence region for the original parameter.

The problem of finding a suitable transformation for a single parameter has been discussed by Hougaard [6], Clarke [3], Cook and Witmer [5] and others. It follows

from their investigations that, as a rule, different criteria would lead to different transformations. Perhaps the best illustration is the Fieller-Creasy problem mentioned above.

As pointed out by Cook and Witmer the obvious transformation in the Fieller-Creasy model $\beta_1 = \Theta_1$, $\beta_2 = \Theta_1\Theta_2$ tends to obscure the parameter of primary interest Θ_2 . Therefore, other transformations have been tried. The transformation $\beta_1 = \Theta_1$, $\beta_2 = \tan^{-1}(\Theta_2)$ suggested by them has the advantage of making the “compansion” terms A_{11}^1 and A_{22}^2 as well as the “arcing” terms A_{22}^1 and A_{11}^2 zero. On the other hand, the “fanning” terms A_{21}^1 and A_{12}^2 are unchanged. It follows that this transformation may produce considerable improvement in situations when there are substantial “compansion” and/or “arcing” effect.

While Clarke [3] in this case has used the transformation $\beta_1 = \Theta_1$, $\beta_2 = \Theta_2^{(1+\hat{\Theta}_2 A_{22}^2 R_{22})}$ we advocate the transformation $\beta_1 = \Theta_1$, $\beta_2 = c \exp(L_{22}^{-1} A_{22}^2 \Theta_2)$, where c is a suitable constant, on the grounds that this transformation sets the parameter-effects curvature for β_2 to zero. We recommend to use this criterion also in the case of a vector parameter. The corresponding problem for a vector parameter is, however, outside the scope of this work and will be dealt with in a separate paper.

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S ú h r n

O BLOKOC H PARAMETRICKÝCH EFEKTOV V N E L I N E Á R N Y C H R E G R E S N Ý C H M O D E L O C H

R A S T I S L A V P O T O C K Ý, T O V A N B A N

V článku sú uvedené vzorce pre výpočet blokov parametrických efektov po reparametrizácii nelineárnych modelov. Tieto vzorce sú užitočné pri konštrukcii oblastí spol'ahlivosti, ktoré sú presnejšie ako doteraz používané oblasti.

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