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Sensitivity analysis in linear models

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Abstract: In this work, we consider the general linear model or its variants with the ordinary least squares, generalised least squares or restricted least squares estimators of the regression coefficients and variance. We propose a newly unified set of definitions for local sensitivity for both situations, one for the estimators of the regression coefficients, and the other for the estimators of the variance. Based on these definitions, we present the estimators' sensitivity results. We include brief remarks on possible links of these definitions and sensitivity results to local influence and other existing results.

Keywords: elliptical distribution; least squares; maximum likelihood; mixed estimation, sensitivity matrix

AMS: 62J05, 62J20, 62M10

1 Introduction

In statistical analysis and applications, the general linear regression model is widely accepted. The ordinary, generalized and restricted least-squares estimators, and several alternatives, are proposed for the regression coefficients and variance in the model or its variants. The local sensitivities of some, but not all, of these estimators are studied. For local sensitivities and diagnostic tests with applications to linear and random effects models, see Magnus and Vasnev [17]. For the sensitivity matrices of least squares estimators and their relevant uses in spatial and panel-spatial autoregressive models, see Liu et al. [12, 14]. The local sensitivities of the posterior mean and precision matrix in the Bayesian context are established as well; see Polasek [19, 20]. These sensitivities are applied to estimator comparisons, regression diagnostics and other issues in several areas. For the interface between these sensitivity results with their applications and some statistical approaches including influence diagnostics see the studies by e.g. Cook [3], Pan et al. [18], Liu et al. [15] and Hao et al. [7]. It is well-known that these sensitivity results are built on the linear models and matrix techniques. For a technical introduction to linear models, see e.g. Magnus and Neudecker [16], Rao et al. [22] and Puntanen et al. [21]. For matrix differential calculus with applications in statistics, econometrics and multivariate analysis, see e.g. Fang and Zhang [5], Liu [10], Magnus and Neudecker [16] and Kollo and von Rosen [8].

In this paper, we focus on the local sensitivities of the ordinary least squares, generalized least squares and restricted least squares estimators in the general linear model or its variants including those with linear restrictions. What is new is that we consider both the regression coefficient and variance estimators, and both an existing approach and a newly proposed approach in which the data and variance schemes for Cook's [3] local influence may be connected.

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We proceed as follows. In section 2, we introduce basic matrix differential calculus and local sensitivity matrix definitions in the context of the linear models we need for the later sections. In section 3, we present the local sensitivity matrix results in the general linear model or its variants, with comments and comparisons in a number of scenarios. In section 4, we make brief concluding remarks to complete the paper.

2 Matrix calculus and local sensitivity

2.1 Matrix calculus

For an $n \times p$ matrix $X = (x_{[1]}, \dots, x_{[i]}, \dots, x_{[n]})' = (x_1, \dots, x_j, \dots, x_p)$, where $()'$ denotes the transpose, $x'_{[i]}$ is the i -th row and x_j is the j -th column ($i = 1, \dots, n$ and $j = 1, \dots, p$), we let $\text{vec}X = (x'_1, \dots, x'_p)'$ denote the $np \times 1$ column-based vectorization vector of X , and $\text{vec}X' = (x'_{[1]}, \dots, x'_{[n]})'$ denote the $np \times 1$ row-based vectorization vector of X . For an $n \times n$ symmetric matrix $V = (v_1, \dots, v_n)$, use $\text{vech}V$ denote the $(n+1)n/2 \times 1$ column-based vectorization vector for the distinct elements of V which stacks the elements on and below the main diagonal of matrix V , and we let $\text{diag}V = v = (v_{11}, \dots, v_{nn})'$ denote the $n \times 1$ diagonal-based vectorization vector which stacks the diagonal elements of matrix V . Let \otimes denote the (right) Kronecker product of two matrices. The following lemmas, definitions and their uses in matrix differential calculus are given by e.g. Magnus and Neudecker [16] and Liu [10].

Lemma 1: Let X be an $n \times p$ matrix. We have

$$\text{vec}X = K_{pn}\text{vec}X',$$

where K_{pn} is the $np \times np$ commutation matrix, with

$$\begin{aligned} K'_{pn}K_{pn} &= I, \\ (A \otimes c')K_{pn} &= c' \otimes A, \\ (z' \otimes B)K_{pn} &= B \otimes z', \\ (z' \otimes c')K_{pn} &= c' \otimes z', \end{aligned}$$

for a $p \times p$ matrix A , a $p \times n$ matrix B , an $n \times 1$ vector c and a $p \times 1$ vector z .

Lemma 2: Let V be an $n \times n$ symmetric matrix. We have

$$\text{vec}V = D\text{vech}V,$$

where D is the $n^2 \times (n+1)n/2$ duplication matrix, with $D'D = I$.

Lemma 3: Let V be an $n \times n$ diagonal matrix. We have

$$\text{vec}V = J\text{diag}V = v,$$

where J is the $n^2 \times n$ selection matrix, with $J'J = I$.

Definition 1: Let $g(x)$ be a scalar function of an $n \times 1$ vector x . The $1 \times n$ derivative vector of $g(x)$ is

$$Dg(x) = \partial g(x) / \partial x'. \quad (1)$$

Definition 2: Let $f(x)$ be an $m \times 1$ vector function of an $n \times 1$ vector x . The $m \times n$ derivative or Jacobian matrix of $f(x)$ is

$$Df(x) = \partial f(x) / \partial x'. \quad (2)$$

2.2 Local sensitivity

Let us consider the general linear model, as given in e.g. Magnus and Neudecker [16], Rao et al. [22] and Puntanen et al. [21]

$$y = X\beta + \epsilon \quad (3)$$

where y is an $n \times 1$ vector of observable random variables, X is an $n \times p$ non-stochastic matrix and ϵ is an $n \times 1$ vector of random disturbances with $E(\epsilon) = 0$ and $E(\epsilon\epsilon') = \sigma^2 V$, where V is an $n \times n$ known positive definite matrix. The $p \times 1$ vector β of regression coefficients and the scalar variance parameter σ^2 are supposed to be fixed but unknown, and therefore need to be estimated.

We assume that we have an estimator of β (say b) and an estimator of σ^2 (say s^2), respectively. Based on Definitions 2 and 1, the following local sensitivity matrices of b and s^2 are defined.

Definition 3: The local sensitivity matrices of b with respect to y , X and V respectively are

$$S_{by} = \partial b / \partial y', \quad (4)$$

$$S_{bX} = \partial b / \partial (\text{vec} X)', \quad (5)$$

$$S_{bX'} = \partial b / \partial (\text{vec} X')', \quad (6)$$

$$S_{bV} = \partial b / \partial (\text{diag} V)', \quad (7)$$

$$S_{bV} = \partial b / \partial (\text{vech} V)', \quad (8)$$

where S_{by} is a $p \times n$ matrix, S_{bX} is a $p \times np$ matrix, $S_{bX'}$ is a $p \times np$ matrix, S_{bV} is a $p \times n$ matrix and S_{bV} is a $p \times (n+1)n/2$ matrix.

Definition 4: The local sensitivity vectors of s^2 with respect to y , X and V respectively are

$$S_{s^2y} = \partial s^2 / \partial y', \quad (9)$$

$$S_{s^2X} = \partial s^2 / \partial (\text{vec} X)', \quad (10)$$

$$S_{s^2X'} = \partial s^2 / \partial (\text{vec} X')', \quad (11)$$

$$S_{s^2V} = \partial s^2 / \partial (\text{diag} V)', \quad (12)$$

$$S_{s^2V} = \partial s^2 / \partial (\text{vech} V)', \quad (13)$$

where S_{s^2y} is a $1 \times n$ vector, S_{s^2X} is a $1 \times np$ vector, $S_{s^2X'}$ is a $1 \times np$ vector, S_{s^2V} is a $1 \times n$ vector and S_{s^2V} is a $1 \times (n+1)n/2$ vector.

Clearly, by definition we see that a sensitivity matrix of an estimator b or s^2 reflects the effects of small changes in y , X or V on the estimator. For example, the sensitivity matrix S_{by} of the estimator b can be used to measure the effects of small changes in y on b .

Actually, the ideas in these definitions are not entirely new. The sensitivity of b to the parameters of the variance matrix in (7) and/or (8) is related to Definition 1 of Magnus and Vasnev (2007). The sensitivity of b to the data in y and X can be connected to Cook's (1986) definition of likelihood displacement; see also Cook (1979). For a study on sensitivity of the variance estimator, see Banerjee and Magnus (1999). In this paper, we simply focus to present the definitions in a systematic approach and provide further results as we see that these sensitivity results are needed and important in dealing with such issues as estimator approximations and comparisons, model mis-specification studies, and regression diagnostics for outliers or influential observations.

Note that the two matrices in definitions (5) and (6) can be equated by the $np \times np$ commutation matrix K_{np} in Lemma 1, same as the two matrices in (10) and (11). However, (6), (8), (11) and (13) are newly proposed to correspond to the perturbation schemes in Cook's local influence diagnostic analysis. The matrix in (5) or (10) uses X 's columns or the variables x_j ($j = 1, \dots, p$), while the matrix in (6) or (11) uses X 's rows or the observations $x_{[i]}$ ($i = 1, \dots, n$) instead, which may reflect the effects of $x_{[i]}$'s minor changes on the estimates of the parameters. In this sense, our sensitivity matrix may be examined to help identifying possible influential observations. The matrix in (7) or the row vector in (12) can be used to examine the effects of $y_{[i]}$ and $x_{[i]}$'s minor changes via the variances v_{ii} , which corresponds to a variance scheme in Cook's influence diagnostic analysis. The largest absolute element of the row vector may indicate the most influential observation in the data. The sensitivities in (8) or (13) can be used to find first-order Tylor approximations for certain estimators; see e.g. Liu et al. [12, 14] for relevant ideas and uses.

In the next section, we use Magnus and Neudecker's [16] matrix differential calculus via Definitions 1 and 2 to establish the sensitivity results, although we do not include detailed derivations for establishing all the

local sensitivity results. The general linear model and some of its variants, with the ordinary least squares, generalized least squares and restricted least squares estimators of β and σ^2 , are considered.

3 General linear model and variants

3.1 Least squares estimators

As the first illustrative example, for the general linear regression model (3)

$$y = X\beta + \epsilon,$$

the following least squares estimators b of β and s^2 of σ^2 are considered, respectively:

$$b = (X'X)^{-1}X'y, \quad (14)$$

$$s^2 = \frac{1}{n-p}(y - Xb)'(y - Xb). \quad (15)$$

Theorem 1: We have

$$S_{by} = (X'X)^{-1}X', \quad (16)$$

$$S_{bX} = (X'X)^{-1} \otimes (y - Xb)' - b' \otimes (X'X)^{-1}X', \quad (17)$$

$$S_{bX'} = (y - Xb)' \otimes (X'X)^{-1} - (X'X)^{-1}X' \otimes b'. \quad (18)$$

To establish (16), we start with (4) for estimator b in (14). We easily find the $p \times n$ local sensitivity matrix of b with respect to y .

To find (17), we use (5). The $p \times np$ local sensitivity matrix of b with respect to X is also given by Magnus and Neudecker [16].

To find (18), we use (6) and the equalities involving the commutation matrix K_{pn} in Lemma 1. We get

$$S_{bX'} = [(X'X)^{-1} \otimes (y - Xb)' - b' \otimes (X'X)^{-1}X']K_{pn},$$

and then (18).

We note that S_{bX} and $S_{bX'}$ involve the residual $y - Xb$. We see from $X'(y - Xb) = 0$ that $S_{bX'}S_{bX'}' = S_{bX}S_{bX}' = (y - Xb)'(y - Xb)(X'X)^{-2} + b'b(X'X)^{-1}$ whose explicit expression is directly dependent on s^2 via the residual. Therefore these sensitivities can be interpreted by the residual in a certain manner.

Theorem 2: We have

$$S_{s^2y} = \frac{2}{n-p}(y - Xb)', \quad (19)$$

$$S_{s^2X} = -\frac{2}{n-p}b' \otimes (y - Xb)', \quad (20)$$

$$S_{s^2X'} = -\frac{2}{n-p}(y - Xb)' \otimes b'. \quad (21)$$

To get (19), we use (9) for estimator s^2 in (15).

To establish (20) and (21), we use (10) and (11) with

$$\begin{aligned}d(y - Xb) &= -(dX)b - Xdb, \\(y - Xb)'X &= 0,\end{aligned}$$

and therefore the differential of s^2 with respect to X

$$\begin{aligned}ds^2 &= \frac{2}{n-p}(y - Xb)'d(y - Xb) \\&= -\frac{2}{n-p}(y - Xb)'(dX)b \\&= -\frac{2}{n-p}b'(dX)'(y - Xb) \\&= -\frac{2}{n-p}(b' \otimes (y - Xb)')dvecX \\&= -\frac{2}{n-p}((y - Xb)' \otimes b')dvecX' .\end{aligned}$$

3.2 Generalized least squares estimators

For model (3)

$$y = X\beta + \epsilon,$$

the generalized least squares estimator of β is

$$\hat{\beta} = (X'V^{-1}X)^{-1}X'V^{-1}y. \quad (22)$$

An unbiased estimator of σ^2 is

$$\hat{\sigma}^2 = \frac{1}{n-p}(y - X\hat{\beta})'V^{-1}(y - X\hat{\beta}). \quad (23)$$

Note that $\hat{\beta}$ and $\hat{\sigma}^2(n-p)/n$ are the maximum likelihood estimators with $(n-p)/n$ as the adjusting constant, if we assume normality for model (3). Hence, we only need to find the sensitivities of $\hat{\beta}$ and $\hat{\sigma}^2$ as defined in Definitions 3 and 4 for both generalized least squares and maximum likelihood estimators.

Theorem 3: We have

$$S_{\hat{\beta}y} = (X'V^{-1}X)^{-1}X'V^{-1}, \quad (24)$$

$$S_{\hat{\beta}X} = (X'V^{-1}X)^{-1} \otimes (y - X\hat{\beta})'V^{-1} - \hat{\beta}' \otimes (X'V^{-1}X)^{-1}X'V^{-1}, \quad (25)$$

$$S_{\hat{\beta}X'} = (y - X\hat{\beta})'V^{-1} \otimes (X'V^{-1}X)^{-1} - (X'V^{-1}X)^{-1}X'V^{-1} \otimes \hat{\beta}', \quad (26)$$

$$S_{\hat{\beta}V} = -[(y - X\hat{\beta})'V^{-1} \otimes (X'V^{-1}X)^{-1}X'V^{-1}]D, \quad (27)$$

$$S_{\hat{\beta}V'} = -[(y - X\hat{\beta})'V^{-1} \otimes (X'V^{-1}X)^{-1}X'V^{-1}]J, \quad (28)$$

where (27) holds for a symmetric matrix V , (28) holds for a diagonal matrix V , and D and J are the duplication and selection matrices, respectively.

To find (24 - 26), we use (4-6) and the matrix differential calculus.

To establish (27) and (28), we first take the differential of (22) to have

$$d\hat{\beta} = -[(y - X\hat{\beta})'V^{-1} \otimes (X'V^{-1}X)^{-1}X'V^{-1}]dvecV. \quad (29)$$

then, if V is an $n \times n$ symmetric matrix, we use $dvecV = DdvecH V$ in Lemma 2 to find (27).

Further, for an $n \times n$ diagonal matrix V , we use $dvec V = Jdv$ in Lemma 3 to establish (28).

Note that $\hat{\beta}$ can be approximated by the first-order Taylor expansion $b + S_{\hat{\beta}V}vechV$. One of such cases may be for a non-diagonal symmetric matrix $V = V(\rho)$ where an AR(1) error structure is involved via the autocorrelation parameter ρ . A first-order Taylor approximation of the generalised least squares estimator in terms of ρ and the sensitivity can be easily established.

Theorem 4: We have

$$S_{\hat{\sigma}^2 y} = \frac{2}{n-p}(y - X\hat{\beta})' V^{-1}, \quad (30)$$

$$S_{\hat{\sigma}^2 X} = -\frac{2}{n-p}\hat{\beta}' \otimes (y - X\hat{\beta})' V^{-1}, \quad (31)$$

$$S_{\hat{\sigma}^2 X'} = -\frac{2}{n-p}(y - X\hat{\beta})' V^{-1} \otimes \hat{\beta}', \quad (32)$$

$$S_{\hat{\sigma}^2 V} = -\frac{1}{n-p}[(y - X\hat{\beta})' V^{-1} \otimes (y - X\hat{\beta})' V^{-1}]D, \quad (33)$$

$$S_{\hat{\sigma}^2 v} = -\frac{1}{n-p}[(y - X\hat{\beta})' V^{-1} \otimes (y - X\hat{\beta})' V^{-1}]J, \quad (34)$$

where (33) holds for a symmetric matrix V , (34) holds for a diagonal matrix V , and D and J are the duplication and selection matrices, respectively.

To get (30), we use (9) to take the differential of estimator $\hat{\sigma}^2$ with respect to y .

To get (31) and (32), we use (10) and (11) with

$$d\hat{\sigma}^2 = -\frac{2}{n-p}[\hat{\beta}' \otimes (y - X\hat{\beta})' V^{-1}]dvecX. \quad (35)$$

We get (33) for a symmetric matrix V , and (34) for a diagonal matrix V , by using (12) and (13) with

$$d\hat{\sigma}^2 = -\frac{1}{n-p}[(y - X\hat{\beta})' V^{-1} \otimes (y - X\hat{\beta})' V^{-1}]dvecV. \quad (36)$$

3.3 Restricted generalized least squares

For the general linear regression model (3)

$$y = X\beta + \epsilon,$$

we consider to have prior information about β in the form of a set of k independent exact linear restrictions expressed as

$$r = R\beta, \quad (37)$$

where R is a $k \times p$ known matrix of rank $k \leq p$ and r is a $k \times 1$ vector of known elements.

The restricted least squares estimators of the parameters in the formulation (3) and (37) are

$$\hat{\beta}_R = \hat{\beta} + (X'V^{-1}X)^{-1}R'[R(X'V^{-1}X)^{-1}R']^{-1}(r - R\hat{\beta}), \quad (38)$$

$$\hat{\sigma}_R^2 = \frac{(y - X\hat{\beta}_R)' V^{-1}(y - X\hat{\beta}_R)}{n - p + k}, \quad (39)$$

where $\hat{\beta} = (X'V^{-1}X)^{-1}X'V^{-1}y$ is the (unrestricted) generalized least squares estimator of β .

Theorem 5: We have

$$S_{\hat{\beta}_{RY}} = M(X'V^{-1}X)^{-1}X'V^{-1}, \tag{40}$$

$$S_{\hat{\beta}_{RX}} = MS_{\hat{\beta}_X} - (\hat{\beta}_R - \hat{\beta})' \otimes M(X'V^{-1}X)^{-1}X'V^{-1} - [(\hat{\beta}_R - \hat{\beta})'X'V^{-1} \otimes M(X'V^{-1}X)^{-1}]K_{pn}, \tag{41}$$

$$S_{\hat{\beta}_{RX'}} = MS_{\hat{\beta}_{X'}} - [(\hat{\beta}_R - \hat{\beta})' \otimes M(X'V^{-1}X)^{-1}X'V^{-1}]K_{pn} - (\hat{\beta}_R - \hat{\beta})'X'V^{-1} \otimes M(X'V^{-1}X)^{-1}, \tag{42}$$

$$S_{\hat{\beta}_{RV}} = MS_{\hat{\beta}_V} + [(\hat{\beta}_R - \hat{\beta})'X'V^{-1} \otimes M(X'V^{-1}X)^{-1}X'V^{-1}]D, \tag{43}$$

$$S_{\hat{\beta}_{RV}} = MS_{\hat{\beta}_V} + [(\hat{\beta}_R - \hat{\beta})'X'V^{-1} \otimes M(X'V^{-1}X)^{-1}X'V^{-1}]J, \tag{44}$$

where (43) holds for a symmetric matrix V , (44) holds for a diagonal matrix V ,

$$M = I - (X'V^{-1}X)^{-1}R'[R(X'V^{-1}X)^{-1}R']^{-1}R$$

is a $p \times p$ idempotent matrix, K_{pn} , D and J are the commutation, duplication and selection matrices, $S_{\hat{\beta}_Y}$, $S_{\hat{\beta}_X}$, $S_{\hat{\beta}_{X'}}$, $S_{\hat{\beta}_V}$ and $S_{\hat{\beta}_V}$ are the same matrices as given in Theorem 3, and $\hat{\beta}_R$ and $\hat{\beta}$ are the restricted and unrestricted generalized least squares estimators of β , respectively.

We establish Theorem 5 using Definition 2 and those results in Theorem 3.

The local sensitivity results of $\hat{\beta}_R$ with respect to X extend a result for which $V = I$ given by Liu and Neudecker [13].

Theorem 6: We have

$$S_{\hat{\sigma}_R^2 Y} = \frac{2}{n-p+k}(y - X\hat{\beta}_R)'V^{-1}(I - XS_{\hat{\beta}_{RY}}), \tag{45}$$

$$S_{\hat{\sigma}_R^2 X} = -\frac{2}{n-p+k}[\hat{\beta}_R' \otimes (y - X\hat{\beta}_R)'V^{-1} - (y - X\hat{\beta}_R)'V^{-1}XS_{\hat{\beta}_{RX}}], \tag{46}$$

$$S_{\hat{\sigma}_R^2 X'} = -\frac{2}{n-p+k}[(y - X\hat{\beta}_R)'V^{-1} \otimes \hat{\beta}_R' - (y - X\hat{\beta}_R)'V^{-1}XS_{\hat{\beta}_{RX'}}], \tag{47}$$

$$S_{\hat{\sigma}_R^2 V} = -\frac{1}{n-p+k}[(y - X\hat{\beta}_R)'V^{-1} \otimes (y - X\hat{\beta}_R)'V^{-1}]D + 2(y - X\hat{\beta}_R)'V^{-1}XS_{\hat{\beta}_{RV}}, \tag{48}$$

$$S_{\hat{\sigma}_R^2 V} = -\frac{1}{n-p+k}[(y - X\hat{\beta}_R)'V^{-1} \otimes (y - X\hat{\beta}_R)'V^{-1}]J + 2(y - X\hat{\beta}_R)'V^{-1}XS_{\hat{\beta}_{RV}}, \tag{49}$$

where (48) holds for a symmetric matrix V , (49) holds for a diagonal matrix V , D and J are the duplication and selection matrices, $S_{\hat{\beta}_{RY}}$, $S_{\hat{\beta}_{RX}}$, $S_{\hat{\beta}_{RX'}}$, $S_{\hat{\beta}_{RV}}$ and $S_{\hat{\beta}_{RV}}$ are the same matrices as given in Theorem 5, and $\hat{\beta}_R$ is the restricted generalized least squares estimator of β .

We establish Theorem 6 using Definition 1.

4 Concluding remarks

Fang et al. [4] studied elliptical distributions and the elliptical distributions based generalized multivariate analysis. Schaffrin and Toutenburg [23], Rao et al. [22], Liu et al. [11] and Leiva et al. [9] discussed mixed estimators for the normal or elliptical distributions based general linear model with stochastic linear restrictions. So we may study sensitivity results for the mixed estimators under normality or elliptical distributional assumptions.

We may further study the maximum likelihood estimators for some of the models covered by Puntanen et al. [21] or the growth curve models studied by e.g. Pan et al. [18] or those discussed in the previous section under elliptical distributions studied by e.g. Fang et al. [4].

We may apply some of these sensitivity results to the first-order approximations of those possible estimators in an approach as taken in section 3.2 and in e.g. Liu et al. [12, 14].

We may conduct numerical studies to examine the possible link of (6) and (11) to Cook's local influence results for the different estimators.

To summarize, we have defined the sensitivities for the general linear model and its variants in a systematic manner, derived the sensitivity results easy to use, and listed possible extensions to further consider.

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