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A Note on Cook's Distance in the Multivariate Linear Model

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Abstract

We propose a version of Cook's distance (called local distance) in the multivariate linear model. The proposed version is a matrix, while the existing version of Cook's distance (called global distance) is a scalar. The existing Cook's distance is the trace of the proposed Cook's distance. In addition, we argue that the proposed Cook's distance has a more natural extension of the Cook's distance in the univariate linear model than the existing Cook's distance. An illustrative example based on a real data set is given.

Keywords: Global distance, influential observations, local distance.

1. Introduction

Most research on regression diagnostics are done for statistical models with one-dimensional response (univariate models); however, studies on multivariate regression diagnostics are relatively limited.

For the influence measures in the multivariate linear model, Caroni (1987) investigated a Studentized residual and suggested a version of Cook's distance (Cook, 1977) based on a confidence ellipsoid analogue. Altunkaynak and Ekni (2002) suggested a useful algorithm to compute the Cook's distance suggested by Caroni (1987). In addition, Diaz-Garcia *et al.* (2003) extended the concept of local influence (Cook, 1986) and likelihood displacement (Cook *et al.*, 1988) in the univariate linear model to the multivariate linear model. However, Tang and Fung (1997) considered case-deletion diagnostics for test statistics and Fung (1999) studied outlier diagnostics in several multivariate samples. For the diagnostics in the repeated measures or the longitudinal data, Preisser and Qaqish (1996) proposed deletion diagnostics for generalized estimating equations, Banerjee and Frees (1997) suggested influence diagnostics for linear longitudinal models, and Lindsey and Lindsey (2000) suggested some diagnostic tools for random effects in the repeated measures growth curve model.

In this paper, we suggest a new version of Cook's distance in the multivariate model. First, we mention the misleading aspect of the existing Cook's distance. The existing Cook's distance of the i^{th} observation on the estimator of regression coefficient matrix is a scalar; however, the proposed Cook's distance in this thesis is a matrix that simultaneously reveals the influence of multiple outputs. We show that the existing version is sum of diagonal elements of the suggested version; therefore, the suggested version contains more diagnostic information than the existing version. In addition, this feature is demonstrated through numerical studies.

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2. Multivariate Linear Model

Consider a multivariate linear model

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{B} + \boldsymbol{U}, \tag{2.1}$$

where $\boldsymbol{Y}$ is $n{\times}q$ response matrix, $\boldsymbol{X}$ is $n{\times}p$ design matrix, $\boldsymbol{B}$ is unknown $p{\times}q$ regression coefficient matrix, and $\boldsymbol{U}$ is $n{\times}q$ error matrix. Specifically let $\boldsymbol{y}_i = (y_{i1}, y_{i2}, \ldots, y_{iq})'$, $\boldsymbol{x}_i = (1, x_{i1}, x_{i2}, \ldots, x_{i,p-1})'$, $\boldsymbol{u}_i = (u_{i1}, u_{i2}, \ldots, u_{iq})'$, $i = 1, 2, \ldots, n$ be the i^{th} row of $\boldsymbol{Y}, \boldsymbol{X}, \boldsymbol{U}$, respectively, and let $\boldsymbol{\beta}_i = (\beta_{i1}, \beta_{i2}, \ldots, \beta_{iq})'$, $i = 1, 2, \ldots, p$ be the i^{th} row of $\boldsymbol{B}$. It is usually assumed that $\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_n$ are independent, and $\mathrm{E}[\boldsymbol{u}_i] = \boldsymbol{0}$ and $\mathrm{Cov}(\boldsymbol{u}_i) = \boldsymbol{\Sigma}$ for all $i = 1, 2, \ldots, n$, where $\boldsymbol{\Sigma}$ is a $q \times q$ variance-covariance matrix of the random vector $\boldsymbol{u}_i$, and has σ_{ij} as its ij^{th} component. The goal is to suggest a new version of Cook's distance and comparing with the existing ones, so that we restrict our attention to the assumption of $\mathrm{Cov}(\boldsymbol{u}_i) = \boldsymbol{\Sigma}$ for all $i = 1, 2, \ldots, n$. For more general cases, see Preisser and Qaqish (1996), Banerjee and Frees (1997), and Lindsey and Lindsey (2000) among others.

If $\boldsymbol{X}'\boldsymbol{X}$ is non-singular, then the least squares estimator of the regression coefficient matrix $\boldsymbol{B}$ is given by

$$\hat{\boldsymbol{B}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{Y}.$$

The fitted matrix can be expressed as $\hat{\boldsymbol{Y}} = \boldsymbol{H}\boldsymbol{Y}$, where $\boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'$ is the hat matrix with $h_{ij} = \boldsymbol{x}_i'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_j$ as the ij^{th} component of $\boldsymbol{H}$. Using this notation, the residual matrix is defined as $\boldsymbol{E} = \boldsymbol{Y} - \hat{\boldsymbol{Y}}$, and let $\boldsymbol{E} = (\boldsymbol{e}_1, \ldots, \boldsymbol{e}_n)'$, where $\boldsymbol{e}_i'$, the i^{th} row of $\boldsymbol{E}$, is the i^{th} residual vector. As an unbiased estimator of $\boldsymbol{\Sigma}$, $\hat{\boldsymbol{\Sigma}} = \boldsymbol{E}'\boldsymbol{E}/(n-p)$ is often used.

2.1. Existing version of Cook's distance C_i^G

In the multivariate linear model $E(\boldsymbol{Y}) = \boldsymbol{X}\boldsymbol{B}$, Cook's distance of the i^{th} observation on the estimator of the regression coefficient matrix $\boldsymbol{B}$ is based on $\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(i)}$, where $\hat{\boldsymbol{B}}_{(i)}$ is the least squares estimator of $\boldsymbol{B}$ based on $n-1$ observations after deleting the i^{th} observation $(\boldsymbol{x}_i, \boldsymbol{y}_i)$. Note that $\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(i)}$ is a $p \times q$ matrix, it is not straightforward to normalize to a scalar. To overcome this situation, by using the vec operation the multivariate linear model in (2.1) can be reexpressed as

$$\mathrm{vec}(\boldsymbol{Y}) = \left(\boldsymbol{I}_q \otimes \boldsymbol{X}\right)\mathrm{vec}(\boldsymbol{B}) + \mathrm{vec}(\boldsymbol{U}).$$

Using this notation, Caroni (1987) and Diaz-Garcia *et al.* (2003) suggested a version of Cook's distance in the multivariate linear model as

$$C_i^G = \frac{1}{p}\left[\mathrm{vec}\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(i)}\right)'\left(\mathrm{Cov}\left(\mathrm{vec}\left(\hat{\boldsymbol{B}}\right)\right)\right)^{-1}\mathrm{vec}\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(i)}\right)\right].$$

Here we call C_i^G a global distance, because it does not distinguish q multiple outputs $(y_{i1}, y_{i2}, \ldots, y_{iq})$, but it computes the effect of q multiple outputs simultaneously. That is to say, C_i^G renders one scalar value as influence of q multiple outputs.

To express C_i^G as a function of basic building blocks, we note that $\mathrm{Cov}(\mathrm{vec}(\hat{\boldsymbol{B}})) = \boldsymbol{\Sigma} \otimes (\boldsymbol{X}'\boldsymbol{X})^{-1}$ and

$$\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(i)} = \frac{(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_i\boldsymbol{e}_i'}{1 - h_{ii}}. \tag{2.2}$$

In addition, if we use

$$(\mathrm{vec}(\boldsymbol{Z}'))'\,(\boldsymbol{A}\otimes\boldsymbol{B}')\,\mathrm{vec}(\boldsymbol{Z}) = \mathrm{tr}(\boldsymbol{A}\boldsymbol{Z}'\boldsymbol{B}\boldsymbol{Z}) \tag{2.3}$$

then, we have

$$C_i^G = \frac{1}{p}\frac{h_{ii}}{1-h_{ii}}\frac{\boldsymbol{e}_i'\hat{\boldsymbol{\Sigma}}^{-1}\boldsymbol{e}_i}{1-h_{ii}}. \tag{2.4}$$

This equation also can be expressed as

$$C_i^G = \frac{1}{p}\frac{r_i^2 h_{ii}}{1-h_{ii}},$$

where

$$r_i^2 = \frac{\boldsymbol{e}_i'\hat{\boldsymbol{\Sigma}}^{-1}\boldsymbol{e}_i}{1-h_{ii}}$$

is a version of studentized residual in the multivariate model.

For the influence of a set of observations, let $K = \{i_1, i_2, \ldots, i_k\}$ be an index set containing k sets. Then the influential set version of the Cook's distance considered above is

$$C_K^G = \frac{1}{p}\left\{\mathrm{vec}\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)}\right)'\left[\boldsymbol{\Sigma}^{-1}\otimes(\boldsymbol{X}'\boldsymbol{X})\right]\mathrm{vec}\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)}\right)\right\}.$$

To express C_K^G as a function of basic building blocks we first note that

$$\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\,\boldsymbol{X}_K'\,(\boldsymbol{I}-\boldsymbol{H}_K)^{-1}\,\boldsymbol{e}_K,$$

where $\boldsymbol{X}_K = (\boldsymbol{x}_{i_1}, \boldsymbol{x}_{i_2}, \ldots, \boldsymbol{x}_{i_k})$ is $k \times p$ matrix, $\boldsymbol{e}_K = (\boldsymbol{e}_{i_1}, \boldsymbol{e}_{i_2}, \ldots, \boldsymbol{e}_{i_k})$ is $k \times q$ matrix, and $\boldsymbol{H}_K = \boldsymbol{X}_K(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}_K'$. Then, by (2.3),

$$\begin{aligned}
C_K^G &= \frac{1}{p}\left\{\mathrm{vec}\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)}\right)'\left[\boldsymbol{\Sigma}^{-1}\otimes(\boldsymbol{X}'\boldsymbol{X})\right]\mathrm{vec}\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)}\right)\right\}\\
&= \frac{1}{p}\,\mathrm{tr}\left(\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)}\right)'\boldsymbol{X}'\boldsymbol{X}\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)}\right)\boldsymbol{\Sigma}^{-1}\right)\\
&= \frac{1}{p}\,\mathrm{tr}\left(\boldsymbol{e}_K'\,(\boldsymbol{I}-\boldsymbol{H}_K)^{-1}\,\boldsymbol{H}_K\,(\boldsymbol{I}-\boldsymbol{H}_K)^{-1}\,\boldsymbol{e}_K\hat{\boldsymbol{\Sigma}}^{-1}\right).
\end{aligned}$$

2.2. A proposed version of Cook's distance $\boldsymbol{C}_i^L$

Recall that Cook's distance for the i^{th} observation in the univariate linear model can be written as

$$\begin{aligned}
D_i &= \frac{1}{p}\left(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{(i)}\right)'\mathrm{Cov}\left(\hat{\boldsymbol{\beta}}\right)^{-1}\left(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{(i)}\right)\\
&= \frac{1}{p}\left(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{(i)}\right)'\sigma^{-2}\,(\boldsymbol{X}'\boldsymbol{X})\left(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{(i)}\right)\\
&= \frac{1}{p}\frac{\left(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{(i)}\right)'}{\sigma}\,(\boldsymbol{X}'\boldsymbol{X})\,\frac{\left(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_{(i)}\right)}{\sigma},
\end{aligned}$$

which motivates Cook's distance in the multivariate linear model as

$$\boldsymbol{C}_i^L = \frac{1}{p}\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(i)}\right)'(\boldsymbol{X}'\boldsymbol{X})\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(i)}\right)\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}.$$

If we use $\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(i)} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_i\boldsymbol{e}_i'/(1 - h_{ii})$, then we can express $\boldsymbol{C}_i^L$ as basic building blocks, *i.e.*,

$$\begin{aligned}\boldsymbol{C}_i^L &= \frac{1}{p}\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}\frac{\boldsymbol{e}_i\boldsymbol{x}_i'(\boldsymbol{X}'\boldsymbol{X})^{-1}}{1 - h_{ii}}(\boldsymbol{X}'\boldsymbol{X})\frac{(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_i\boldsymbol{e}_i'}{1 - h_{ii}}\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}\\ &= \frac{1}{p}\frac{h_{ii}}{(1 - h_{ii})^2}\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}\boldsymbol{e}_i\boldsymbol{e}_i'\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}},\end{aligned}$$

where $\boldsymbol{e}_i = \boldsymbol{y}_i - \boldsymbol{x}_i'\hat{\boldsymbol{B}}$ and $h_{ii} = \boldsymbol{x}_i'(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{x}_i$. Note that $\boldsymbol{C}_i^L$ is not scalar but a $q \times q$ matrix. In addition, it is clear that $\text{tr}(\boldsymbol{C}_i^L) = C_i^G$.

2.3. Remarks on local influence and global influence

There is a serious disadvantage in C_i^G. Note that some of the diagonal elements of the local distance $\boldsymbol{C}_i^L$ could be small or large, and therefore, C_i^G may not reveal the actual influence of the i^{th} observation. For example, $C_i^G = 2.0$ is due to either $\boldsymbol{C}_i^L(1,1) = 1.0$, $\boldsymbol{C}_i^L(2,2) = 1.0$ or $\boldsymbol{C}_i^L(1,1) = 1.9$, $\boldsymbol{C}_i^L(2,2) = 0.1$. Hence, $\boldsymbol{C}_i^L$ is more informative measure than C_i^G to represent actual influence of the i^{th} observation.

To see further relations between $\boldsymbol{C}_i^L$ and C_i^G, note that $\boldsymbol{e}_i'\hat{\boldsymbol{\Sigma}}^{-1}\boldsymbol{e}_i$ in C_i^G is replaced by $\hat{\boldsymbol{\Sigma}}^{-1/2}\boldsymbol{e}_i\boldsymbol{e}_i'\hat{\boldsymbol{\Sigma}}^{-1/2}$ in $\boldsymbol{C}_i^L$. To compare these two terms we assume, for simplicity, that $q = 2$ and correlation between y_{i1} and y_{i2} is close to zero. Then, $\boldsymbol{e}_i'\hat{\boldsymbol{\Sigma}}^{-1}\boldsymbol{e}_i \simeq e_{i1}^2/\hat{\sigma}_1^2 + e_{i2}^2/\hat{\sigma}_2^2$, but

$$\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}\boldsymbol{e}_i\boldsymbol{e}_i'\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}} \simeq \begin{bmatrix} \dfrac{e_{i1}^2}{\hat{\sigma}_1^2} & \dfrac{e_{i1}e_{i2}}{\hat{\sigma}_1\hat{\sigma}_2} \\ \dfrac{e_{i1}e_{i2}}{\hat{\sigma}_1\hat{\sigma}_2} & \dfrac{e_{i2}^2}{\hat{\sigma}_2^2} \end{bmatrix}.$$

Therefore, if we assume weak correlations between responses, we may say that the j^{th} diagonal element $\boldsymbol{C}_i^L(jj)$ represents the influence of y_{ij} and $\boldsymbol{x}_i$ on $\hat{\boldsymbol{B}}$. Of course, if q responses are highly correlated, then interpretations on each component of $\boldsymbol{C}_i^L$ will be very complicated. Hence, $\boldsymbol{C}_i^L$ can be called the local distance representing the influence of each response separately for the i^{th} observation. On the other hand, C_i^G, sum of diagonal elements of $\boldsymbol{C}_i^L$, can be called the global distance representing the influence of all the q responses simultaneously for the i^{th} observation.

We can easily extend $\boldsymbol{C}_i^L$ to $\boldsymbol{C}_K^L$, local Cook's distance for the set of observations in $K = (i_1, i_2, \ldots, i_k)$, *i.e.*,

$$\boldsymbol{C}_K^L = \frac{1}{p}\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)}\right)'(\boldsymbol{X}'\boldsymbol{X})\left(\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)}\right)\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}. \qquad (2.5)$$

To express $\boldsymbol{C}_K^L$ as a function of basic building blocks, we use

$$\hat{\boldsymbol{B}} - \hat{\boldsymbol{B}}_{(K)} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}_K'(\boldsymbol{I} - \boldsymbol{H}_K)^{-1}\boldsymbol{e}_K.$$

Then the local Cook's distance for the set of observations in K can be reexpressed as

$$\boldsymbol{C}_K^L = \frac{1}{p}\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}\boldsymbol{e}_K'(\boldsymbol{I} - \boldsymbol{H}_K)^{-1}\boldsymbol{H}_K(\boldsymbol{I} - \boldsymbol{H}_K)^{-1}\boldsymbol{e}_K\hat{\boldsymbol{\Sigma}}^{-\frac{1}{2}}. \qquad (2.6)$$

Table 1: Two versions of Cook's distance C_K^G and $\boldsymbol{C}_K^L$ when $K = \{i\}$ in the automobile tire data.

K	$\boldsymbol{C}_K^L$		C_K^G
1	0.317	0.093	0.344
	0.093	0.027	
2	0.247	−0.330	0.688
	−0.330	0.441	
3	0.303	−0.073	0.321
	−0.073	0.018	
4	0.067	0.066	0.131
	0.066	0.064	
5	0.024	−0.081	0.298
	−0.081	0.274	
6	0.132	−0.066	0.165
	−0.066	0.033	
7	0.010	0.109	1.196
	0.109	1.186	
8	0.010	−0.025	0.073
	−0.025	0.063	
9	0.704	−0.785	1.580
	−0.785	0.876	
10	0.038	0.037	0.073
	0.037	0.035	

Table 2: Five largest Cook's distances for C_K^G and $\boldsymbol{C}_K^L$ when $K = \{i, j\}$ in the automobile tire data.

K	$\boldsymbol{C}_K^L$		C_K^G
5, 9	13.1654	0.7721	13.3879
	0.7721	0.2225	
7, 9	4.9712	3.3713	8.0197
	3.3713	3.0485	
5, 7	1.4881	2.8318	7.1213
	2.8318	5.6332	
3, 7	1.9939	2.9972	6.9868
	2.9972	4.9929	
3, 9	0.2126	−0.3611	6.9321
	−0.3611	6.7195	

If we assume, for simplicity, that $q = 2$, $K = \{i, j\}$ and correlation between y_{i1} and y_{i2} is close to zero, then the first diagonal element of $\boldsymbol{C}_K^L$ represents the influence of y_{i1} and y_{j1} on $\hat{\boldsymbol{B}}$, and the second diagonal element of $\boldsymbol{C}_K^L$ represents the influence of y_{i2} and y_{j2} on $\hat{\boldsymbol{B}}$; however, C_K^G shows only the sum of two influences of $\{y_{i1}, y_{j1}\}$ and $\{y_{i2}, y_{j2}\}$ on $\hat{\boldsymbol{B}}$.

3. Example

As an illustrative example for two versions of Cook's distance C_K^G and $\boldsymbol{C}_K^L$, we take automobile tire data described in Green (1978). The data consist of 2 responses and 4 covariates, and the number of observations is 10, *i.e.*, $q = 2$, $p = 5$ and $n = 10$.

After fitting a multivariate linear model $\boldsymbol{Y} = \boldsymbol{XB} + \boldsymbol{U}$, we evaluate two influence measures in Table 1. First, the global Cook's distance C_i^G reveals that the 9^{th} observation is very influential, and the 7^{th} observation is also quite influential. If we see the local Cook's distance $\boldsymbol{C}_i^L$, then the global influence of the 9^{th} observation 1.580 is sum 0.704 (local influence of $y_{9,1}$) and 0.876 (local influence of $y_{9,2}$); however, the global influence of the 7^{th} observation 1.196 is sum of 0.010 (local influence of $y_{7,1}$) and 1.186 (local influence of $y_{7,2}$). Therefore, the high influence of the 7^{th} observation is mainly due to the 2^{nd} component of the response $y_{7,2}$. For the influence of two observations (Table 2), we see that $\{5, 9\}$ has the largest global Cook's distance mainly due to y_{51} and y_{91}; in addition, the contribution of y_{52} and y_{92} is almost negligible.

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