

Multiple Deletions in Logistic Regression Models

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Abstract

We extended the results of Roy and Guria (2008) to multiple deletions in logistic regression models. Since single deletions may not exactly detect outliers or influential observations due to swamping effects and masking effects, it needs multiple deletions. We developed conditional deletion diagnostics which are designed to overcome problems of masking effects. We derived the closed forms for several statistics in logistic regression models. They give useful diagnostics on the statistics.

Keywords: Conditional deletions, logistic regression models, masking effects, multiple deletions, outliers, swamping effects.

1. Introduction

Regression models are efficient under certain assumptions. These are violated by outliers or influential observations. The detection of outliers or influential observations has a long history. Many diagnostic measures have been proposed in classical linear regression model (Belsley *et al.*, 1980; Cook and Weisberg, 1982). A few works that treat detection of influential observations for general types of linear model are found. Among them, Pregibon (1981) proposed the Pearson residuals for a binary model through logistic regression and Thomas and Cook (1989) studied the local influence in the generalized linear model (GLM), which was suggested by Cook (1986). Those diagnostics are based on the perturbation schemes.

Deletion statistics are basic tools in regression diagnostics. However, deletion statistics in GLM are complicated, because the models use the maximum likelihood estimators (MLE) instead of the least squares estimators. In GLM the MLEs are usually obtained using iteratively reweighted least squares, a kind of least squares estimates which is known to be sensitive to outliers or influential observations. The diagnostics in GLM with Gaussian linear models used the Pearson residual, the deviance residual, the hat matrix and the Cook distance (Dobson, 2002, pp. 127–130). Roy and Guria (2008) proposed deletion diagnostics for logistic regression models, based on the Newton-Raphson approximation formula. Since these diagnostics are single case deletion methods, they cannot detect unusually multiple observations and overcome the errors of masking or swamping effects (Jung, 2007).

In this work we extend the results of Roy and Guria (2008) to multiple deletions for regression parameters and statistics which are very useful for regression diagnostics in GLM. In Section 2 we review the logistic regression model and introduce some notations used in this paper. We derive the multiple deletion regression coefficients for the maximum likelihood estimators. And we develop a conditional deletion diagnostics which are designed to overcome problems of masking effects. In Section 3 we derive multiple deletion diagnostics related to statistics for the logistic regression model.

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In Section 4 an illustrative example is given and the result shows that multiple deletions are useful to check whether the swamping effects or masking effects exist or not.

2. Multiple Deletions for Regression Coefficients

For $i = 1, \dots, n$ let consider the model $y_i = \mu_i + \epsilon_i$, where $\mu_i = \mathbf{x}_i^T \boldsymbol{\beta}$ and ϵ_i follows $N(0, \sigma^2)$. Nelder and Wedderburn (1972) extended this normal linear model to the GLM with considering the non-normal response variables and the link function $g(\mu_i) = \mathbf{x}_i^T \boldsymbol{\beta}$, where $\boldsymbol{\beta} = (\beta_1, \dots, \beta_p)^T$ is the parameter vector of regression coefficients. When the link function is the logit function we call this model a logistic regression model with a binary response variable having values 0 or 1. The logistic regression model can be written as

$$P_i = P(y_i = 1 | \mathbf{x}_i) = \frac{e^{\mathbf{x}_i^T \boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i^T \boldsymbol{\beta}}}$$

and $P(y_i = 0) = 1 - P_i$. The log-likelihood function becomes

$$L(\boldsymbol{\beta}) = \sum_{i=1}^n \{y_i \mathbf{x}_i^T \boldsymbol{\beta} - \ln(1 + e^{\mathbf{x}_i^T \boldsymbol{\beta}})\}. \quad (2.1)$$

Let $s_i = y_i - P_i$, $v_i = P_i(1 - P_i)$, $\mathbf{s} = (s_1, \dots, s_n)$, $\mathbf{V} = \text{diag}(v_1, \dots, v_n)$ and $\mathbf{Z} = \mathbf{V}^{1/2} \mathbf{X}$. Then the maximum likelihood estimator of $\boldsymbol{\beta}$ can be obtained iteratively by

$$\hat{\boldsymbol{\beta}}^1 = \boldsymbol{\beta}^0 + (\mathbf{Z}^T \mathbf{Z})^{-1} (\mathbf{Z}^T \mathbf{V}^{-1/2} \mathbf{s}), \quad (2.2)$$

where $\boldsymbol{\beta}^0$ is an initial solution of $\boldsymbol{\beta}$. And the matrices \mathbf{Z} , \mathbf{s} and \mathbf{V} are evaluated at $\boldsymbol{\beta}^0$.

Now we derive deletion statistics when the observations corresponding to the index set J with length m of $\{1, \dots, n\}$ are omitted. The log-likelihood function with the deletion of the index set J becomes

$$L^{(J)}(\boldsymbol{\beta}) = \sum_{i=1, i \notin J}^n \{y_i \mathbf{x}_i^T \boldsymbol{\beta} - \ln(1 + e^{\mathbf{x}_i^T \boldsymbol{\beta}})\}. \quad (2.3)$$

Then

$$\frac{\partial L^{(J)}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = \mathbf{X}^T \mathbf{s} - \sum_{j \notin J} \mathbf{x}_j s_j$$

and

$$-\frac{\partial^2 L^{(J)}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^T} = \mathbf{Z}^T \mathbf{Z} - \sum_{j \notin J} \mathbf{z}_j \mathbf{z}_j^T,$$

where $\mathbf{z}_i = \sqrt{v_i} \mathbf{x}_i$. Without observations for the index set J the first approximation to $\hat{\boldsymbol{\beta}}^{1(J)}$ becomes

$$\hat{\boldsymbol{\beta}}^{1(J)} = \boldsymbol{\beta}^{0(J)} + \left(\mathbf{Z}^T \mathbf{Z} - \sum_{j \notin J} \mathbf{z}_j \mathbf{z}_j^T \right)^{-1} \left(\mathbf{X}^T \mathbf{s} - \sum_{j \notin J} \mathbf{x}_j s_j \right), \quad (2.4)$$

where $\boldsymbol{\beta}^{0(J)}$ is an initial solution with the deletion of observations corresponding to the index set J . It is usual to set $\boldsymbol{\beta}^0$ as the least squares estimate $(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$ for a linear regression model. It is natural

to use

$$\begin{aligned}\beta^{0(J)} &= \left(\mathbf{X}^T \mathbf{X} - \sum_{j \notin J} \mathbf{x}_j \mathbf{x}_j^T \right)^{-1} \left(\mathbf{X}^T \mathbf{y} - \sum_{j \notin J} \mathbf{x}_j y_j \right) \\ &= \beta^0 - (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}_J^T (\mathbf{I} - \mathbf{H}_J)^{-1} \mathbf{e}_J,\end{aligned}\quad (2.5)$$

where \mathbf{H}_J is the $m \times m$ minor of $\mathbf{H} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$ given by the intersection of the rows and columns indexed by J , that is $\mathbf{H}_J = \mathbf{X}_J(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}_J^T$ and $\mathbf{e}_J = \mathbf{y}_J - \mathbf{X}_J^T \beta^0$.

We simplify the second term in (2.4). Since

$$\left(\mathbf{Z}^T \mathbf{Z} - \sum_{j \notin J} \mathbf{z}_j \mathbf{z}_j^T \right)^{-1} = (\mathbf{Z}^T \mathbf{Z})^{-1} + (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_J^T (\mathbf{I} - \mathbf{H}_J^*)^{-1} \mathbf{Z}_J (\mathbf{Z}^T \mathbf{Z})^{-1},$$

where $\mathbf{H}_J^* = \mathbf{Z}_J (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_J^T$, some calculation yields

$$(\mathbf{Z}^T \mathbf{Z} - \mathbf{Z}_J^T \mathbf{Z}_J)^{-1} (\mathbf{X}^T \mathbf{s} - \mathbf{X}_J^T s_J) = (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{X}^T \mathbf{s} - (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_J^T (\mathbf{I} - \mathbf{H}_J^*)^{-1} \mathbf{e}_J^*, \quad (2.6)$$

where $\mathbf{e}_J^* = \mathbf{V}_J^{-1/2} \mathbf{s}_J - \mathbf{Z}_J (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_J^T \mathbf{V}_J^{-1/2} \mathbf{s}$ which can be obtained by residual for regressing $\mathbf{V}_J^{-1/2} \mathbf{s}_J$ on \mathbf{Z}_J . Also the statistics are evaluated at β^0 . Then from (2.5) and (2.6) we have the regression estimate (2.4) with the deletion of the index set J

$$\hat{\beta}^{1(J)} = \hat{\beta}^1 - (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_J^T (\mathbf{I} - \mathbf{H}_J^*)^{-1} \mathbf{e}_J^* - (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}_J^T (\mathbf{I} - \mathbf{H}_J)^{-1} \mathbf{e}_J. \quad (2.7)$$

Equation (2.7) may get more exact influence information than single deletions which cannot detect outliers when data have swamping or masking effects.

If we use a fully iterated estimate instead of the initial estimate, the deletion estimate in (2.7) becomes

$$\begin{aligned}\hat{\beta}^{(J)} &= \hat{\beta} + (\mathbf{Z}^T \mathbf{Z})^{-1} (\mathbf{Z}^T \mathbf{V}^{-1/2} \mathbf{S}) - (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_J^T (\mathbf{I} - \mathbf{H}_J^*)^{-1} \mathbf{e}_J^* \\ &= \hat{\beta} - (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_J^T (\mathbf{I} - \mathbf{H}_J^*)^{-1} \mathbf{e}_J^*,\end{aligned}\quad (2.8)$$

where the last term on the right hand side of (2.8) is evaluated at $\hat{\beta}$. Since the last terms are calculated on the full set, it does not need running the regression again without the index set J .

Lawrance (1995) developed a conditional deletion diagnostic designed to detect and overcome problems of masking within datasets under the ordinary least squares model. We have extended Lawrance's conditional deletion diagnostic to the logistic regression model. The quantities calculated are the estimate for the K cases after deletion of the J cases. It arises from assessing conditional influence on the deletion of the other case. The conditional influence is denoted by $\hat{\beta}^{K(J)}$ and is exactly equal to the difference of $\hat{\beta}^{(J,K)}$ and $\hat{\beta}^{(J)}$. Thus we have

$$\begin{aligned}\hat{\beta}^{1K(J)} &= -(\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_{J,K}^T (\mathbf{I} - \mathbf{H}_{J,K}^*)^{-1} \mathbf{e}_{J,K}^* - (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}_{J,K}^T (\mathbf{I} - \mathbf{H}_{J,K})^{-1} \mathbf{e}_{J,K} \\ &\quad + (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_J^T (\mathbf{I} - \mathbf{H}_J^*)^{-1} \mathbf{e}_J^* + (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}_J^T (\mathbf{I} - \mathbf{H}_J)^{-1} \mathbf{e}_J.\end{aligned}\quad (2.9)$$

Also the conditional deletions for the converged estimate are similarly derived as (2.8).

3. Multiple Deletions for Statistics

In this section we derive multiple deletions of a scalar instead of the deletion impact of the regression coefficient vector β . The influence information on the observation of β can be reserved as a form of linear combination between covariates and the regression coefficients. We consider the estimated linear predictor $\eta_i = \mathbf{x}_i^T \hat{\beta}$ and compute the deletion statistics

$$\begin{aligned} \text{DFFIT}_i^{(J)} &= \hat{\eta}_i^1 - \hat{\eta}_i^{(J)} \\ &= v_i^{-\frac{1}{2}} \mathbf{z}_i^T (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}_J^T (\mathbf{I} - \mathbf{H}_J^*)^{-1} \mathbf{e}_J + \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}_J^T (\mathbf{I} - \mathbf{H}_J)^{-1} \mathbf{e}_J. \end{aligned} \tag{3.1}$$

A large value of $\text{DFFIT}_i^{(J)}$ implies that the observation i has large impact on the regression coefficient without observations J in the sense of the regression coefficient vector rather than each components of the vector. For the final iterated estimate instead of the initial estimate we get the statistic DFFIT_i without the index set J by the first term of (3.1).

Next we considered a diagnostic which is a scalar for the regression coefficient vector. Cook (1977) proposed Cook's distance, $(\hat{\beta}^{(j)} - \hat{\beta})^T \mathbf{X} \mathbf{X} (\hat{\beta}^{(j)} - \hat{\beta}) / ps^2$ in linear regression. For logistic regressions the change in likelihood gives Cook's distance as the scaled likelihood difference

$$\text{LD}^{(j)} = \frac{2 \left\{ L^{(j)}(\hat{\beta}^{(j)}) - L(\hat{\beta}^1) \right\}}{p}, \tag{3.2}$$

where

$$L^{(j)}(\hat{\beta}^{(j)}) = \sum_{i=1, i \notin J}^n \left\{ y_i \mathbf{x}_i^T \hat{\beta}^{(j)} - \ln(1 + e^{\mathbf{x}_i^T \hat{\beta}^{(j)}}) \right\}.$$

The definition of P_i yields

$$L^{(j)}(\hat{\beta}^{(j)}) = \sum_{i \notin J}^n \sum_{k=0}^1 I(y_i = k) \ln \hat{P}^{(j)}(y_i = k),$$

where $I(\cdot)$ denotes the indicator function and $\hat{P}^{(j)}(y_i = 1) = \hat{P}_i^{(j)} = e^{\mathbf{x}_i^T \hat{\beta}^{(j)}} / (1 + e^{\mathbf{x}_i^T \hat{\beta}^{(j)}})$, $\hat{P}^{(j)}(y_i = 0) = 1 - \hat{P}_i^{(j)}$ and they are followed by (2.8). Also we have the conditional deletions

$$\hat{P}^{K(j)}(y_i = 1) = \hat{P}_i^{K(j)} = \frac{e^{\mathbf{x}_i^T \hat{\beta}^{1K(j)}}}{1 + e^{\mathbf{x}_i^T \hat{\beta}^{1K(j)}},$$

where $\hat{\beta}^{1K(j)}$ is followed by (2.9).

Then (3.2) becomes

$$\text{LD}^{(j)} = 2 \sum_{i \notin J}^n \sum_{k=0}^1 I(y_i = k) \left\{ \ln \frac{\hat{P}^{(j)}(y_i = k)}{\hat{P}(y_i = k)} \right\} / p. \tag{3.3}$$

We have the conditional deletions $\text{LD}^{K(j)}$

$$\text{LD}^{K(j)} = \frac{2 \left\{ L^{(K,j)}(\hat{\beta}^{1(j,K)}) - L^{(K)}(\hat{\beta}^{1(j)}) \right\}}{p}.$$

Another statistic to measure the impact of the observations is deviance which can be defined as $D = 2(L(y) - L(\hat{\beta}))$. It can be a statistic for goodness of fit of a model. A substantial decrease in the deviance after the deletion of the index set J implies that the observations are misfits (Roy and Guria, 2008). In this case $Y = 1$ or $Y = 0$, the deviance becomes

$$D = -2 \sum_{i=1}^n \left[\hat{P}_i \ln \frac{\hat{P}_i}{1 - \hat{P}_i} + \ln(1 - \hat{P}_i) \right].$$

See page 30 of Faraway (2006). And we have the deviance without the index set J

$$D^{(J)} = -2 \sum_{i \notin J} \left[\hat{P}_i^{(J)} \ln \frac{\hat{P}_i^{(J)}}{1 - \hat{P}_i^{(J)}} + \ln(1 - \hat{P}_i^{(J)}) \right].$$

Thus we have

$$\begin{aligned} \text{DDEV}^{(J)} &= D - D^{(J)} \\ &= D + 2 \sum_{i \notin J} \left[\frac{e^{x_i^T \hat{\beta}^{(J)}}}{1 + e^{x_i^T \hat{\beta}^{(J)}}} - \ln(1 + e^{x_i^T \hat{\beta}^{(J)}}) \right]. \end{aligned} \tag{3.4}$$

The multiple index set J having large $\text{DDEV}^{(J)}$ indicates a set of outliers. Similarly we define the conditional deletions for DDEV by $\text{DDEV}^{K(J)} = D^{(J)} - D^{(J,K)}$.

4. Numerical Example

In this section we illustrate how the multiple deletions given in Sections 2 and 3 provide influence information about the parameters and statistics in logistic regression models. We investigate the influence of observations on the regression coefficients using (2.7), (3.1), (3.3) and (3.4).

Finney (1947) provided the data on the effect of the rate and volume of air inspired on a transient vasco-constriction in the skin of the digits. See Pregibon (1981). The response variable describes whether the occurrence of vasco-constriction ($Y = 1$) or nonoccurrence ($Y = 0$). The predictors are the logarithm of RATE and VOLUME.

We consider the model $\eta = \beta_1 + \beta_2 \log(\text{RATE}) + \beta_3 \log(\text{VOLUME})$. The Newton-Raphson method gives the MLEs of β as

$$\hat{\beta} = (\hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3)^T = (-2.875, 5.179, 4.562)^T.$$

The single deletions are summarized in Pregibon (1981). They concluded that observations 4 and 18 are most influential for the regression parameters.

We conducted regression diagnostics using multiple deletions developed in Sections 2 and 3. Table 1 summarizes single deletions for regression parameters and DFFIT, LD, DDEV based on the fully iterated estimate given in the above paragraph. That is, the matrices \mathbf{Z}, \mathbf{H} are evaluated at the points instead of the initial estimate. The numbers are arranged to the absolute difference between the estimates without corresponding observations and those based on the full data. The number in the parenthesis denotes the corresponding index. Table 1 shows that observations 4 and 18 are most influential for all parameters and statistics. However it does not imply that there are not masking effects or swamping effects. We should conduct multiple deletions on the statistics.

Tables 2 and 3 are summarized on the double deletions and triple deletions for the vasco-constriction data. The most influential observations are 4 and 18. From Table 2 the difference between the largest

Table 1: Single deletions for the vasco-constriction data

β_1	β_2	β_3	DFFIT	LD	DDEV
1.42 (4)	-1.89 (4)	-1.70 (4)	1.27 (4)	0.46 (4)	4.45 (4)
1.26 (18)	-1.58 (18)	-1.52 (18)	0.99 (18)	0.34 (18)	3.97 (18)
-0.34 (19)	0.33 (13)	0.37 (19)	0.45 (31)	0.05 (19)	2.14 (24)
0.31 (29)	0.30 (12)	-0.35 (29)	0.36 (29)	0.05 (29)	1.82 (33)
-0.25 (23)	0.26 (38)	0.31 (6)	0.24 (6)	0.04 (24)	1.55 (19)

Table 2: Double deletions for the vasco-constriction data

β_1	β_2	β_3	LD	DDEV
2.98 (4, 18)	-3.86 (4, 18)	-3.59 (4, 18)	1.99 (4, 18)	7.67 (4, 18)
1.79 (4, 29)	-2.06 (4, 24)	-2.14 (4, 29)	0.66 (4, 29)	6.32 (4, 24)
1.66 (18, 29)	-1.94 (4, 26)	-1.98 (18, 29)	0.55 (18, 29)	6.12 (4, 33)
1.57 (4, 31)	-1.93 (4, 21)	-1.89 (4, 31)	0.51 (4, 31)	5.94 (4, 19)
1.46 (4, 39)	-1.93 (4, 30)	-1.75 (4, 30)	0.47 (3, 39)	5.86 (4, 23)

Table 3: Triple deletions for the vasco-constriction data

β_1	β_2	β_3	LD	DDEV
3.47 (4, 18, 29)	-4.07 (4, 18, 22)	-4.16 (4, 18, 29)	2.42 (4, 18, 29)	9.29 (4, 18, 29)
3.16 (4, 18, 31)	-4.06 (4, 18, 26)	-3.80 (4, 18, 31)	2.05 (4, 18, 31)	9.25 (4, 18, 24)
3.16 (4, 18, 22)	-4.00 (4, 18, 38)	-3.80 (4, 18, 22)	2.05 (4, 18, 39)	9.19 (4, 18, 33)
3.12 (4, 18, 26)	-4.00 (4, 18, 21)	-3.77 (4, 18, 26)	2.03 (4, 18, 26)	8.99 (4, 18, 31)
3.10 (4, 18, 30)	-4.00 (4, 18, 24)	-3.75 (4, 18, 30)	2.02 (4, 18, 21)	8.92 (4, 18, 19)

Table 4: Conditional deletions for the vasco-constriction data when $J = \{4, 18\}$ and $K = 1, \dots, n$

β_1	β_2	β_3	LD	DDEV
0.49 (29)	0.26 (31)	-0.57 (29)	0.43 (29)	1.62 (29)
-0.26 (19)	-0.21 (22)	0.29 (19)	-0.24 (28)	1.57 (24)
-0.19 (23)	-0.20 (26)	0.28 (6)	-0.24 (37)	1.51 (33)
0.18 (31)	0.14 (13)	-0.21 (31)	-0.24 (23)	1.32 (31)
0.18 (22)	-0.14 (38)	-0.21 (22)	-0.23 (8)	1.24 (19)

influence and the second largest influence is somewhat large. It means that observation 4 or 18 impacts influence on the statistics. But the difference between the largest influence and the second largest influence is not large. It means that there may not be swamping or masking effects and only observations 4 and 18 have large influence. In Table 3 we can see the same phenomenon. It is sure that observations 4 and 18 are only influential.

To show the non-existence of swamping effects and masking effects we performed the conditional deletions when $J = \{4, 18\}$ and $K = 1, \dots, 39$. The results are summarized in Table 4. We can see that the values in Table 4 are smaller than those in Table 1. If there are other influential observations except observations 4 and 18, DDEV of Table 4 will have the difference as large as 4.45, that of Table 1. But the largest DDEV of Table 4 is 1.62 which is corresponding to the fifth largest DDEV of Table 1. It implies that there are not large influence on statistics except observations 4 and 18.

We conclude that the vasco-constriction data has only two influential observations 4 and 18. Also there are not swamping effects and masking effects and observations 4 and 18 have individual influence on the statistics. The conclusion can be illustrated by only multiple deletions which are easily obtained from our derivations.

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