

0.1 Case Deletion Diagnostics

Since the pioneering work of Cook in 1977, deletion measures have been applied to many statistical models for identifying influential observations. Case-deletion diagnostics provide a useful tool for identifying influential observations and outliers.

The key to making deletion diagnostics useable is the development of efficient computational formulas, allowing one to obtain the case deletion diagnostics by making use of basic building blocks, computed only once for the full model.

The computation of case deletion diagnostics in the classical model is made simple by the fact that estimates of β and σ^2 , which exclude the i -th observation, can be computed without re-fitting the model.

? describes two type of diagnostics. When the set consists of only one observation, the type is called ‘*observation-diagnostics*’. For multiple observations, Preisser describes the diagnostics as ‘*cluster-deletion*’ diagnostics. When applied to LME models, such update formulas are available only if one assumes that the covariance parameters are not affected by the removal of the observation in question. However, this is rarely a reasonable assumption.

0.2 Case Deletion Diagnostics

CPJ develops case deletion diagnostics, in particular the equivalent of Cook’s distance, for diagnosing influential observations when estimating the fixed effect parameters and variance components.

0.2.1 Deletion Diagnostics

Since the pioneering work of Cook in 1977, deletion measures have been applied to many statistical models for identifying influential observations.

Deletion diagnostics provide a means of assessing the influence of an observation (or groups of observations) on inference on the estimated parameters of LME models.

Data from single individuals, or a small group of subjects may influence non-linear mixed effects model selection. Diagnostics routinely applied in model building may identify such individuals, but these methods are not specifically designed for that purpose and are, therefore, not optimal. We describe two likelihood-based diagnostics for identifying individuals that can influence the choice between two competing models.

Case-deletion diagnostics provide a useful tool for identifying influential observations and outliers.

The computation of case deletion diagnostics in the classical model is made simple by the fact that estimates of β and σ^2 , which exclude the i th observation, can be computed without re-fitting the model. Such update formulas are available in the mixed model only if you assume that the covariance parameters are not affected by the removal of the observation in question. This is rarely a reasonable assumption.

0.2.2 Extension of Diagnostic Methods to LME models

? noted the case deletion diagnostics techniques had not been applied to linear mixed effects models and seeks to develop methodologies in that respect. ? develops these techniques in the context of REML.

? develops case deletion diagnostics, in particular the equivalent of Cook's distance, a well-known metric, for diagnosing influential observations when estimating the fixed effect parameters and variance components. Deletion diagnostics provide a means of

assessing the influence of an observation (or groups of observations) on inference on the estimated parameters of LME models. We shall provide a fuller discussion of Cook’s distance in due course.

? extends several regression diagnostic techniques commonly used in linear regression, such as leverage, infinitesimal influence, case deletion diagnostics, Cook’s distance, and local influence to the linear mixed-effects model. In each case, the proposed new measure has a direct interpretation in terms of the effects on a parameter of interest, and reduces to the familiar linear regression measure when there are no random effects.

The new measures that are proposed by ? are explicitly defined functions and do not require re-estimation of the model, especially for cluster deletion diagnostics. The basis for both the cluster deletion diagnostics and Cook’s distance is a generalization of Miller’s simple update formula for case deletion for linear models. Furthermore ? shows how Pregibon’s infinitesimal case deletion diagnostics is adapted to the linear mixed-effects model.

? proposes two likelihood-based diagnostics for identifying individuals that can influence the choice between two competing models.

0.3 Matrix Notation for Case Deletion

0.3.1 Case deletion notation

For notational simplicity, $\mathbf{A}(i)$ denotes an $n \times m$ matrix \mathbf{A} with the i -th row removed, a_i denotes the i -th row of \mathbf{A} , and a_{ij} denotes the (i, j) -th element of \mathbf{A} .

0.3.2 Partitioning Matrices

Without loss of generality, matrices can be partitioned as if the i -th omitted observation is the first row; i.e. $i = 1$.

0.4 Case Deletion Diagnostics

Christensen, Pearson and Johnson (1992) studied case deletion diagnostics, in particular the equivalent of Cook's distance, for diagnosing influential observations when estimating the fixed effect parameters and variance components.

0.4.1 Case Deletion Diagnostics

Case-deletion diagnostics provide a useful tool for identifying influential observations and outliers.

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0.5 Effects on fitted and predicted values

$$\hat{e}_{i(U)} = y_i - x\hat{\beta}_{(U)} \tag{1}$$

0.5.1 Deletion Diagnostics

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Data from single individuals, or a small group of subjects may influence non-linear mixed effects model selection. Diagnostics routinely applied in model building may identify such individuals, but these methods are not specifically designed for that purpose and are, therefore, not optimal. We describe two likelihood-based diagnostics for identifying individuals that can influence the choice between two competing models.

0.6 Case Deletion Diagnostics for LME models

? remark that linear mixed effects models didn't experience a corresponding growth in the use of deletion diagnostics, adding that ? makes no mention of diagnostics whatsoever.

? describes three propositions that are required for efficient case-deletion in LME models. The first proposition describes how to efficiently update V when the i th element is deleted.

$$V_{[i]}^{-1} = \Lambda_{[i]} - \frac{\lambda\lambda'}{\nu ii} \quad (2)$$

The second of christensen's propositions is the following set of equations, which are variants of the Sherman Woodbury updating formula.

$$X'_{[i]} V_{[i]}^{-1} X_{[i]} = X' V^{-1} X - \frac{\hat{x}_i \hat{x}_i'}{s_i} \quad (3)$$

$$(X'_{[i]} V_{[i]}^{-1} X_{[i]})^{-1} = (X' V^{-1} X)^{-1} + \frac{(X' V^{-1} X)^{-1} \hat{x}_i \hat{x}_i' (X' V^{-1} X)^{-1}}{s_i - \bar{h}_i} \quad (4)$$

$$X'_{[i]} V_{[i]}^{-1} Y_{[i]} = X' V^{-1} Y - \frac{\hat{x}_i \hat{y}_i'}{s_i} \quad (5)$$

In LME models, fitted by either ML or REML, an important overall influence measure is the likelihood distance (?). The procedure requires the calculation of the

full data estimates $\hat{\psi}$ and estimates based on the reduced data set $\hat{\psi}_{(U)}$. The likelihood distance is given by determining

$$LD_{(U)} = 2\{l(\hat{\psi}) - l(\hat{\psi}_{(U)})\} \quad (6)$$

$$RLD_{(U)} = 2\{l_R(\hat{\psi}) - l_R(\hat{\psi}_{(U)})\} \quad (7)$$

0.6.1 Case Deletion Diagnostics for Mixed Models

? notes the case deletion diagnostics techniques have not been applied to linear mixed effects models and seeks to develop methodologies in that respect.

? develops these techniques in the context of REML

0.7 Case Deletion Diagnostics for LME models

? remark that linear mixed effects models didn't experience a corresponding growth in the use of deletion diagnostics, adding that ? makes no mention of diagnostics whatsoever.

? examines the use and implementation of influence measures in LME models.

Influence is understood to be the ability of a single or multiple data points, through their presences or absence in the data, to alter important aspects of the analysis, yield qualitatively different inferences, or violate assumptions of the statistical model (?).

Outliers are the most noteworthy data points in an analysis, and an objective of influence analysis is how influential they are, and the manner in which they are influential.

? describes a simple procedure for quantifying influence. Firstly a model should be fitted to the data, and estimates of the parameters should be obtained. The second step is that either single or multiple data points, specifically outliers, should be omitted

from the analysis, with the original parameter estimates being updated. This is known as ‘leave one out’ ‘leave k out’ analysis. The final step of the procedure is comparing the sets of estimates computed from the entire and reduced data sets to determine whether the absence of observations changed the analysis.

A residual is the difference between an observed quantity and its estimated or predicted value. In LME models, there are two types of residuals, marginal residuals and conditional residuals. A marginal residual is the difference between the observed data and the estimated marginal mean. A conditional residual is the difference between the observed data and the predicted value of the observation. In a model without random effects, both sets of residuals coincide.

? notes that it is not always possible to derive influence statistics necessary for comparing full- and reduced-data parameter estimates. ? offers an procedure to assess the influences for the variance components within the linear model, complementing the existing methods for the fixed components. The essential problem is that there is no useful updating procedures for \hat{V} , or for \hat{V}^{-1} . ? propose an alternative , and computationally inexpensive approach, making use of the ‘delete=replace’ identity.

? considers the effect of ‘leave k out’ calculations on the parameters β and σ^2 , using several key results from ? on partitioned matrices.

In LME models, fitted by either ML or REML, an important overall influence measure is the likelihood distance (?). The procedure requires the calculation of the full data estimates $\hat{\psi}$ and estimates based on the reduced data set $\hat{\psi}_{(U)}$. The likelihood distance is given by determining

$$LD_{(U)} = 2\{l(\hat{\psi}) - l(\hat{\psi}_{(U)})\} \quad (8)$$

$$RLD_{(U)} = 2\{l_R(\hat{\psi}) - l_R(\hat{\psi}_{(U)})\} \quad (9)$$

0.7.1 Case Deletion Diagnostics

? develops case deletion diagnostics, in particular the equivalent of Cook's distance, for diagnosing influential observations when estimating the fixed effect parameters and variance components.

0.7.2 Effects on fitted and predicted values

$$\hat{e}_{i(U)} = y_i - x\hat{\beta}_{(U)} \quad (10)$$

0.7.3 Case Deletion Diagnostics for Mixed Models

? notes the case deletion diagnostics techniques have not been applied to linear mixed effects models and seeks to develop methodologies in that respect.

? develops these techniques in the context of REML

A general method for comparing nested models fit by maximum likelihood is the likelihood ratio test. This test can be used for models fit by REML (restricted maximum likelihood), but only if the fixed terms in the two models are invariant, and both models have been fit by REML. Otherwise, the argument: `method=ML` must be employed (ML = maximum likelihood).

Example of a likelihood ratio test used to compare two models:

```
!"
```

The output will contain a p-value, and this should be used in conjunction with the AIC scores to judge which model is preferred. Lower AIC scores are better.

Generally, likelihood ratio tests should be used to evaluate the significance of terms on the random effects portion of two nested models, and should not be used to determine the significance of the fixed effects.

A simple way to more reliably test for the significance of fixed effects in an LME model is to use conditional F-tests, as implemented with the `simple anova` function.

Example: `" !"`

will give the most reliable test of the fixed effects included in `model1`.

0.7.4 Methods and Measures

The key to making deletion diagnostics useable is the development of efficient computational formulas, allowing one to obtain the case deletion diagnostics by making use of basic building blocks, computed only once for the full model.

`?` lists several established methods of analyzing influence in LME models. These methods include

- Cook's distance for LME models,
- likelihood distance,

- the variance (information) ratio,
- the Cook-Weisberg statistic,
- the Andrews-Prebigon statistic.

0.7.5 Matrix Notation for Case Deletion

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0.7.7 Partitioning Matrices

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0.7.8 Case Deletion Diagnostics

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0.7.10 Case Deletion Diagnostics

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0.7.11 Deletion Diagnostics

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Data from single individuals, or a small group of subjects may influence non-linear mixed effects model selection. Diagnostics routinely applied in model building may identify such individuals, but these methods are not specifically designed for that purpose and are, therefore, not optimal. We describe two likelihood-based diagnostics for identifying individuals that can influence the choice between two competing models.

Case-deletion diagnostics provide a useful tool for identifying influential observations and outliers.

The computation of case deletion diagnostics in the classical model is made simple by the fact that estimates of β and σ^2 , which exclude the i th observation, can be computed without re-fitting the model. Such update formulas are available in the mixed model only if you assume that the covariance parameters are not affected by the removal of the observation in question. This is rarely a reasonable assumption.

0.8 Case Deletion Diagnostics for LME models

Christensen (19XX) describes three propositions that are required for efficient case-deletion in LME models. The first proposition describes how to efficiently update V when the i th element is deleted.

$$V_{[i]}^{-1} = \Lambda_{[i]} - \frac{\lambda\lambda'}{\nu ii} \quad (11)$$

The second of Christensen's propositions is the following set of equations, which are variants of the Sherman Woodbury updating formula.

$$X'_{[i]} V_{[i]}^{-1} X_{[i]} = X' V^{-1} X - \frac{\hat{x}_i \hat{x}_i'}{s_i} \quad (12)$$

$$(X'_{[i]} V_{[i]}^{-1} X_{[i]})^{-1} = (X' V^{-1} X)^{-1} + \frac{(X' V^{-1} X)^{-1} \hat{x}_i \hat{x}_i' (X' V^{-1} X)^{-1}}{s_i - \bar{h}_i} \quad (13)$$

$$X'_{[i]} V_{[i]}^{-1} Y_{[i]} = X' V^{-1} Y - \frac{\hat{x}_i \hat{y}_i'}{s_i} \quad (14)$$

In LME models, fitted by either ML or REML, an important overall influence measure is the likelihood distance (?). The procedure requires the calculation of the full data estimates $\hat{\psi}$ and estimates based on the reduced data set $\hat{\psi}_{(U)}$. The likelihood distance is given by determining

$$LD_{(U)} = 2\{l(\hat{\psi}) - l(\hat{\psi}_{(U)})\} \quad (15)$$

$$RLD_{(U)} = 2\{l_R(\hat{\psi}) - l_R(\hat{\psi}_{(U)})\} \quad (16)$$

0.9 Terminology for Case Deletion diagnostics

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0.12.1 Matrix Notation for Case Deletion

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