# Contents

0.1	Introduction and Classical Approach		
	0.1.1	Diagnostic Methods for OLS models	3
	0.1.2	Cook's 1986 paper on Local Influence	4
	0.1.3	Cook's 1986 paper on Local Influence	4
	0.1.4	Influence Diagnostics: Basic Idea and Statistics	5
	0.1.5	Case Deletion Diagnostics	5
0.2	Termi	nology for Case Deletion diagnostics	6
	0.2.1	Deletion Diagnostics	6
	0.2.2	Influence Diagnostics: Basic Idea and Statistics	7
	0.2.3	What is Influence	8
0.3	Influence analysis for LME Models		
	0.3.1	Influence Analysis for LME Models	9
	0.3.2	Computation Matters	10
	0.3.3	Extension of techniques to LME Models	11
	0.3.4	Analyzing Influence in LME models	11
	0.3.5	Influence in LME models (schab)	12
0.4	Overall Influence and Iterative Influence Analysis		14
	0.4.1	Overall Influence	14
	0.4.2	Iterative Influence Analysis	14
	0.4.3	Iterative Influence Analysis	14
	0.4.4	Iterative and non-iterative influence analysis	15
	0.4.5	Local Influence	16

0.5	A Pro	cedure for Quantifying Influence	17
0.6	Influer	nce Statistics for LME models	18
	0.6.1	Cook's Distance	18
	0.6.2	Variance Ratio	18
	0.6.3	Cook-Weisberg statistic	18
	0.6.4	Zewotir Measures of Influence in LME Models	19
	0.6.5	Andrews-Pregibon statistic	19
	0.6.6	Zewotir Measures of Influence in LME Models	19
	0.6.7	Computation and Notation	21
	0.6.8	Cook's Distance	21
	0.6.9	Information Ratio	22

## 0.1 Introduction and Classical Approach

## 0.1.1 Diagnostic Methods for OLS models

Influence diagnostics are formal techniques allowing for the identification of observations that exert substantial influence on the estimates of fixed effects and variance covariance parameters.

The idea of influence diagnostics for a given observation is to quantify the effect of omission of this observation from the data on the results of the model fit. To this aim, the concept of likelihood displacement is used.

Cook (1977) greatly expanded the study of residuals and influence measures. Cook's Distance, denoted as  $D_{(i)}$ , is a well known diagnostic technique used in classical linear models, used as an overall measure of the combined impact of the *i*th case of all estimated regression coefficients. Cook's key observation was the effects of deleting each observation in turn could be calculated with little additional computation. That is to say,  $D_{(i)}$  can be calculated without fitting a new regression coefficient each time an observation is deleted. Consequently deletion diagnostics have become an integral part of assessing linear models.

The focus of this analysis is related to the estimation of point estimates (i.e. regression coefficients). It must be pointed out that the effect on the precision of estimates is separate from the effect on the point estimates. Data points that have a small Cook's distance, for example, can still greatly affect hypothesis tests and confidence intervals, if their influence on the precision of the estimates is large.

As well as individual observations, Cook's distance can be used to analyse the influence of observations in subset U on a vector of parameter estimates (Cook, 1977).

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

$$\delta_{(U)} = \hat{\beta} - \hat{\beta}_{(U)} \tag{2}$$

### 0.1.2 Cook's 1986 paper on Local Influence

Cook 1986 introduced methods for local influence assessment. These methods provide a powerful tool for examining perturbations in the assumption of a model, particularly the effects of local perturbations of parameters of observations.

Cook (1977) greatly expanded the study of residuals and influence measures. Cook's key observation was the effects of deleting each observation in turn could be calculated with little additional computation. That is to say,  $D_{(i)}$  can be calculated without fitting a new regression coefficient each time an observation is deleted. Consequently deletion diagnostics have become an integral part of assessing linear models. Cook proposed a measure that combines the information of leverage and residual of the observation, now known simply as the Cook's Distance. Cook's Distance, denoted as  $D_{(i)}$ , is a well known diagnostic technique used in classical linear models, used as an overall measure of the combined impact of the i-th case of all estimated regression coefficients.

## 0.1.3 Cook's 1986 paper on Local Influence

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The local-influence approach to influence assessment is quitedifferent from the case deletion approach, comparisons are of interest. Cook (1986) introduces powerful tools for local-influence assessment and examining perturbations in the assumptions of a model. In particular the effect of local perturbations of parameters or observations are examined

The local-influence approach to influence assessment is quite different from the case deletion approach, comparisons are of interest.

## 0.1.4 Influence Diagnostics: Basic Idea and Statistics

The general idea of quantifying the influence of one or more observations relies on computing parameter estimates based on all data points, removing the cases in question from the data, refitting the model, and computing statistics based on the change between full-data and reduced-data estimation.

## 0.1.5 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 Terminology for Case Deletion diagnostics

Preisser (1996) 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.

### 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  $\beta$  and  $\sigma^2$ , which exclude the ith 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.

#### Effects on fitted and predicted values

$$\hat{e}_{i(U)} = y_i - x\hat{\beta}_{(U)} \tag{3}$$

### 0.2.2 Influence Diagnostics: Basic Idea and Statistics

Broadly defined, "influence is understood as the ability of a single or multiple data points, through their presence or absence in the data, to alter important aspects of the analysis, yield qualitatively different inferences, or violate assumptions of the statistical model.

The goal of influence analysis is not primarily to mark data points for deletion so that a better model fit can be achieved for the reduced data, although this might be a result of influence analysis. The goal is rather to determine which cases are influential and the manner in which they are important to the analysis. Outliers, for example, may be the most noteworthy data points in an analysis. They can point to a model breakdown and lead to development of a better model.

The general idea of quantifying the influence of one or more observations relies on computing parameter estimates based on all data points, removing the cases in question from the data, refitting the model, and computing statistics based on the change between full-data and reduced-data estimation.

## 0.2.3 What is Influence

Broadly defined, influence is understood as the ability of a single or multiple data points, through their presence or absence in the data, to alter important aspects of the analysis, yield qualitatively different inferences, or violate assumptions of the statistical model. The goal of influence analysis is not primarily to mark data points for deletion so that a better model fit can be achieved for the reduced data, although this might be a result of influence analysis (Schabenberger, 2004).

## 0.3 Influence analysis for LME Models

Model diagnostic techniques, well established for classical models, have since been adapted for use with linear mixed effects models. Diagnostic techniques for LME models are inevitably more difficult to implement, due to the increased complexity.

Likelihood based estimation methods, such as ML and REML, are sensitive to unusual observations. Influence diagnostics are formal techniques that assess the influence of observations on parameter estimates for  $\beta$  and  $\theta$ . A common technique is to refit the model with an observation or group of observations omitted.

West et al. (2007) examines a group of methods that examine various aspects of influence diagnostics for LME models. For overall influence, the most common approaches are the 'likelihood distance' and the 'restricted likelihood distance'.

### 0.3.1 Influence Analysis for LME Models

The linear mixed effects model is a useful methodology for fitting a wide range of models. However, linear mixed effects models are known to be sensitive to outliers. Christensen et al. (1992) advises that identification of outliers is necessary before conclusions may be drawn from the fitted model.

Standard statistical packages concentrate on calculating and testing parameter estimates without considering the diagnostics of the model. The assessment of the effects of perturbations in data, on the outcome of the analysis, is known as statistical influence analysis. Influence analysis examines the robustness of the model. Influence analysis methodologies have been used extensively in classical linear models, and provided the basis for methodologies for use with LME models. Computationally inexpensive diagnostics tools have been developed to examine the issue of influence (Zewotir and Galpin, 2005).

Studentized residuals, error contrast matrices and the inverse of the response variance covariance matrix are regular components of these tools.

Influence arises at two stages of the LME model. Firstly when V is estimated by

 $\hat{V}$ , and subsequent estimations of the fixed and random regression coefficients  $\beta$  and u, given  $\hat{V}$ .

### 0.3.2 Computation Matters

Key to the implementations of influence diagnostics in the MIXED procedure is the attempt to quantify influence, where possible, by drawing on the basic definitions of the various statistics in the classical linear model.

On occasion, quantification is not possible. Assume, for example, that a data point is removed and the new estimate of the G matrix is not positive definite. This may occur if a variance component estimate now falls on the boundary of the parameter space. Thus, it may not be possible to compute certain influence statistics comparing the full-data and reduced-data parameter estimates. However, knowing that a new singularity was encountered is important qualitative information about the data points influence on the analysis.

### 0.3.3 Extension of techniques to LME Models

Model diagnostic techniques, well established for classical models, have since been adapted for use with linear mixed effects models. Diagnostic techniques for LME models are inevitably more difficult to implement, due to the increased complexity.

Beckman, Nachtsheim and Cook (1987) Beckman et al. (1987) applied the local influence method of Cook (1986) to the analysis of the linear mixed model.

While the concept of influence analysis is straightforward, implementation in mixed models is more complex. Update formulae for fixed effects models are available only when the covariance parameters are assumed to be known.

If the global measure suggests that the points in U are influential, the nature of that influence should be determined. In particular, the points in U can affect the following

- the estimates of fixed effects,
- the estimates of the precision of the fixed effects,
- the estimates of the covariance parameters,
- the estimates of the precision of the covariance parameters,
- fitted and predicted values.

## 0.3.4 Analyzing Influence in LME models

"Influence is defined by Schabenberger (2005) as "the ability of a single or multiple data points, through their presence or absence in the data, to alter important aspects of the analysis, yield qualitatively different inferences, or violate assumptions of the statistical model". The goal of influence analysis is rather to identify influential cases and the manner in which they are important to the analysis. A consequence of this that cases may be to mark data points for deletion so that a better model fit can be achieved for the reduced data (Schabenberger, 2005).

Schabenberger (2005) considers several important aspects of the use and implementation of influence measures in LME models. *schabenberger* notes that it is not always possible to derive influence statistics necessary for comparing full- and reduced-data parameter estimates.

Schabenberger (2005) 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.

## 0.3.5 Influence in LME models (schab)

Likelihood based estimation methods, such as ML and REML, are sensitive to unusual observations. Influence diagnostics are formal techniques that assess the influence of observations on parameter estimates for  $\beta$  and  $\theta$ . A common technique is to refit the model with an observation or group of observations omitted. West et al. (2007) examines a group of methods that examine various aspects of influence diagnostics for LME models. For overall influence, the most common approaches are the 'likelihood distance' and the 'restricted likelihood distance'.

schab 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 (schabenberger).

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. schab 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 of multiple data points, specifically outliers, should be omitted from the analysis, with the original parameter estimates being updated.

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In recent years, mixed models have become invaluable tools in the analysis of experimental and observational data. In these models, more than one term can be subject to random variation. Mixed model technology enables you to analyze complex experimental data with hierarchical random processes, temporal, longitudinal, and spatial data, to name just a few important applications.

schab remarks that the concept of critiquing the model-data agreement applies in mixed models in the same way as in linear fixed-effects models. In fact, because of the more complex model structure, you can argue that model and data diagnostics are even more important. For example, you are not only concerned with capturing the important variables in the model. You are also concerned with "distributing them correctly between the fixed and random components of the model. The mixed model structure presents unique and interesting challenges that prompt us to reexamine the traditional ideas of influence and residual analysis.

# 0.4 Overall Influence and Iterative Influence Analysis

An overall influence statistic measures the change in the objective function being minimized. For example, in OLS regression, the residual sums of squares serves that purpose. In linear mixed models fit by maximum likelihood (ML) or restricted maximum likelihood (REML), an overall influence measure is the likelihood distance [Cook and Weisberg].

#### 0.4.1 Overall Influence

An overall influence statistic measures the change in the objective function being minimized. For example, in OLS regression, the residual sums of squares serves that purpose. In linear mixed models fit by maximum likelihood (ML) or restricted maximum likelihood (REML), an overall influence measure is the likelihood distance [Cook and Weisberg].

## 0.4.2 Iterative Influence Analysis

Schabenberger (2004) describes the choice between iterative influence analysis and noniterative influence analysis.

## 0.4.3 Iterative Influence Analysis

For linear models, the implementation of influence analysis is straightforward. However, for LME models, the process is more complex. Update formulas for the fixed effects are available only when the covariance parameters are assumed to be known. A measure of total influence requires updates of all model parameters. This can only be achieved in general is by omitting observations, then refitting the model.

Schabenberger (2004) describes the choice between iterative influence analysis and non-iterative influence analysis.

## 0.4.4 Iterative and non-iterative influence analysis

Schabenberger (2004) highlights some of the issue regarding implementing mixed model diagnostics.

A measure of total influence requires updates of all model parameters.

however, this doesnt increase the procedures execution time by the same degree.

## 0.4.5 Local Influence

Beckman et al. (1987) applied the local influence method of Cook (1986) to the analysis of the LME model. While the concept of influence analysis is straightforward, implementation in mixed models is more complex. Update formulae for fixed effects models are available only when the covariance parameters are assumed to be known.

If the global measure suggests that the points in U are influential, the nature of that influence should be determined. In particular, the points in U can affect the following

- the estimates of fixed effects,
- the estimates of the precision of the fixed effects,
- the estimates of the covariance parameters,
- the estimates of the precision of the covariance parameters,
- fitted and predicted values.

## 0.5 A Procedure for Quantifying Influence

The basic procedure for quantifying influence is simple:

- 1. Fit the model to the data and obtain estimates of all parameters.
- 2. Remove one or more data points from the analysis and compute updated estimates of model parameters.
- 3. Based on full- and reduced-data estimates, contrast quantities of interest to determine how the absence of the observations changes the analysis.

We use the subscript (U) to denote quantities obtained without the observations in the set U. For example, (U) denotes the fixed-effects *leave-U-out* estimates. Note that the set U can contain multiple observations.

If the global measure suggests that the points in U are influential, you should next determine the nature of that influence. In particular, the points can affect

- the estimates of fixed effects
- the estimates of the precision of the fixed effects
- the estimates of the covariance parameters
- the estimates of the precision of the covariance parameters
- fitted and predicted values

It is important to further decompose the initial finding to determine whether data points are actually troublesome. Simply because they are influential somehow, should not trigger their removal from the analysis or a change in the model. For example, if points primarily affect the precision of the covariance parameters without exerting much influence on the fixed effects, then their presence in the data may not distort hypothesis tests or confidence intervals about  $\beta$ .

## 0.6 Influence Statistics for LME models

Influence statistics can be coarsely grouped by the aspect of estimation that is their primary target:

- overall measures compare changes in objective functions: (restricted) likelihood distance (Cook and Weisberg 1982, Ch. 5.2)
- influence on parameter estimates: Cook's (Cook 1977, 1979), MDFFITS (Belsley, Kuh, and Welsch 1980, p. 32)
- influence on precision of estimates: CovRatio and CovTrace
- influence on fitted and predicted values: PRESS residual, PRESS statistic (Allen 1974), DFFITS (Belsley, Kuh, and Welsch 1980, p. 15)
- outlier properties: internally and externally studentized residuals, leverage

#### 0.6.1 Cook's Distance

• For variance components  $\gamma$ 

Diagnostic tool for variance components

$$C_{\theta i} = (\hat{(\theta)}_{[i]} - \hat{(\theta)})^T \operatorname{cov}(\hat{(\theta)})^{-1} (\hat{(\theta)}_{[i]} - \hat{(\theta)})$$

#### 0.6.2 Variance Ratio

• For fixed effect parameters  $\beta$ .

#### 0.6.3 Cook-Weisberg statistic

• For fixed effect parameters  $\beta$ .

#### 0.6.4 Zewotir Measures of Influence in LME Models

Zewotir and Galpin (2005) describes a number of approaches to model diagnostics, investigating each of the following;

- Variance components
- Fixed effects parameters
- Prediction of the response variable and of random effects
- likelihood function

## 0.6.5 Andrews-Pregibon statistic

• For fixed effect parameters  $\beta$ .

The Andrews-Pregibon statistic  $AP_i$  is a measure of influence based on the volume of the confidence ellipsoid. The larger this statistic is for observation i, the stronger the influence that observation will have on the model fit.

#### 0.6.6 Zewotir Measures of Influence in LME Models

Zewotir describes a number of approaches to model diagnostics, investigating each of the following;

- Variance components
- Fixed effects parameters
- Prediction of the response variable and of random effects
- likelihood function

## Random Effects

A large value for  $CD(u)_i$  indicates that the i-th observation is influential in predicting random effects.

## 0.6.7 Computation and Notation

with V unknown, a standard practice for estimating  $X\beta$  is the estime the variance components  $\sigma_j^2$ , compute an estimate for V and then compute the projector matrix A,  $X\hat{\beta} = AY$ .

Zewotir remarks that D is a block diagonal with the i-th block being uI

#### 0.6.8 Cook's Distance

- For variance components  $\gamma$ :  $CD(\gamma)_i$ ,
- For fixed effect parameters  $\beta$ :  $CD(\beta)_i$ ,
- For random effect parameters u:  $CD(u)_i$ ,
- For linear functions of  $\hat{beta}$ :  $CD(\psi)_i$

Diagnostic tool for variance components

$$C_{\theta i} = (\hat{\theta})_{[i]} - \hat{\theta})^T \operatorname{cov}(\hat{\theta})^{-1} (\hat{\theta})_{[i]} - \hat{\theta})$$

## Random Effects

A large value for  $CD(u)_i$  indicates that the i-th observation is influential in predicting random effects.

## linear functions

 $CD(\psi)_i$  does not have to be calculated unless  $CD(\beta)_i$  is large.

## 0.6.9 Information Ratio

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