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0.0.1 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, 20XX).

0.1 Introduction

In classical linear models model diagnostics have become a required part of any statistical analysis, and the methods are commonly available in statistical packages and standard textbooks on applied regression. However it has been noted by several papers that model diagnostics do not often accompany LME model analyses. Model diagnostic techniques determine whether or not the distributional assumptions are satisfied, and to assess the influence of unusual observations.

0.1.1 What is Influence

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0.1.2 Quantifying Influence

The basic procedure for quantifying influence is simple as follows:

- Fit the model to the data and obtain estimates of all parameters.

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

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.

0.1.3 Model Data Agreement

Schabenberger(20XX) describes the examination of model-data agreement as comprising several elements;

- residual analysis,
- goodness of fit,
- collinearity diagnostics
- influence analysis.

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 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].

0.1.6 Quantifying Influence

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0.1.9 Residual diagnostics

For classical linear models, residual diagnostics are typically implemented as a plot of the observed residuals and the predicted values. A visual inspection for the presence of trends inform the analyst on the validity of distributional assumptions, and to detect outliers and influential observations.

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) 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.

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.

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: Cooks (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

For linear models for uncorrelated data, it is not necessary to refit the model after removing a data point in order to measure the impact of an observation on the model. The change in fixed effect estimates, residuals, residual sums of squares, and the variance-covariance matrix of the fixed effects can be computed based on the fit to the full data alone. By contrast, in mixed models several important complications arise. Data points can affect not only the fixed effects but also the covariance parameter estimates on which the fixed-effects estimates depend.

Furthermore, closed-form expressions for computing the change in important model quantities might not be available. This section provides background material for the various influence diagnostics available with the MIXED procedure. See the section Mixed Models Theory for relevant expressions and definitions. The parameter vector

denotes all unknown parameters in the β and Σ matrix. The observations whose influence is being ascertained are represented by the set S and referred to simply as "the observations in S ." The estimate of a parameter vector, such as β , obtained from all observations except those in the set S is denoted $\hat{\beta}_{-S}$. In case of a matrix Σ , the notation Σ_{-S} represents the matrix with the rows in S removed; these rows are collected in Σ_S . If Σ is symmetric, then notation Σ_{-S} implies removal of rows and columns. The vector y_{-S} comprises the responses of the data points being removed, and Σ_{-S} is the variance-covariance matrix of the remaining observations. When S is a single point, lowercase notation emphasizes that single points are removed, such as $\hat{\beta}_{-i}$.

SUMMARY AND CONCLUSIONS

Standard residual and influence diagnostics for linear models can be extended to linear mixed models. The dependence of fixed-effects solutions on the covariance parameter estimates has important ramifications in perturbation analysis. To gauge the full impact of a set of observations on the analysis, covariance parameters need to be updated, which requires refitting of the model.

The experimental INFLUENCE option of the MODEL statement in the MIXED procedure (SAS 9.1) enables you to perform iterative and noniterative influence analysis for individual observations and sets of observations. The conditional (subject-specific) and marginal (population-averaged) formulations in the linear mixed model enable you to consider conditional residuals that use the estimated BLUPs of the random effects, and marginal residuals which are deviations from the overall mean. Residuals using the BLUPs are useful to diagnose whether the random effects components in the model are specified correctly, marginal residuals are useful to diagnose the fixed-effects components. Both types of residuals are available in SAS 9.1 as an experimental option of the MODEL statement in the MIXED procedure. It is important to note that influence analyses are performed under the assumption that the chosen model is correct. Changing the model structure can alter the conclusions. Many other variance models have been fit to the data presented in the repeated measures example. You need to see the conclusions about which model component is affected in light of the model being fit. For example, modeling these data with a random intercept and random slope for each child or an unstructured covariance matrix will affect your conclusions about which children are influential on the analysis and how this influence manifests itself.

0.1.10 Summary of Paper

Standard residual and influence diagnostics for linear models can be extended to LME models. The dependence of the fixed effects solutions on the covariance parameters has important ramifications on the perturbation analysis. Calculating the studentized

residuals-And influence statistics whereas each software procedure can calculate both conditional and marginal raw residuals, only SAS Proc Mixed is currently the only program that provide studentized residuals Which are preferred for model diagnostics. The conditional Raw residuals are not well suited to detecting outliers as are the studentized conditional residuals. (schabenbege r)

LME are flexible tools for the analysis of clustered and repeated measurement data. LME extend the capabilities of standard linear models by allowing unbalanced and missing data, as long as the missing data are MAR. Structured covariance matrices for both the random effects G and the residuals R . missing at Random.

A conditional residual is the difference between the observed value and the predicted value of a dependent variable- Influence diagnostics are formal techniques that allow the identification observation that heavily influence estimates of parameters. To alleviate the problems with the interpretation of conditional residuals that may have unequal variances, we consider scaling. Residuals obtained in this manner are called studentized residuals.

0.1.11 ITERATIVE VS. NONITERATIVE INFLUENCE ANALYSIS

While the basic idea of influence analysis is straightforward, the implementation in mixed models can be tricky. For example, update formulas for the fixed effects are available only when the covariance parameters are assumed to be known. At most the profiled residual variance can be updated without refitting the model. A measure of total influence requires updates of all model parameters, and the only way that this can be achieved in general is by removing the observations in question and refitting the model. Because this brute-force method involves iterative reestimation of the covariance parameters, it is termed iterative influence analysis. Reliance on closed-form update formulas for the fixed effects without updating the (un-profiled) covariance parameters is termed a noniterative influence analysis. An iterative analysis seems like a costly,

computationally intensive enterprise. If you compute iterative influence diagnostics for all n observations, then a total of $n + 1$ mixed models are fit iteratively. This does not imply, of course, that the procedures execution time increases n -fold. Keep in mind that

- iterative reestimation always starts at the converged full-data estimates. If a data point is not influential, then its removal will have little effect on the objective function and parameter estimates. Within one or two iterations, the process should arrive at the reduced-data estimates.
- if complete reestimation does require many iterations, then this is important information in itself. The likelihood surface has probably changed drastically, and the reduced-data estimates are moving away

from the full-data estimates.

0.1.12 Residual Plots

A residual plot is a graph that shows the residuals on the vertical axis and the independent variable on the horizontal axis. If the points in a residual plot are randomly dispersed around the horizontal axis, a linear regression model is appropriate for the data; otherwise, a non-linear model is more appropriate.

Below the table on the left shows inputs and outputs from a simple linear regression analysis, and the chart on the right displays the residual (e) and independent variable (X) as a residual plot.

x	60	70	80	85	95
y	70	65	70	95	85
y.hat	65.411	71.849	78.288	81.507	87.945
e	4.589	-6.849	-8.288	13.493	-2.945

The residual plot shows a fairly random pattern - the first residual is positive, the next two are negative, the fourth is positive, and the last residual is negative. This random pattern indicates that a linear model provides a decent fit to the data.

Below, the residual plots show three typical patterns. The first plot shows a random pattern, indicating a good fit for a linear model. The other plot patterns are non-random (U-shaped and inverted U), suggesting a better fit for a non-linear model.

0.1.13 Introduction

In statistics and optimization, statistical errors and residuals are two closely related and easily confused measures of the deviation of an observed value of an element of a statistical sample from its "theoretical value". The error (or disturbance) of an observed value is the deviation of the observed value from the (unobservable) true function value, while the residual of an observed value is the difference between the observed value and the estimated function value.

The distinction is most important in regression analysis, where it leads to the concept of studentized residuals.

0.1.14 Residual

Residual (or error) represents unexplained (or residual) variation after fitting a regression model. It is the difference (or left over) between the observed value of the variable and the value suggested by the regression model.

The difference between the observed value of the dependent variable (y) and the predicted value (\hat{y}) is called the residual (e). Each data point has one residual.

Residual = Observed value - Predicted value

$$e = y - \hat{y}$$

Both the sum and the mean of the residuals are equal to zero. That is, $\sum e = 0$ and $\bar{e} = 0$.

0.1.15 Residual

A residual (or fitting error), on the other hand, is an observable estimate of the unobservable statistical error. Consider the previous example with men's heights and suppose we have a random sample of n people. The sample mean could serve as a good estimator of the population mean. Then we have:

The difference between the height of each man in the sample and the unobservable population mean is a statistical error, whereas The difference between the height of each man in the sample and the observable sample mean is a residual. Note that the sum of the residuals within a random sample is necessarily zero, and thus the residuals are necessarily not independent. The statistical errors on the other hand are independent, and their sum within the random sample is almost surely not zero.

Other uses of the word "error" in statistics:

The use of the term "error" as discussed in the sections above is in the sense of a deviation of a value from a hypothetical unobserved value. At least two other uses also occur in statistics, both referring to observable prediction errors:

- Mean square error or mean squared error (abbreviated MSE) and root mean

square error (RMSE) refer to the amount by which the values predicted by an estimator differ from the quantities being estimated (typically outside the sample from which the model was estimated).

- Sum of squared errors, typically abbreviated SSE or SSe, refers to the residual sum of squares (the sum of squared residuals) of a regression; this is the sum of the squares of the deviations of the actual values from the predicted values, within the sample used for estimation. Likewise, the sum of absolute errors (SAE) refers to the sum of the absolute values of the residuals, which is minimized in the least absolute deviations approach to regression.

0.1.16 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.

0.1.17 Standardization

A random variable is said to be standardized if the difference from its mean is scaled by its standard deviation. The residuals above have mean zero but their variance is unknown, it depends on the true values of θ . Standardization is thus not possible in practice.

0.1.18 Studentization

Instead, you can compute studentized residuals by dividing a residual by an estimate of its standard deviation.

0.1.19 Internal and External Studentization

If that estimate is independent of the i -th observation, the process is termed ‘external studentization’. This is usually accomplished by excluding the i -th observation when computing the estimate of its standard error. If the observation contributes to the standard error computation, the residual is said to be internally studentized.

Externally studentized residual require iterative influence analysis or a profiled residuals variance.

0.1.20 Computation

The computation of internally studentized residuals relies on the diagonal entries of $\mathbf{V}(\hat{\theta}) - \mathbf{Q}(\hat{\theta})$, where $\mathbf{Q}(\hat{\theta})$ is computed as

$$\mathbf{Q}(\hat{\theta}) = \mathbf{X}(\mathbf{X}'\mathbf{Q}(\hat{\theta})^{-1}\mathbf{X})\mathbf{X}^{-1}$$

0.1.21 Standardized and studentized residuals

To alleviate the problem caused by inconstant variance, the residuals are scaled (i.e. divided) by their standard deviations. This results in a ‘standardized residual’. Because true standard deviations are frequently unknown, one can instead divide a residual by the estimated standard deviation to obtain the ‘studentized residual’.

0.1.22 Standardization

A random variable is said to be standardized if the difference from its mean is scaled by its standard deviation. The residuals above have mean zero but their variance is unknown, it depends on the true values of θ . Standardization is thus not possible in practice.

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Instead, you can compute studentized residuals by dividing a residual by an estimate of its standard deviation.

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If that estimate is independent of the i –th observation, the process is termed ‘external studentization’. This is usually accomplished by excluding the i –th observation when computing the estimate of its standard error. If the observation contributes to the standard error computation, the residual is said to be internally studentized.

Externally studentized residual require iterative influence analysis or a profiled residuals variance.

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The computation of internally studentized residuals relies on the diagonal entries of $V(\hat{\theta}) - Q(\hat{\theta})$, where $Q(\hat{\theta})$ is computed as

$$\mathbf{Q}(\hat{\theta}) = \mathbf{X}(\mathbf{X}'\mathbf{Q}(\hat{\theta})^{-1}\mathbf{X})\mathbf{X}^{-1}$$

0.1.26 Pearson Residual

Another possible scaled residual is the ‘Pearson residual’, whereby a residual is divided by the standard deviation of the dependent variable. The Pearson residual can be used when the variability of $\hat{\beta}$ is disregarded in the underlying assumptions.

0.1.27 Standardized and studentized residuals

To alleviate the problem caused by inconstant variance, the residuals are scaled (i.e. divided) by their standard deviations. This results in a ‘standardized residual’. Because true standard deviations are frequently unknown, one can instead divide a residual by the estimated standard deviation to obtain the ‘studentized residual’.

0.1.28 Standardization

A random variable is said to be standardized if the difference from its mean is scaled by its standard deviation. The residuals above have mean zero but their variance is unknown, it depends on the true values of θ . Standardization is thus not possible in practice.

0.1.29 Studentization

Instead, you can compute studentized residuals by dividing a residual by an estimate of its standard deviation.

0.1.30 Internal and External Studentization

If that estimate is independent of the i –th observation, the process is termed ‘external studentization’. This is usually accomplished by excluding the i –th observation when computing the estimate of its standard error. If the observation contributes to the standard error computation, the residual is said to be internally studentized.

Externally studentized residual require iterative influence analysis or a profiled residuals variance.

0.1.31 Computation

The computation of internally studentized residuals relies on the diagonal entries of $V(\hat{\theta}) - Q(\hat{\theta})$, where $Q(\hat{\theta})$ is computed as

$$\mathbf{Q}(\hat{\theta}) = \mathbf{X}(\mathbf{X}'\mathbf{Q}(\hat{\theta})^{-1}\mathbf{X})\mathbf{X}^{-1}$$

0.1.32 Pearson Residual

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0.1.34 Covariance Parameters

The unknown variance elements are referred to as the covariance parameters and collected in the vector θ .

0.2 Standardized and studentized residuals

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If that estimate is independent of the i –th observation, the process is termed ‘external studentization’. This is usually accomplished by excluding the i –th observation when computing the estimate of its standard error. If the observation contributes to the standard error computation, the residual is said to be internally studentized.

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$$\mathbf{Q}(\hat{\theta}) = \mathbf{X}(\mathbf{X}'\mathbf{Q}(\hat{\theta})^{-1}\mathbf{X})\mathbf{X}^{-1}$$

0.2.5 Studentization

In statistics, a studentized residual is the quotient resulting from the division of a residual by an estimate of its standard deviation. Typically the standard deviations of residuals in a sample vary greatly from one data point to another even when the errors all have the same standard deviation, particularly in regression analysis; thus it does not make sense to compare residuals at different data points without first studentizing. It is a form of a Student's t-statistic, with the estimate of error varying between points.

This is an important technique in the detection of outliers. It is named in honor of William Sealey Gosset, who wrote under the pseudonym Student, and dividing by an estimate of scale is called studentizing, in analogy with standardizing and normalizing: see Studentization.

0.3 Standardized and studentized residuals

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$$\mathbf{Q}(\hat{\theta}) = \mathbf{X}(\mathbf{X}'\mathbf{Q}(\hat{\theta})^{-1}\mathbf{X})\mathbf{X}^{-1}$$

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0.5.5 Pearson Residual

Another possible scaled residual is the ‘Pearson residual’, whereby a residual is divided by the standard deviation of the dependent variable. The Pearson residual can be used when the variability of $\hat{\beta}$ is disregarded in the underlying assumptions.

0.5.6 Marginal and Conditional Residuals

A marginal residual is the difference between the observed data and the estimated (marginal) mean, $r_{mi} = y_i - x_0'\hat{b}$. A conditional residual is the difference between the observed data and the predicted value of the observation, $r_{ci} = y_i - x_i'\hat{b} - z_i'\hat{\gamma}$.

In linear mixed effects models, diagnostic techniques may consider ‘conditional’ residuals. A conditional residual is the difference between an observed value y_i and the conditional predicted value \hat{y}_i .

$$\epsilon_{i|X_i} = y_i - \hat{y}_i = y_i - (X_i\hat{\beta} + Z_i\hat{\gamma})$$

However, using conditional residuals for diagnostics presents difficulties, as they tend to be correlated and their variances may be different for different subgroups, which can lead to erroneous conclusions.

$$r_{mi} = x_i^T \hat{\beta} \tag{1}$$

0.5.7 Marginal Residuals

$$\begin{aligned} \hat{\beta} &= (X^T R^{-1} X)^{-1} X^T R^{-1} Y \\ &= BY \end{aligned}$$

0.5.8 Marginal and Conditional Residuals

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$$r_{mi} = x_i^T \hat{\beta} \tag{2}$$

0.5.9 Marginal Residuals

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However, using conditional residuals for diagnostics presents difficulties, as they tend to be correlated and their variances may be different for different subgroups, which can lead to erroneous conclusions.

Residuals

Residuals are used to examine model assumptions and to detect outliers and potentially influential data point. The raw residuals r_{mi} and r_{ci} are usually not well suited for these purposes.

- Conditional Residuals r_{ci}
- Marginal Residuals r_{mi}
-

Conditional Residuals

Marginal Residuals

Distinction From Linear Models

- The differences between perturbation and residual analysis in the linear model and the linear mixed model are connected to the important facts that b and b depend on the estimates of the covariance parameters, that b has the form of an (estimated) generalized least squares (GLS) estimator, and that b is a random vector.
- In a mixed model, you can consider the data in a conditional and an unconditional sense. If you imagine a particular realization of the random effects, then you are considering the conditional distribution $Y|b$ —
- If you are interested in quantities averaged over all possible values of the random effects, then you are interested in Y ; this is called the marginal formulation. In a clinical trial, for example, you may be interested in drug efficacy for a particular patient. If random effects vary by patient, that is a conditional problem. If you are interested in the drug efficacy in the population of all patients, you are using a marginal formulation. Correspondingly, there will be conditional and marginal residuals, for example.
- The estimates of the fixed effects depend on the estimates of the covariance parameters. If you are interested in determining the influence of an observation on the analysis, you must determine whether this is influence on the fixed effects for a given value of the covariance parameters, influence on the covariance parameters, or influence on both.
- Mixed models are often used to analyze repeated measures and longitudinal data. The natural experimental or sampling unit in those studies is the entity that is repeatedly observed, rather than each individual repeated observation. For example, you may be analyzing monthly purchase records by customer.

- An influential data point is then not necessarily a single purchase. You are probably more interested in determining the influential customer. This requires that you can measure the influence of sets of observations on the analysis, not just influence of individual observations.
- The computation of case deletion diagnostics in the classical model is made simple by the fact that 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.
- The application of well-known concepts in model-data diagnostics to the mixed model can produce results that are at first counter-intuitive, since our understanding is steeped in the ordinary least squares (OLS) framework. As a consequence, we need to revisit these important concepts, ask whether they are portable to the mixed model, and gain new appreciation for their changed properties. An important example is the ostensibly simple concept of leverage.
- The definition of leverage adopted by the MIXED procedure can, in some instances, produce negative values, which are mathematically impossible in OLS. Other measures that have been proposed may be non-negative, but trade other advantages. Another example are properties of residuals. While OLS residuals necessarily sum to zero in any model (with intercept), this not true of the residuals in many mixed models.

0.6 Residual diagnostics

For classical linear models, residual diagnostics are typically implemented as a plot of the observed residuals and the predicted values. A visual inspection for the presence of trends inform the analyst on the validity of distributional assumptions, and to detect outliers and influential observations.

0.6.1 Residuals diagnostics in mixed models

The marginal and conditional means in the linear mixed model are $E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta}$ and $E[\mathbf{Y}|\mathbf{u}] = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u}$, respectively.

A residual is the difference between an observed quantity and its estimated or predicted value. In the mixed model you can distinguish marginal residuals r_m and conditional residuals r_c .

0.6.2 Marginal and Conditional Residuals

A marginal residual is the difference between the observed data and the estimated (marginal) mean, $r_{mi} = y_i - x_0'\hat{b}$ A conditional residual is the difference between the observed data and the predicted value of the observation, $r_{ci} = y_i - x_i'\hat{b} - z_i'\hat{\gamma}$

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$$\epsilon_{i|} = y_i - \hat{y}_i = y_i - (X_i\hat{\beta} + Z_i\hat{\gamma})$$

However, using conditional residuals for diagnostics presents difficulties, as they tend to be correlated and their variances may be different for different subgroups, which can lead to erroneous conclusions.

$$r_{mi} = x_i^T \hat{\beta} \tag{3}$$

0.6.3 Marginal Residuals

$$\begin{aligned}\hat{\beta} &= (X^T R^{-1} X)^{-1} X^T R^{-1} Y \\ &= BY\end{aligned}$$

0.7 Conditional and Marginal Residuals

Conditional residuals include contributions from both fixed and random effects, whereas marginal residuals include contribution from only fixed effects.

Suppose the linear mixed-effects model `lme` has an $n \times p$ fixed-effects design matrix \mathbf{X} and an $n \times q$ random-effects design matrix \mathbf{Z} .

Also, suppose the p -by-1 estimated fixed-effects vector is $\hat{\beta}$, and the q -by-1 estimated best linear unbiased predictor (BLUP) vector of random effects is \hat{b} . The fitted conditional response is

$$\hat{y}_{Cond} = X\hat{\beta} + Z\hat{b}$$

and the fitted marginal response is

$$\hat{y}_{Mar} = X\hat{\beta}$$

residuals can return three types of residuals:

- raw,
- Pearson, and
- standardized.

For any type, you can compute the conditional or the marginal residuals. For example, the conditional raw residual is

$$r_{Cond} = y - X\hat{\beta} - Z\hat{b}$$

and the marginal raw residual is

$$r_{Mar} = y - X\hat{\beta}$$

Cox and Snell (1968, JRSS-B): general definition of residuals for models with single source of variability Hilden-Minton (1995, PhD thesis UCLA), Verbeke and Lesaffre (1997, CSDA) or Pinheiro and Bates (2000, Springer): extension to define three types of residuals that accommodate the extra source of variability present in linear mixed models, namely:

- i) Marginal residuals,
predictors of marginal errors,
- ii) Conditional residuals,

$$be = yX\hat{\beta}Zbb = \hat{\sigma}Q\hat{y}$$

, predictors of conditional errors

$$e = yE[y|b] = yX\beta Zb$$

- iii) BLUP, Zbb , predictors of random effects,

$$Zb = E[y|b]E[y]$$

Marginal residuals

$$y - X\beta = Z\eta + \epsilon$$

- Should be mean 0, but may show grouping structure
- May not be homoskedastic.
- Good for checking fixed effects, just like linear regr.

Conditional residuals

$$y - X\beta - Z\eta = \epsilon$$

- Should be mean zero with no grouping structure
- Should be homoscedastic.
- Good for checking normality of outliers

Random effects

$$y - X\beta - \epsilon = Z\eta$$

- Should be mean zero with no grouping structure
- May not be be homoscedastic.

0.8 Residual diagnostics

For classical linear models, residual diagnostics are typically implemented as a plot of the observed residuals and the predicted values. A visual inspection for the presence of trends inform the analyst on the validity of distributional assumptions, and to detect outliers and influential observations.

0.8.1 Residuals diagnostics in mixed models

The marginal and conditional means in the linear mixed model are $E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta}$ and $E[\mathbf{Y}|\mathbf{u}] = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u}$, respectively.

A residual is the difference between an observed quantity and its estimated or predicted value. In the mixed model you can distinguish marginal residuals r_m and conditional residuals r_c .

0.8.2 Marginal and Conditional Residuals

A marginal residual is the difference between the observed data and the estimated (marginal) mean, $r_{mi} = y_i - x'_0\hat{b}$. A conditional residual is the difference between the observed data and the predicted value of the observation, $r_{ci} = y_i - x'_i\hat{b} - z'_i\hat{\gamma}$.

In linear mixed effects models, diagnostic techniques may consider ‘conditional’ residuals. A conditional residual is the difference between an observed value y_i and the conditional predicted value \hat{y}_i .

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However, using conditional residuals for diagnostics presents difficulties, as they tend to be correlated and their variances may be different for different subgroups, which can lead to erroneous conclusions.

$$r_{mi} = x_i^T \hat{\beta} \tag{4}$$

0.8.3 Marginal Residuals

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0.8.4 Confounded Residuals

Hilden-Minton (1995, PhD thesis, UCLA): residual is pure for a specific type of error if it depends only on the fixed components and on the error that it is supposed to predict. Residuals that depend on other types of errors are called *confounded residuals*.

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.

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.

0.9 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.

0.9.1 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.

0.10 Effects on fitted and predicted values

$$\hat{e}_{i(U)} = y_i - x\hat{\beta}_{(U)} \tag{5}$$

0.10.1 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. ? 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.

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0.10.4 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.

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0.10.6 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

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0.10.8 Residuals diagnostics in mixed models

The marginal and conditional means in the linear mixed model are $E[\mathbf{Y}] = \mathbf{X}\boldsymbol{\beta}$ and $E[\mathbf{Y}|\mathbf{u}] = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{u}$, respectively.

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0.10.9 Standardized and studentized residuals

To alleviate the problem caused by inconstant variance, the residuals are scaled (i.e. divided) by their standard deviations. This results in a ‘standardized residual’. Because true standard deviations are frequently unknown, one can instead divide a residual by the estimated standard deviation to obtain the ‘studentized residual’.

0.10.10 Residual Analysis for Linear Models, LME models and GLMs

Keywords:

- Residuals (*Beginners*),
- Testing the Assumption of Normality (*Beginners*)
- Diagnostic Plots with the `plot` function
- Cook’s Distance
- DFFits and DFBeta
- Standardized and Studentized Residuals
- Influence Leverage and Outlierness

0.10.11 Identifying outliers with a LME model object

The process is slightly different than with standard LME model objects, since the *influence* function does not work on lme model objects. Given *mod.lme*, we can use the plot function to identify outliers.

0.10.12 Diagnostics for Random Effects

Empirical best linear unbiased predictors EBLUPS provide the a useful way of diagnosing random effects.

EBLUPs are also known as “shrinkage estimators” because they tend to be smaller than the estimated effects would be if they were computed by treating a random factor as if it was fixed (West et al)

0.10.13 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.

0.10.14 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

0.10.15 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.

Zewotir and Galpin (2005) lists several established methods of analyzing influence in LME models. These methods include

- Cook's distance for LME models,
- likelihood distance,
- the variance (information) ration,
- the Cook-Weisberg statistic,
- the Andrews-Prebigon statistic.

0.10.16 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.

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

0.11 Leverage and Influence

0.11.1 Influence

The influence of an observation can be thought of in terms of how much the predicted scores for other observations would differ if the observation in question were not included.

Cook's D is a good measure of the influence of an observation and is proportional to the sum of the squared differences between predictions made with all observations in the analysis and predictions made leaving out the observation in question. If the predictions are the same with or without the observation in question, then the observation has no influence on the regression model. If the predictions differ greatly when the observation is not included in the analysis, then the observation is influential.

0.11.2 Interpreting Cook's Distance

A common rule of thumb is that an observation with a value of Cook's D over 1.0 has too much influence. As with all rules of thumb, this rule should be applied judiciously and not thoughtlessly.

0.11.3 Leverage

The leverage of an observation is based on how much the observation's value on the predictor variable differs from the mean of the predictor variable. The greater an observation's leverage, the more potential it has to be an influential observation.

For example, an observation with a value equal to the mean on the predictor variable has no influence on the slope of the regression line regardless of its value on the criterion

variable. On the other hand, an observation that is extreme on the predictor variable has the potential to affect the slope greatly.

Calculation of Leverage (h)

The first step is to standardize the predictor variable so that it has a mean of 0 and a standard deviation of 1. Then, the leverage (h) is computed by squaring the observation's value on the standardized predictor variable, adding 1, and dividing by the number of observations.

0.11.4 Summary of Influence Statistics

- **Studentized Residuals** Residuals divided by their estimated standard errors (like t-statistics). Observations with values larger than 3 in absolute value are considered outliers.
- **Leverage Values (Hat Diag)** Measure of how far an observation is from the others in terms of the levels of the independent variables (not the dependent variable). Observations with values larger than $2(k + 1)/n$ are considered to be potentially highly influential, where k is the number of predictors and n is the sample size.
- **DFFITS** Measure of how much an observation has effected its fitted value from the regression model. Values larger than $2\sqrt{(k + 1)/n}$ in absolute value are considered highly influential.
- **DFBETAS** Measure of how much an observation has effected the estimate of a regression coefficient (there is one DFBETA for each regression coefficient, including the intercept). Values larger than $2/\sqrt{n}$ in absolute value are considered highly influential.

The measure that measures how much impact each observation has on a particular predictor is DFBETAs The DFBETA for a predictor and for a particular

observation is the difference between the regression coefficient calculated for all of the data and the regression coefficient calculated with the observation deleted, scaled by the standard error calculated with the observation deleted.

- **Cooks D** Measure of aggregate impact of each observation on the group of regression coefficients, as well as the group of fitted values. Values larger than $4/n$ are considered highly influential.

0.12 Influence analysis

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 β and θ . 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’.

0.13 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.

0.13.1 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.

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0.14.1 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.

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

0.14.2 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].

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

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

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- outlier properties: internally and externally studentized residuals, leverage

0.14.3 Quantifying Influence

The basic procedure for quantifying influence is simple as follows:

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

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.

0.15 Measures 2

0.15.1 Cook's Distance

- For variance components γ

Diagnostic tool for variance components

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

0.15.2 Variance Ratio

- For fixed effect parameters β .

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0.15.4 Cook-Weisberg statistic

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0.15.5 Andrews-Pregibon statistic

- For fixed effect parameters β .

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.

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Diagnostic tool for variance components

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0.17 Zewotir Measures of Influence in LME Models

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

- Variance components
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- 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.

linear functions

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

0.17.1 Information Ratio

0.18 Computation and Notation

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

Zewotir remarks that \mathbf{D} is a block diagonal with the i -th block being $u\mathbf{I}$

0.19 Measures of Influence

The impact of an observation on a regression fitting can be determined by the difference between the estimated regression coefficient of a model with all observations and the estimated coefficient when the particular observation is deleted. The measure DFBETA is the studentized value of this difference.

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 $\boldsymbol{\beta}$ and u , given \hat{V} .

0.19.1 DFFITS

DFFITS is a statistical measure designed to show how influential an observation is in a statistical model. It is closely related to the studentized residual.

$$DFFITS = \frac{\hat{y}_i - \widehat{y}_{i(k)}}{s_{(k)}\sqrt{h_{ii}}}$$

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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 β and u , given \hat{V} .

0.20.1 DFBETA

$$DFBETA_a = \hat{\beta} - \hat{\beta}_{(a)} \quad (6)$$

$$= B(Y - Y_{\bar{a}}) \quad (7)$$

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0.20.3 PRESS

The prediction residual sum of squares (PRESS) is an value associated with this calculation. When fitting linear models, PRESS can be used as a criterion for model selection, with smaller values indicating better model fits.

$$PRESS = \sum (y - y^{(k)})^2 \quad (8)$$

- $e_{-Q} = y_Q - x_Q \hat{\beta}^{-Q}$
- $PRESS_{(U)} = y_i - x_i \hat{\beta}_{(U)}$

0.20.4 DFBETA

$$DFBETA_a = \hat{\beta} - \hat{\beta}_{(a)} \quad (9)$$

$$= B(Y - Y_{\bar{a}}) \quad (10)$$

0.20.5 Influential Observations : DFBeta and DFBetas

Cook's distance refers to how far, on average, predicted y-values will move if the observation in question is dropped from the data set. dfbeta refers to how much a parameter estimate changes if the observation in question is dropped from the data set. Note that with k covariates, there will be k+1 dfbetas (the intercept, β_0 , and 1 β for each covariate). Cook's distance is presumably more important to you if you are doing predictive modeling, whereas dfbeta is more important in explanatory modeling.

schabenberger 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.

schabenberger 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’ or ‘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.

schabenberger notes that it is not always possible to derive influence statistics necessary for comparing full- and reduced-data parameter estimates.

Abstract

This paper reviews the use of diagnostic measures for LME models in SAS. This text has been widely cited by texts that don't deal with SAS implementations.

Schabenberger: Summary and Conclusions

- Standard residual and influence diagnostics for linear models can be extended to linear mixed models. The dependence of fixed-effects solutions on the covariance parameter estimates has important ramifications in perturbation analysis.
- To gauge the full impact of a set of observations on the analysis, covariance parameters need to be updated, which requires refitting of the model.
- The experimental INFLUENCE option of the MODEL statement in the MIXED procedure (SAS 9.1) enables you to perform iterative and noniterative influence analysis for individual observations and sets of observations.
- The conditional (subject-specific) and marginal (population-averaged) formulations in the linear mixed model enable you to consider conditional residuals that use the estimated BLUPs of the random effects, and marginal residuals which are deviations from the overall mean.
- Residuals using the BLUPs are useful to diagnose whether the random effects components in the model are specified correctly, marginal residuals are useful to diagnose the fixed-effects components.
- Both types of residuals are available in SAS 9.1 as an experimental option of the MODEL statement in the MIXED procedure.
- It is important to note that influence analyses are performed under the assumption that the chosen model is correct. Changing the model structure can alter the conclusions. Many other variance models have been fit to the data presented in the repeated measures example. You need to see the conclusions about which model component is affected in light of the model being fit.
- For example, modeling these data with a random intercept and random slope for each child or an unstructured covariance matrix will affect your conclusions about which children are influential on the analysis and how this influence manifests itself.

0.21 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.

0.21.1 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.

0.22 Efficient Updating Theorem

Zewotir and Galpin (2005) describes the basic theorem of efficient updating.

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$$m_i = \frac{1}{c_{ii}}$$

0.23 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
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1.2.1 Cook's Distance

- For variance components γ : $CD(\gamma)_i$,

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1.2.2 Information Ratio

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

? remarks that \mathbf{D} is a block diagonal with the i -th block being $u\mathbf{I}$

1.4 Haslett's Analysis

For fixed effect linear models with correlated error structure Haslett (1999) showed that the effects on the fixed effects estimate of deleting each observation in turn could be cheaply computed from the fixed effects model predicted residuals.

A general theory is presented for residuals from the general linear model with correlated errors. It is demonstrated that there are two fundamental types of residual associated with this model, referred to here as the marginal and the conditional residual.

These measure respectively the distance to the global aspects of the model as represented by the expected value and the local aspects as represented by the conditional expected value.

These residuals may be multivariate.

Haslett and Hayes (1998) develop some important dualities which have simple implications for diagnostics.

1.5 Demidenko's I Influence

The concept of I Influence is generalized to the non linear regression model.

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Diagnostics for repeated measurements in LME models.

Most currently available methods for detecting discordant subjects and observations in linear mixed effects model fits adapt existing methods for single-level regression data. The most common methods are generalizations of deletion-based approaches, primarily Cook's distance. This article describes the limitations of modifications to Cook's distance and local influence, and suggests a new nondeletion subject-level method, studentized residual sum of squares (TRSS) plots. We also suggest a new observation-level deletion method that detects discordant observations as an application of TRSS plots.

TRSS Plots

The proposed method provides greater information on repeated measurements by utilizing revised residuals and efficiently evaluating the effect of discordant subjects and observations on the estimation of parameters including variance components. We compare the performance of the proposed methods with current methods by using the orthodontic growth data: a longitudinal dataset with 27 subjects each observed four times. TRSS plots successfully identified discordant subjects that were missed by modified Cook's distance methods and the local influence approach.

- Diagnostics for repeated measurements in linear mixed effects models
- Most currently available methods for detecting discordant subjects and observations in linear mixed effects model fits adapt existing methods for single-level regression data.
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- We also suggest a new observation-level deletion method that detects discordant observations as an application of TRSS plots. The proposed method provides greater information on repeated measurements by utilizing revised residuals and efficiently evaluating the effect of discordant subjects and observations on the estimation of parameters including variance components.
- We compare the performance of the proposed methods with current methods by using the orthodontic growth data: a longitudinal dataset with 27 subjects each observed four times.
- TRSS plots successfully identified discordant subjects that were missed by modified Cook's distance methods and the local influence approach.

3.5.1 Case Deletion Diagnostics

Christensen et al. (1992) 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.

3.5.2 Effects on fitted and predicted values

$$\hat{e}_{i(U)} = y_i - x\hat{\beta}_{(U)} \quad (3.1)$$

3.5.3 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`.

3.5.4 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.

Zewotir and Galpin (2005) lists several established methods of analyzing influence in LME models. These methods include

- Cook’s distance for LME models,
- likelihood distance,
- the variance (information) ration,
- the Cook-Weisberg statistic,

- the Andrews-Prebigon statistic.

3.5.5 Matrix Notation for Case Deletion

3.5.6 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} .

3.5.7 Partitioning Matrices

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

3.5.8 Case Deletion Diagnostics

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3.5.10 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.

3.5.11 Case Deletion Diagnostics

Christensen et al. (1992) 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.

3.5.12 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.

3.5.13 Terminology for Case Deletion diagnostics

Preisser(19XX) 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.

3.5.14 Cook's Distance

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3.5.15 Information Ratio

Cook's Distance

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 computed without undue additional computational expense. Consequently deletion diagnostics have become an integral part of assessing linear models.

Cook (1986) gave a completely general method for assessing influence of local departures from assumptions in statistical models.

Cook's Distance

In classical linear regression, a commonly used measure of influence is Cook's distance. It is used as a measure of influence on the regression coefficients.

Cook's Distance

Cook's Distance (D_i) is an overall measure of the combined impact of the i th case on all estimated regression coefficients. It uses the same structure for measuring the combined impact of the differences in the estimated regression coefficients when the i -th case is deleted.

Importantly, $D_{(i)}$ can be calculated without fitting a new regression coefficient each time an observation is deleted.

3.5.16 Cook's Distance

Cook's D statistics (i.e. colloquially Cook's Distance) is a measure of the influence of observations in subset U on a vector of parameter estimates.

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

If V is known, Cook's D can be calibrated according to a chi-square distribution with degrees of freedom equal to the rank of \mathbf{X} .

For LME models, Cook's distance can be extended to model influence diagnostics by defining.

It is also desirable to measure the influence of the case deletions on the covariance matrix of $\hat{\beta}$.

3.6 Cook's Distance for LMEs

Diagnostic methods for fixed effects are generally analogues of methods used in classical linear models. Diagnostic methods for variance components are based on ‘one-step’ methods. Cook (1986) gives a completely general method for assessing the influence of local departures from assumptions in statistical models.

For fixed effects parameter estimates in LME models, the Cook's distance can be extended to measure influence on these fixed effects.

$$CD_i(\beta) = \frac{(c_{ii} - r_{ii}) \times t_i^2}{r_{ii} \times p}$$

For random effect estimates, the Cook's distance is

$$CD_i(b) = g'_{(i)}(I_r + \text{var}(\hat{b})D)^{-2}\text{var}(\hat{b})g_{(i)}.$$

Large values for Cook's distance indicate observations for special attention.

3.7 Cook's Distance for LMEs

Diagnostic methods for fixed effects are generally analogues of methods used in classical linear models. Diagnostic methods for variance components are based on ‘one-step’ methods. *cook86* gives a completely general method for assessing the influence of local departures from assumptions in statistical models.

3.7.1 Cook's Distance

Cooks Distance (D_i) is an overall measure of the combined impact of the i th case of all estimated regression coefficients. It uses the same structure for measuring the combined impact of the differences in the estimated regression coefficients when the k th case is deleted. $D_{(k)}$ can be calculated without fitting a new regression coefficient each time an observation is deleted.

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 computed

without undue additional computational expense. Consequently deletion diagnostics have become an integral part of assessing linear models.

Cook's Distance is a well known diagnostic technique used in classical linear models, extended to LME models. For LME models, two formulations exist; a Cook's distance that examines the change in fixed fixed parameter estimates, and another that examines the change in random effects parameter estimates. The outcome of either Cook's distance is a scaled change in either β or θ .

Cook's D statistics (i.e. colloquially Cook's Distance) is a measure of the influence of observations in subset U on a vector of parameter estimates (Cook, 1977).

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

If V is known, Cook's D can be calibrated according to a chi-square distribution with degrees of freedom equal to the rank of \mathbf{X} (?).

In classical linear regression, a commonly used measure of influence is Cook's distance. It is used as a measure of influence on the regression coefficients.

For linear mixed effects models, Cook's distance can be extended to model influence diagnostics by defining.

$$C_{\beta i} = \frac{(\hat{\beta} - \hat{\beta}_{[i]})^T (\mathbf{X}' \mathbf{V}^{-1} \mathbf{X}) (\hat{\beta} - \hat{\beta}_{[i]})}{p}$$

It is also desirable to measure the influence of the case deletions on the covariance matrix of $\hat{\beta}$.

For fixed effects parameter estimates in LME models, the Cook's distance can be extended to measure influence on these fixed effects.

$$CD_i(\beta) = \frac{(c_{ii} - r_{ii}) \times t_i^2}{r_{ii} \times p}$$

For random effect estimates, the Cook's distance is

$$CD_i(b) = g'_{(i)} (I_r + \text{var}(\hat{b}) D)^{-2} \text{var}(\hat{b}) g_{(i)}.$$

Large values for Cook's distance indicate observations for special attention.

3.7.2 Change in the precision of estimates

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.

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3.8 Cook's Distance

3.8.1 Cook's Distance

Cooks Distance (D_i) is an overall measure of the combined impact of the i th case of all estimated regression coefficients. It uses the same structure for measuring the combined impact of the differences in the estimated regression coefficients when the k th case is deleted. $D_{(k)}$ can be calculated without fitting a new regression coefficient each time an observation is deleted.

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It is also desirable to measure the influence of the case deletions on the covariance matrix of $\hat{\beta}$.

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

If V is known, Cook's D can be calibrated according to a chi-square distribution with degrees of freedom equal to the rank of \mathbf{X} (?).

3.8.4 Cook's Distance

In statistics, Cook's Distance or Cook's D is a commonly used estimate of the influence of a data point when performing least squares regression analysis.[1] In a practical ordinary least squares analysis, Cook's distance can be used in several ways: to indicate data points that are particularly worth checking for validity; to indicate regions of the design space where it would be good to be able to obtain more data points. It is named after the American statistician R. Dennis Cook, who introduced the concept in 1977.

Interpretation

Specifically D_i can be interpreted as the distance one's estimates move within the confidence ellipsoid that represents a region of plausible values for the parameters.[clarification needed] This is shown by an alternative but equivalent representation of Cook's distance in terms of changes to the estimates of the regression parameters between the cases where the particular observation is either included or excluded from the regression analysis.

3.8.5 Cook's Distance

Some texts tell you that points for which Cook's distance is higher than 1 are to be considered as influential. Other texts give you a threshold of $4/N$ or $4/(Nk1)$, where N is the number of observations and k the number of explanatory variables. In your case the latter formula should yield a threshold around 0.1 .

John Fox (1), in his booklet on regression diagnostics is rather cautious when it comes to giving numerical thresholds. He advises the use of graphics and to examine in closer details the points with "values of D that are substantially larger than the rest". According to Fox, thresholds should just be used to enhance graphical displays.

In your case the observations 7 and 16 could be considered as influential. Well, I would at least have a closer look at them. The observation 29 is not substantially different from a couple of other observations.

(1) Fox, John. (1991). Regression Diagnostics: An Introduction. Sage Publications.

3.9 Influence analysis

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 β and θ . 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'.

3.9.1 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.

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

3.9.2 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].

3.10 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.

3.11 Cook's Distance

3.11.1 Cook's Distance

Cooks Distance (D_i) is an overall measure of the combined impact of the i th case of all estimated regression coefficients. It uses the same structure for measuring the combined impact of the differences in the estimated regression coefficients when the k th case is deleted. $D_{(k)}$ can be calculated without fitting a new regression coefficient each time an observation is deleted.

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 computed without undue additional computational expense. Consequently deletion diagnostics have become an integral part of assessing linear models.

Cook's Distance is a well known diagnostic technique used in classical linear models, extended to LME models. For LME models, two formulations exist; a Cook's distance that examines the change in fixed fixed parameter estimates, and another that examines the change in random effects parameter estimates. The outcome of either Cook's distance is a scaled change in either β or θ .

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Cook's D statistics (i.e. colloquially Cook's Distance) is a measure of the influence of observations in subset U on a vector of parameter estimates (Cook, 1977).

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

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3.11.3 Cook's Distance

In classical linear regression, a commonly used measure of influence is Cook's distance. It is used as a measure of influence on the regression coefficients.

For linear mixed effects models, Cook's distance can be extended to model influence diagnostics by defining.

$$C_{\beta i} = \frac{(\hat{\beta} - \hat{\beta}_{[i]})^T (\mathbf{X}' \mathbf{V}^{-1} \mathbf{X}) (\hat{\beta} - \hat{\beta}_{[i]})}{p}$$

It is also desirable to measure the influence of the case deletions on the covariance matrix of $\hat{\beta}$.

3.12 Cook's Distance for LMEs

Diagnostic methods for fixed effects are generally analogues of methods used in classical linear models. Diagnostic methods for variance components are based on ‘one-step’ methods. Cook (1986) gives a completely general method for assessing the influence of local departures from assumptions in statistical models.

For fixed effects parameter estimates in LME models, the Cook's distance can be extended to measure influence on these fixed effects.

$$CD_i(\beta) = \frac{(c_{ii} - r_{ii}) \times t_i^2}{r_{ii} \times p}$$

For random effect estimates, the Cook's distance is

$$CD_i(b) = g_{I(i)}(I_r + \text{var}(\hat{b})D)^{-2} \text{var}(\hat{b})g_{(i)}.$$

Large values for Cook's distance indicate observations for special attention.

3.12.1 Change in the precision of estimates

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.

3.12.2 Cook's Distance

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

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.

3.12.3 Information Ratio

3.13 Computation and Notation

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

Zewotir and Galpin (2005) remarks that \mathbf{D} is a block diagonal with the i -th block being $u\mathbf{I}$

3.14 Cook's Distance for LMEs

Cook's Distance is a well known diagnostic technique used in classical linear models, extended to LME models. For LME models, two formulations exist; a Cook's distance that examines the change in fixed fixed parameter estimates, and another that examines the change in random effects parameter estimates. The outcome of either Cook's distance is a scaled change in either $\boldsymbol{\beta}$ or $\boldsymbol{\theta}$.

Diagnostic methods for fixed effects are generally analogues of methods used in classical linear models. Diagnostic methods for variance components are based on 'one-step' methods. *Cook (1986)* gives a completely general method for assessing the influence of local departures from assumptions in statistical models.

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3.15 CPJ's Three Propositions

3.16 The CPJ Paper

3.16.1 Case-Deletion results for Variance components

Christensen et al. (1992) examines case deletion results for estimates of the variance components, proposing the use of one-step estimates of variance components for examining case influence. The method describes focuses on REML estimation, but can easily be adapted to ML or other methods.

This paper develops their global influences for the deletion of single observations in two steps: a one-step estimate for the REML (or ML) estimate of the variance components, and an ordinary case-deletion diagnostic for a weighted regression problem (conditional on the estimated covariance matrix) for fixed effects.

3.16.2 CPJ Notation

$$\mathbf{C} = \mathbf{H}^{-1} = \begin{bmatrix} c_{ii} & \mathbf{c}'_i \\ \mathbf{c}_i & \mathbf{C}_{[i]} \end{bmatrix}$$

Christensen et al. (1992) noted the following identity:

$$\mathbf{H}^{-1}_{[i]} = \mathbf{C}_{[i]} - \frac{1}{c_{ii}} \mathbf{c}_{[i]} \mathbf{c}'_{[i]}$$

Christensen et al. (1992) use the following as building blocks for case deletion statistics.

- \check{x}_i
- \check{z}_i
- \check{z}_{ij}
- \check{y}_i
- p_i

- m_i

All of these terms are a function of a row (or column) of \mathbf{H} and $\mathbf{H}_{[i]}^{-1}$

3.17 Matrix Notation for Case Deletion

3.17.1 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} .

3.17.2 Partitioning Matrices

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

3.18 The CPJ Paper

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All of these terms are a function of a row (or column) of \mathbf{H} and $\mathbf{H}_{[i]}^{-1}$

3.23 CPJ's Three Propositions

Proposition 1

$$\mathbf{V}^{-1} = \begin{bmatrix} \nu^{ii} & \lambda'_i \\ \lambda_i & \Lambda_{[i]} \end{bmatrix}$$

$$\mathbf{V}_{[i]}^{-1} = \Lambda_{[i]} - \frac{\lambda_i \lambda'_i}{\lambda_i}$$

3.23.1 Proposition 2

$$(i) \quad \mathbf{X}_{[i]}^T \mathbf{V}_{[i]}^{-1} \mathbf{X}_{[i]} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{X}$$

$$(ii) \quad = (\mathbf{X}' \mathbf{V}^{-1} \mathbf{Y})^{-1}$$

$$(iii) \quad \mathbf{X}_{[i]}^T \mathbf{V}_{[i]}^{-1} \mathbf{Y}_{[i]} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{Y}$$

3.23.2 Proposition 3

This proposition is similar to the formula for the one-step Newtown Raphson estimate of the logistic regression coefficients given by Pregibon (1981) and discussed in Cook Weisberg.

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3.24.1 Case-Deletion results for Variance components

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Proposition 1

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$$(i) \quad \mathbf{X}_{[i]}^T \mathbf{V}_{[i]}^{-1} \mathbf{X}_{[i]} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{X}$$

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3.26 CPJ's Three Propositions

3.26.1 Proposition 2

$$(i) \mathbf{X}_{[i]}^T \mathbf{V}_{[i]}^{-1} \mathbf{X}_{[i]} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{X}$$

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$$(iii) \mathbf{X}_{[i]}^T \mathbf{V}_{[i]}^{-1} \mathbf{Y}_{[i]} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{Y}$$

3.26.2 Proposition 3

This proposition is similar to the formula for the one-step Newtown Raphson estimate of the logistic regression coefficients given by Pregibon (1981) and discussed in Cook Weisberg.

3.27 CPJ's Three Propositions

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$$\mathbf{V}_{[i]}^{-1} = \Lambda_{[i]} - \frac{\lambda_i \lambda'_i}{\lambda_i}$$

3.28.1 Proposition 2

$$(i) \quad \mathbf{X}_{[i]}^T \mathbf{V}_{[i]}^{-1} \mathbf{X}_{[i]} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{X}$$

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$$(iii) \quad \mathbf{X}_{[i]}^T \mathbf{V}_{[i]}^{-1} \mathbf{Y}_{[i]} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{Y}$$

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$$\mathbf{V}_{[i]}^{-1} = \Lambda_{[i]} - \frac{\lambda_i \lambda'_i}{\lambda_i}$$

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$$(iii) \quad \mathbf{X}_{[i]}^T \mathbf{V}_{[i]}^{-1} \mathbf{Y}_{[i]} = \mathbf{X}' \mathbf{V}^{-1} \mathbf{Y}$$

3.29.3 Likelihood Distance

The likelihood distance gives the amount by which the log-likelihood of the full data changes if one were to evaluate it at the reduced-data estimates. The important point is that $l(\psi_{(U)})$ is not the log-likelihood obtained by fitting the model to the reduced data set.

It is obtained by evaluating the likelihood function based on the full data set (containing all n observations) at the reduced-data estimates.

The likelihood distance is a global, summary measure, expressing the joint influence of the observations in the set U on all parameters in ψ that were subject to updating.

$$LD(\omega) = 2[L\hat{\theta} - \hat{\theta}_\omega]$$

Large values indicate that $\hat{\theta}$ and $\hat{\theta}_\omega$ differ considerably.

3.30 Likelihood Distance

The likelihood distance gives the amount by which the log-likelihood of the full data changes if one were to evaluate it at the reduced-data estimates. The important point is that $l(\psi_U)$ is not the log-likelihood obtained by fitting the model to the reduced data set.

It is obtained by evaluating the likelihood function based on the full data set (containing all n observations) at the reduced-data estimates.

The likelihood distance is a global, summary measure, expressing the joint influence of the observations in the set U on all parameters in ψ that were subject to updating.

3.30.1 Likelihood Distance

The likelihood distance is a global, summary measure, expressing the joint influence of the observations in the set U on all parameters in ϕ that were subject to updating.

3.31 Likelihood Distance

The likelihood distance gives the amount by which the log-likelihood of the full data changes if one were to evaluate it at the reduced-data estimates. The important point is that $l(\psi_U)$ is not the log-likelihood obtained by fitting the model to the reduced data set.

It is obtained by evaluating the likelihood function based on the full data set (containing all n observations) at the reduced-data estimates.

The likelihood distance is a global, summary measure, expressing the joint influence of the observations in the set U on all parameters in ψ that were subject to updating.

3.31.1 Likelihood Distance

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3.32 Likelihood Distance

The likelihood distance gives the amount by which the log-likelihood of the full data changes if one were to evaluate it at the reduced-data estimates. The important point is that $l(\psi_U)$ is not the log-likelihood obtained by fitting the model to the reduced data set.

It is obtained by evaluating the likelihood function based on the full data set (containing all n observations) at the reduced-data estimates.

The likelihood distance is a global, summary measure, expressing the joint influence of the observations in the set U on all parameters in ψ that were subject to updating.

3.32.1 Likelihood Distance

The likelihood distance is a global, summary measure, expressing the joint influence of the observations in the set U on all parameters in ϕ that were subject to updating.

3.33 Likelihood Distance

The likelihood distance gives the amount by which the log-likelihood of the full data changes if one were to evaluate it at the reduced-data estimates. The important point is that $l(\psi_U)$ is not the log-likelihood obtained by fitting the model to the reduced data set.

It is obtained by evaluating the likelihood function based on the full data set (containing all n observations) at the reduced-data estimates.

The likelihood distance is a global, summary measure, expressing the joint influence of the observations in the set U on all parameters in ψ that were subject to updating.

3.33.1 Likelihood Distance

The likelihood distance is a global, summary measure, expressing the joint influence of the observations in the set U on all parameters in ϕ that were subject to updating.

3.33.2 Likelihood Distance

The likelihood distance is a global, summary measure, expressing the joint influence of the observations in the set U on all parameters in ϕ that were subject to updating.

3.33.3 Key Definitions

Residual The difference between the predicted value (based on the regression equation) and the actual, observed value.

Outlier In linear regression, an outlier is an observation with large residual. In other words, it is an observation whose dependent-variable value is unusual given its value on the predictor variables. An outlier may indicate a sample peculiarity or may indicate a data entry error or other problem.

Leverage An observation with an extreme value on a predictor variable is a point with high leverage. Leverage is a measure of how far an independent variable deviates from its mean. High leverage points can have a great amount of effect on the estimate of regression coefficients.

Influence An observation is said to be influential if removing the observation substantially changes the estimate of the regression coefficients. Influence can be thought of as the product of leverage and outlierness.

Cook's distance A measure that combines the information of leverage and residual of the observation.

3.33.4 Leverage

In statistics, leverage is a term used in connection with regression analysis and, in particular, in analyses aimed at identifying those observations that are far away from corresponding average predictor values. Leverage points do not necessarily have a large effect on the outcome of fitting regression models.

Leverage points are those observations, if any, made at extreme or outlying values of the independent variables such that the lack of neighboring observations means that the fitted regression model will pass close to that particular observation.[1]

Modern computer packages for statistical analysis include, as part of their facilities for regression analysis, various quantitative measures for identifying influential observations: among these measures is partial leverage, a measure of how a variable contributes to the leverage of a datum.

3.33.5 Leverage in LME models

For the general mixed model, leverage can be defined through the projection matrix that results from a transformation of the model with the inverse of the Cholesky decomposition of \mathbf{V} , or through an oblique projector. The MIXED procedure follows the latter path in the computation of influence diagnostics. The leverage value reported for the i th observation is the i th diagonal entry of the matrix

which is the weight of the observation in contributing to its own predicted value, \hat{y}_i . While \mathbf{H} is idempotent, it is generally not symmetric and thus not a projection matrix in the narrow sense. The properties of these leverages are generalizations of the properties in models with diagonal variance-covariance matrices. For example, $\sum h_{ii} = p$, and in a model with intercept and $p-1$ predictors, the leverage values

are $1/n$ and $1/n + \frac{1}{n-1} \sum_{j=1}^{p-1} x_{ij}^2$. The lower bound for h_{ii} is achieved in an intercept-only model, and the upper bound is achieved in a saturated model. The trace of \mathbf{H} equals the rank of \mathbf{X} . If h_{ij} denotes the element in row i , column j of \mathbf{H} , then for a model containing only an intercept the diagonal elements of \mathbf{H} are

Because is a sum of elements in the i th row of the inverse variance-covariance matrix, can be negative, even if the correlations among data points are nonnegative. In case of a saturated model with n , .

Nobre Singer : Mixed Model Residuals

Usually one assumes

- $b_i \sim N_q(0, G)$ $i = 1, \dots, m$
- $e_i \sim N_{n_i}(0, \sigma_i)$
- b_i and e_i independent
- G and σ_i are $(q \times q)$ and $(n_i \times n_i)$ positive definite matrices with elements expressed as functions of a vector of covariance parameters θ not functionally related to β
- If $\sigma_i = I_{n_i} \sigma^2$: homoskedastic conditional independence model

$$\begin{bmatrix} \mathbf{b} \\ \mathbf{e} \end{bmatrix} \sim \mathcal{N}_{qm+n}$$

$$\mathbf{Q} = \mathbf{V}^{-1} - \mathbf{V}^{-1} \mathbf{X} (\mathbf{X}^T \mathbf{V}^{-1} \mathbf{X})^{-1}$$

Sensitivity and residual analysis of the underlying assumptions constitute important tools for evaluating the fit of any model to given data.

Generalized Leverage

3.34 Case Deletion Diagnostics for LME models

Haslett & Dillane (19XX) remark that linear mixed effects models didn't experience a corresponding growth in the use of deletion diagnostics, adding that McCullough and Searle (2001) makes no mention of diagnostics whatsoever.

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.

$$V_{[i]}^{-1} = \Lambda_{[i]} - \frac{\lambda\lambda'}{\nu ii} \quad (3.2)$$

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

$$X'_{[i]} V_{[i]}^{-1} X_{[i]} = X' V^{-1} X - \frac{\hat{x}_i \hat{x}_i'}{s_i} \quad (3.3)$$

$$(X'_{[i]} V_{[i]}^{-1} X_{[i]})^{-1} = (X' V^{-1} X)^{-1} + \frac{(X' V^{-1} X)^{-1} \hat{x}_i \hat{x}_i' (X' V^{-1} X)^{-1}}{s_i - \bar{h}_i} \quad (3.4)$$

$$X'_{[i]} V_{[i]}^{-1} Y_{[i]} = X' V^{-1} Y - \frac{\hat{x}_i \hat{y}_i'}{s_i} \quad (3.5)$$

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

$$LD_{(U)} = 2\{l(\hat{\psi}) - l(\hat{\psi}_{(U)})\} \quad (3.6)$$

$$RLD_{(U)} = 2\{l_R(\hat{\psi}) - l_R(\hat{\psi}_{(U)})\} \quad (3.7)$$

Haslett & Dillane (199X) 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} . Haslett & Dillane (199X) propose an alternative, and computationally inexpensive approach, making use of the 'delete=replace' identity.

Haslett (1999) considers the effect of 'leave k out' calculations on the parameters β and σ^2 , using several key results from Haslett and Hayes (1998) on partitioned matrices.

Haslett and Hayes - Residuals

Haslett and Hayes (1998) and Haslett (1999) considered the case of an LME model with correlated covariance structure.

3.34.1 Residual Diagnostics in LME models

- A **residual** is the difference between the observed quantity and the predicted value. In LME models a distinction is made between marginal residuals and conditional residuals.
- A **Marginal residual** is the difference between the observed data and the estimated marginal mean (Schabenberger pg3) The computation of case deletion diagnostics in the classical model is made simple by the fact that important estimates can be computed without refitting the model.
- Such update formulae 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. Schabenberger remarks that this is not a reasonable assumption.

Basic procedure for quantifying influence is simple

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

The likelihood distance is a global summary measure expressing the joint influence of the observations in the set U on all parameters in Ψ that were subject to updating.

3.35 Case Deletion Diagnostics for LME models

Haslett and Dillane (2004) remark that linear mixed effects models didn't experience a corresponding growth in the use of deletion diagnostics, adding that McCullough and Searle (2001) 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.

$$V_{[i]}^{-1} = \Lambda_{[i]} - \frac{\lambda\lambda'}{\nu ii} \quad (3.8)$$

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

$$X'_{[i]} V_{[i]}^{-1} X_{[i]} = X' V^{-1} X - \frac{\hat{x}_i \hat{x}_i'}{s_i} \quad (3.9)$$

$$(X'_{[i]} V_{[i]}^{-1} X_{[i]})^{-1} = (X' V^{-1} X)^{-1} + \frac{(X' V^{-1} X)^{-1} \hat{x}_i \hat{x}_i' (X' V^{-1} X)^{-1}}{s_i - \bar{h}_i} \quad (3.10)$$

$$X'_{[i]} V_{[i]}^{-1} Y_{[i]} = X' V^{-1} Y - \frac{\hat{x}_i \hat{y}_i'}{s_i} \quad (3.11)$$

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

$$LD_{(U)} = 2\{l(\hat{\psi}) - l(\hat{\psi}_{(U)})\} \quad (3.12)$$

$$RLD_{(U)} = 2\{l_R(\hat{\psi}) - l_R(\hat{\psi}_{(U)})\} \quad (3.13)$$

3.36 Turkan's LMEs

The linear mixed model is considerably sensitive to outliers and influential observations. It is known that outliers and influential observations affect substantially the results of analysis. So it is very important to be aware of these observations.

Some diagnostics which are analogue of diagnostics in multiple linear regression were developed to detect outliers and influential observations in the linear mixed model. *In this paper, the new diagnostic measure which is analogue of the Pena's influence statistic is developed for the linear mixed model.*

Estimation and Building blocks in LME models

$$\hat{u} = DZ^T H^{-1}(y - X\hat{\beta})$$

$$\hat{y} = (I_n - H^{-1})y + H^{-1}X\hat{\beta}$$

The proposed diagnostic Measure.

Influence.ME: Tools for Detecting Influential Data in Mixed Effects Models

- *The previous Section (Section 4) is a literary review of residual diagnostics and influence procedures for Linear Mixed Effects Models, drawing heavily on Schabenberger and Zewotir.*
- *Section 4 begins with an introduction to key topics in residual diagnostics, such as influence, leverage, outliers and Cook's distance. Other concepts such as DF-FITS and DFBETAs will be introduced briefly, mostly to explain why they are not particularly useful for the Method Comparison context, and therefore are not elaborated upon.*
- *In brief, Variable Selection is not applicable to Method Comparison Studies, in the commonly used context. Testing a rather simplistic specified model against one with more random effects terms is tractable, but this research question is of secondary importance.*

Appendix to Section 4

As an appendix to section 4, an appraisal of the current state of development (or lack thereof) for current implemenations for LME models, particularly for `nlme` and `lme4` fitted models.

Crucially, a review of internet resources indicates that almost all of the progress in this regard has been done for `lme4` fitted models, specifically the *Influence.ME* R package. (Nieuwenhuis et 2012)

Conversely there is very little for `nlme` models. To delve into this mor, one would immediately investigate the current development workflow for both packages.

As an aside, Douglas Bates was arguably the most prominent R developer working in the LME area. However Bates has now prioritised the development of LME models in another computing environment , i.e Julia.

The `nlme` package

With regards to `nlme`, the torch has been passed to Galecki Galecki & Burzykowski (UMich. and Hasselt respecitely). Galecki & Burzykowski published *Linear Mixed Effects Models using R*. Also, the accompanying R package, `nlmeU` package is under current development, with a version being released XXXX.

The `lme4` package

The `lme4` package is also under active development, under the leadership of Ben Bolker (McMaster University). According to CRAN, the LME4 package, fits linear and generalized linear mixed-effects models

The models and their components are represented using S4 classes and methods. The core computational algorithms are implemented using the Eigen C++ library for numerical linear algebra and RcppEigen "glue".
(CRAN)

The key issue is that `nlme` allows for the particular specification of Roy’s Model, specifically direct specification of the VC matrices for within subject and between subject residuals. The `lme4` package does not allow for this. To advance the ideas that emanate from Roys’ paper, one is required to use the `nlme` context. However, to take advantage of the infrastructure already provided for `lme4` models, one may change the research question away from that of Roy’s paper. To this end, an exploration of what `textit`influence.ME can accomplish is merited. As a complement to this, one can also consider how to properly employ the R^2 measure, in the context of Method Comparison Studies, further to the work by Edwards et al, namely “An R^2 statistic for fixed effects in the linear mixed model”.

Abstract for “An R^2 statistic for fixed effects in the linear mixed model” Statisticians most often use the linear mixed model to analyze Gaussian longitudinal data.

The value and familiarity of the R^2 statistic in the linear univariate model naturally creates great interest in extending it to the linear mixed model. We define and describe how to compute a model R^2 statistic for the linear mixed model by using only a single model.

The proposed R^2 statistic measures multivariate association between the repeated outcomes and the fixed effects in the linear mixed model. The R^2 statistic arises as a 11 function of an appropriate F statistic for testing all fixed effects (except typically the intercept) in a full model.

The statistic compares the full model with a null model with all fixed effects deleted (except typically the intercept) while retaining exactly the same covariance structure.

Furthermore, the R^2 statistic leads immediately to a natural definition of a partial R^2 statistic. A mixed model in which ethnicity gives a very small p-value as a longitudinal predictor of blood pressure (BP) compellingly illustrates the value of the statistic.

In sharp contrast to the extreme p-value, a very small R^2 , a measure of statistical and scientific importance, indicates that ethnicity has an almost negligible association with the repeated BP outcomes for the study.

Leave-One-Out Diagnostics with `lmeU`

Galecki et al discuss the matter of LME influence diagnostics in their book, although not into great detail.

The command `lmeU` fits a model with a particular subject removed. The identifier of the subject to be removed is passed as the only argument

A plot of the per-observation diagnostics individual subject log-likelihood contributions can be rendered.

Likelihood Displacement

Missing Data in Method Comparison Studies

The matter of missing data has not been commonly encountered in either Method Comparison Studies or Linear Mixed Effects Modelling. However Roy (2009) deals with the relevant assumptions regarding missing data.

Galecki & Burzykowski (2013) tackles the subject of missing data in LME Modelling.

Furthermore the nlmeU package includes the `patMiss` function, which “allows to compactly present pattern of missing data in a given vector/matrix/data frame or combination of thereof”.

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