

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 Model Data Agreement

? describes the examination of model-data agreement as comprising several elements; residual analysis, goodness of fit, collinearity diagnostics and influence analysis.

0.1.2 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.

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

0.1.4 Influence Statistics for LME models

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

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

0.1.5 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 (?).

0.1.6 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.

? 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.

0.2 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.

0.3 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’.

0.3.1 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.

0.3.2 Studentization

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

0.3.3 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.

0.3.4 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

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

0.3.5 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.

0.4 Covariance Parameters

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

0.4.1 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.

0.5 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.

0.5.1 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 .

0.5.2 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 .

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

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.

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

0.5.3 Marginal Residuals

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

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, $r_{ci} = y_i - x_i'\hat{b} - z_i'\hat{\gamma}$.

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 .

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

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.

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

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 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’.

0.7.1 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.

0.7.2 Studentization

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

0.7.3 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.

0.7.4 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

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

0.7.5 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.

0.7.6 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

0.8 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’.

0.8.1 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.

0.8.2 Studentization

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

0.8.3 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.

0.8.4 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

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

0.8.5 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.

0.9 Diagnostics

0.9.1 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.

0.9.2 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 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.

0.10.1 Model Data Agreement

? describes the examination of model-data agreement as comprising several elements; residual analysis, goodness of fit, collinearity diagnostics and influence analysis.

0.10.2 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.

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

0.10.4 Influence Statistics for LME models

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

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

0.10.5 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 (?).

0.10.6 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.

? 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.

0.11 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.

0.11.1 Case Deletion Diagnostics for Mixed Models

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

? develops these techniques in the context of REML

0.11.2 Methods and Measures

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

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

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

0.11.3 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.

0.11.4 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].

0.11.5 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 (?).

0.11.6 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.

? 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.

0.12 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.

0.13 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.

0.13.1 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 .

0.13.2 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 .

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

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.