

Chapter 1

Model Diagnostics

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Abstract

This chapter is broken into two parts. The first part is a review of diagnostics methods for linear models, intended to acquaint the reader with the subject, and also to provide a basis for material covered in the second part. Particular attention is drawn to graphical methods.

The second part of the chapter looks at diagnostics techniques for LME models, firstly covering the theory, then proceeding to a discussion on implementing these using R code.

While a substantial body of work has been developed in this area, there is still areas worth exploring. In particular the development of graphical techniques pertinent to LME models should be looked at.

1.1 Model Validation Framework

In statistical modelling, the process of model validation is a critical step of model fitting process, but also a step that is too often overlooked. A very simple procedure is to examine commonly-used metrics, such as the R^2 value. However, using a small handful of simple measures and methods is insufficient to properly assess the quality of a fitted model. To do so properly, a full and comprehensive analysis that tests of all of the assumptions, as far as possible, must be carried out.

? describes the model validation framework as comprised of the following tasks

- overall measures of goodness-of-fit
- the informal, graphical examination of estimates of model errors to assess the quality of distributional assumptions: residual analysis
- the quantitative assessment of the inter-relationship of model components; for example, collinearity diagnostics
- the qualitative and quantitative assessment of influence of cases on the analysis, i.e. influence analysis.

Residual analysis is a widely used model validation technique. A residual is simply the difference between an observed value and the corresponding fitted value, as predicted by the model. The rationale is that, if the model is properly fitted to the model, then the residuals would approximate the random errors that one should expect. that is to say, if the residuals behave randomly, with no discernible trend, the model has fitted the data well. If some sort of non-random trend is evident in the model, then the model can be considered to be poorly fitted.

Statistical software environments, such as the R Programming language, provides a suite of tests and graphical procedure sfor appraising a fitted linear model, with several of these procedures analysing the model residuals.

For LME models the matter of residual is more complex. ? describes 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. We shall revert to this matter in due course.

Further to the analysis of residuals, ? recommends the examination of the following questions.

- Does the model-data agreement support the model assumptions?
- Should model components be refined, and if so, which components? For example, should regressors be added or removed, and is the covariation of the observations modeled properly?
- Are the results sensitive to model and/or data? Are individual data points or groups of cases particularly influential on the analysis?

1.1.1 Outliers and Leverage

The question of whether or not a point should be considered an outlier must also be addressed. An outlier is an observation whose true value is unusual given its value on the predictor variables. The leverage of an observation is a further consideration. Leverage describes an observation with an extreme value on a predictor variable is a point with high leverage. High leverage points can have a great amount of effect on the estimate of regression coefficients.

Influence can be thought of as the product of leverage and outlierness. An observation is said to be influential if removing the observation substantially changes the estimate of the regression coefficients. The R programming language has a variety of methods used to study each of the aspects for a linear model. While linear models and GLMS can be studied with a wide range of well-established diagnostic techniques, the choice of methodology is much more restricted for the case of LMEs.

For classical linear models, residual diagnostics are typically conducted using 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.

1.2 Case Deletion Diagnostics

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

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

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

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

1.2.1 Extension of Diagnostic Methods to LME models

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

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

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

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

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

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

Cook's distance

In the study of Linear model diagnostics, Cook proposed a measure that combines the information of leverage and residual of the observation, now known simply as the Cook's Distance. ? would later adapt the Cook's distance measure for the analysis of LME models.

1.3 Cook's Distance

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

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

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

$$\hat{e}_{i(U)} = y_i - x\hat{\beta}_{(U)} \quad (1.1)$$

$$\delta_{(U)} = \hat{\beta} - \hat{\beta}_{(U)} \quad (1.2)$$

1.4 Exention of Cook's Distance methodology to LME models

Cook's Distance is 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 .

Diagnostic methods for variance components are based on 'one-step' methods. ? 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.

Cook's Distance was extended from classical linear models to LME models. For linear mixed effects models, Cook's distance can be extended to model influence diagnostics by definining.

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

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

1.4.1 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 $\hat{\beta}$: $CD(\psi)_i$

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

1.5 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. ? 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.

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

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.

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 .

1.5.1 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.

1.6 Analysis of Influence

1.6.1 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 (?).

1.6.2 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].

1.6.3 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.

1.6.4 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.

1.7 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.

1.7.1 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.

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

1.7.2 PRESS

The prediction residual sum of squares (PRESS) is a 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.

$$PRESS = \sum (y - \hat{y}^{(k)})^2 \quad (1.3)$$

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

DFBETA

$$DFBETA_a = \hat{\beta} - \hat{\beta}_{(a)} \quad (1.4)$$

$$= B(Y - Y_{\bar{a}}) \quad (1.5)$$

1.8 Influence in 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.

1.8.1 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

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.

1.9 Influence analysis for LME Models

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.

? 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’.

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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.

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} .

Influence Analysis for LME Models

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1.9.4 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 (?).

1.9.5 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.

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- 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.

1.11 Likelihood Distance

The likelihood distance is a global summary measure that expresses the joint influence of the subsets of observations, U , on all parameters in ϕ that were subject to updating. ? points out the likelihood distance gives the amount by which the log-likelihood of the model fitted from the full data changes if one were to estimate the model from a reduced-data estimates. Importantly $LD(\psi_U)$ 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.

$$LD((\mathbf{U})) = 2[l(\hat{\phi}) - l\hat{\phi}_{\omega}]$$

$$RLD((\mathbf{U})) = 2[l_R(\hat{\phi}) - l_R(\hat{\phi})_{\omega}]$$