

Chapter 1

Residual Analysis

1.1 Introduction to Residual 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.

1.2 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.

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.

1.3 Fundamentals of Residuals

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.

1.3.1 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.

1.4 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.

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 .

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

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.

1.4.1 Residuals

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

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

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

1.5 Framework for Model Validation using Residual Diagnostics

In statistical modelling, the process of model validation is a critical step, but also a step that is too often overlooked. A very simple procedure is to examine commonly encountered 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. A statistical model, whether of the fixed-effects or mixed-effects variety, represents how you think your data were generated. Following model specification and estimation, it is of interest to explore the model-data agreement by raising questions such as

- 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?

1.5.1 Residual Analysis

In classical linear models, an examination of model-data agreement has traditionally revolved around

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.

1.5.2 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.

1.6 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’.

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.

1.6.1 Studentization

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

1.6.2 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 .

1.6.3 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 $\bar{e} = 0$.

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.

1.6.4 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.

1.6.5 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.

1.6.6 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

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

1.6.7 Standardized and studentized residuals

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

1.6.8 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’.

1.6.9 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.

1.6.10 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

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

1.6.11 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.

1.6.12 Computation

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

1.7 Covariance Parameters

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

1.7.1 Standardized and studentized residuals

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Chapter 2

Residuals for LME Models

2.1 Residual Analysis for LME Models

In classical linear models model diagnostics have been 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.

Cite:Zewotir 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.

2.1.1 LME REsiduals

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,

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

2.1.2 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.

2.1.3 Residuals diagnostics in mixed models

A residual is the difference between an observed quantity and its estimated or predicted value. In the mixed model you can distinguish marginal residuals rm and conditional residuals rc . A marginal residual is the difference between the observed data and the estimated (marginal) mean.

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.

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2.3 Marginal and Conditional Residuals

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 . 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, $r_{ci} = y_i - x'_i\hat{b} - z'_i\hat{\gamma}$

2.3.1 Marginal and Conditional Residuals

$$r_{mi} = x_i^T \hat{\beta} \tag{2.1}$$

2.3.2 Marginal Residuals

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

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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.

$$r_{mi} = x_i^T \hat{\beta} \tag{2.2}$$

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$$r_{mi} = x_i^T \hat{\beta} \quad (2.3)$$

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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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2.3.7 Residuals diagnostics in LME 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.

$$r_{mi} = x_i^T \hat{\beta} \quad (2.4)$$

2.3.8 Marginal Residuals

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

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}
-

2.4 Residual diagnostics

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2.4.1 Marginal Residuals

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

2.4.2 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*.

2.5 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

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

and the fitted marginal response is

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

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

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

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

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 homoscedastic.

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 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 —
- 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.

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$$r_{mi} = x_i^T \hat{\boldsymbol{\beta}} \tag{2.5}$$

2.5.2 Marginal Residuals

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

2.6 Diagnostic Tools for the nlme package

With the nlme package, the generic function `lme()` fits a linear mixed-effects model in the formulation described in Laird and Ware (1982) but allowing for nested random effects.

The within-group errors are allowed to be correlated and/or have unequal variances, which is very important in fitting the models for Roy's Tests

The nlme package has a limited set of diagnostic tools that can be used to assess the model fit. A review of the package manual is sufficient to get a sense of the package's capability in that regard.

2.7 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} , $\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{A}\mathbf{Y}$.

Bibliography

Cook, R. (1986). Assessment of local influence. *Journal of the Royal Statistical Society. Series B (Methodological)* 48(2), 133–169.