

STAT 574 Linear and Nonlinear Mixed Models

Lecture 10: Diagnoses and Influence Analysis

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Influence analysis

- ▶ Influence analysis is a set of techniques used to identify and assess the impact of individual data points on the overall model fit and parameter estimates.
- ▶ In this lecture, we consider the **influence analysis** as a **sensitivity analysis** of the model fit to the data.
- ▶ Data influence: the sensitivity of the model to a infinitesimal perturbation in the data.
- ▶ Model influence: the sensitivity of the model to the assumptions.

Linear Regression Model

Consider a linear regression model:

$$y_i = \boldsymbol{\beta}^T \mathbf{x}_i + \epsilon_i \quad \forall i.$$

The OLS estimator of $\boldsymbol{\beta}$ is given by

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = \left(\sum_i \mathbf{x}_i \mathbf{x}_i^T \right)^{-1} \sum_i \mathbf{x}_i y_i,$$

where \mathbf{X} is the design matrix and \mathbf{y} is the response vector.

Leverage

The **leverage** of the i -th observation is defined as the i -th diagonal element of the hat matrix

$$\mathbf{H} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T.$$

That is

$$h_i = (\mathbf{H})_{ii} = \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i.$$

Leverage

The sum of the leverages is equal to the number of parameters in the model:

$$\begin{aligned}\sum_{i=1}^n h_i &= \text{tr}(\mathbf{H}) \\ &= \text{tr}(\mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T) \\ &= \text{tr}((\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{X}) \\ &= \text{tr}(\mathbf{I}) \\ &= m,\end{aligned}$$

where m is the number of parameters in the model.

- ▶ Observations with high leverage are called **influential observations**.
- ▶ It measures how the predicted value is influenced by the i -th observation.

Leave-one-out

Another measure of influence is to check the change in the estimates of the parameters when the i -th observation is removed from the data set.

The estimated parameter $\hat{\beta}_{(i)}$ when the i -th observation is removed is given by

$$\hat{\beta}_{(i)} = (\mathbf{X}_{(i)}^T \mathbf{X}_{(i)})^{-1} \mathbf{X}_{(i)}^T \mathbf{y}_{(i)},$$

where $\mathbf{X}_{(i)}$ and $\mathbf{y}_{(i)}$ are the design matrix and response vector with the i -th observation removed.

Leave-one-out

We notice that

$$(\mathbf{X}_{(i)}^T \mathbf{X}_{(i)})^{-1} = (\mathbf{X}^T \mathbf{X} - \mathbf{x}_i \mathbf{x}_i^T)^{-1} = (\mathbf{X}^T \mathbf{X})^{-1} + \frac{(\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{x}_i \mathbf{x}_i^T) (\mathbf{X}^T \mathbf{X})^{-1}}{1 - \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i}$$

Then

$$\begin{aligned} \hat{\beta}_{(i)} &= (\mathbf{X}^T \mathbf{X} - \mathbf{x}_i \mathbf{x}_i^T)^{-1} (\mathbf{X}^T \mathbf{y} - \mathbf{x}_i y_i) \\ &= [(\mathbf{X}^T \mathbf{X})^{-1} + (1 - h_i)^{-1} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1}] (\mathbf{X}^T \mathbf{y} - \mathbf{x}_i y_i) \\ &= \hat{\beta} + (1 - h_i)^{-1} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} - (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i y_i \\ &\quad - (1 - h_i)^{-1} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i y_i \\ &= \hat{\beta} + (1 - h_i)^{-1} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i \hat{y}_i - (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i y_i - \frac{h_i}{1 - h_i} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i y_i \\ &= \hat{\beta} - \frac{y_i - \hat{y}_i}{1 - h_i} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i. \end{aligned}$$

Cook's distance

The confidence region for the estimator $\hat{\beta}$ is given by

$$\left\{ \beta : (\beta - \hat{\beta})^T (\mathbf{X}^T \mathbf{X})^{-1} (\beta - \hat{\beta}) \leq m s^2 F_{\alpha, m, n-m} \right\}$$

The **Cook's distance** is defined as

$$D_i = \frac{1}{m s^2} (\hat{\beta}_{(i)} - \hat{\beta})^T (\mathbf{X}^T \mathbf{X})^{-1} (\hat{\beta}_{(i)} - \hat{\beta})$$

By previous result, we have

$$D_i = \frac{(y_i - \hat{y}_i)^2}{m s^2} \frac{h_i}{(1 - h_i)^2}$$

Large values of D_i indicate that the i -th observation has a large influence on the fitted model.

Infinitesimal Influence (I-influence)

- ▶ \mathbf{D} : data vector including all the observed values.
- ▶ $t(\mathbf{D})$: a statistic of interest.
- ▶ The **infinitesimal data influence** is

$$\lim_{\Delta D \rightarrow 0} \frac{t(\mathbf{D} + \Delta D e_i) - t(\mathbf{D})}{\Delta D} = \frac{\partial t(\mathbf{D})}{\partial D_i}$$

Infinitesimal Influence (I-influence)

- ▶ Let $\ell(\boldsymbol{\theta})$ be the log-likelihood function of the model.
- ▶ Consider a more general model $\ell(\boldsymbol{\theta} \mid \boldsymbol{\omega})$ such that $\boldsymbol{\omega} = 0$ corresponds to the model of interest.
- ▶ The **infinitesimal model influence** is defined as

$$\left. \frac{\partial t}{\partial \boldsymbol{\omega}} \right|_{\boldsymbol{\omega}=0}$$

Influence of the Dependent Variable

We consider the influence of y_i on the estimated parameters $\hat{\beta}$.

- ▶ The OLS solution is

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} = (\mathbf{X}^T \mathbf{X})^{-1} \sum_i \mathbf{x}_i y_i.$$

- ▶ The influence of y_i on $\hat{\beta}$ is given by

$$\frac{\partial \hat{\beta}}{\partial y_i} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i.$$

- ▶ Two possibilities that the size of the influence is large:
 - ▶ $|\mathbf{x}_i|$ is large: the i -th observation is far from the center of the data.
 - ▶ The direction of \mathbf{x}_i is close to the direction of the eigenvector of $\mathbf{X}^T \mathbf{X}$ corresponding to the smallest eigenvalue.

Influence of the Continuous Explanatory Variable

In particular, we are interested in

$$\frac{\partial \hat{\boldsymbol{\beta}}}{\partial x_{ik}},$$

where x_{ik} is the k -th element of \mathbf{x}_i .

Use matrix calculus, we have (by considering \mathbf{x}_i as the only variable)

$$\begin{aligned}d\hat{\boldsymbol{\beta}} &= (\mathbf{X}^T \mathbf{X})^{-1} d(\mathbf{X}^T \mathbf{y}) + (d(\mathbf{X}^T \mathbf{X})^{-1}) (\mathbf{X}^T \mathbf{y}) \\&= (\mathbf{X}^T \mathbf{X})^{-1} y_i d\mathbf{x}_i - (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{x}_i d\mathbf{x}_i^T + (d\mathbf{x}_i) \mathbf{x}_i^T) (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \mathbf{y}) \\&= (\mathbf{X}^T \mathbf{X})^{-1} y_i d\mathbf{x}_i - (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i (d\mathbf{x}_i)^T \hat{\boldsymbol{\beta}} - (\mathbf{X}^T \mathbf{X})^{-1} (d\mathbf{x}_i) \hat{y}_i \\&= (\mathbf{X}^T \mathbf{X})^{-1} (y_i - \hat{y}_i) d\mathbf{x}_i - (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i \hat{\boldsymbol{\beta}}^T d\mathbf{x}_i.\end{aligned}$$

Therefore,

$$\frac{\partial \hat{\boldsymbol{\beta}}}{\partial \mathbf{x}_i} = (\mathbf{X}^T \mathbf{X})^{-1} \left((y_i - \hat{y}_i) \mathbf{I} - \mathbf{x}_i \hat{\boldsymbol{\beta}}^T \right)$$

Influence of the Continuous Explanatory Variable

Now we have

$$\frac{\partial \hat{\beta}}{\partial x_{ik}} = (\mathbf{X}^T \mathbf{X})^{-1} \left((y_i - \hat{y}_i) \mathbf{e}_k - \hat{\beta}_k \mathbf{x}_i \right)$$

- ▶ First component: normalized residual.
- ▶ Second component: the influence through the dependent variable.

It is also connected to Cook's local influence, which is measured by

$$\text{local influence of } x_{ik} \text{ on } \hat{\beta}_k = y_i - \hat{y}_i - \hat{\beta}_k q_i$$

where q_i is the residual of the regression of $\mathbf{x}^{(k)}$ on the other variables.

Influence of the Binary Explanatory Variable

Now we assume x_{ik} is a binary variable.

- ▶ A binary variable can be misclassified.
- ▶ We assume x_{ik} is an observation for the true binary variable z_{ik} such that misclassification occurs with probability q_i .
- ▶ The true model should be

$$E(y_i | z_{ik}) = \alpha + \beta_k z_{ik}$$

- ▶ But now

$$E(y_i | x_{ik}) = \alpha + \beta_k(x_{ik} + (1 - 2x_{ik})q_i)$$

- ▶ The influence of the misclassification is given by

$$\left. \frac{\partial \hat{\beta}}{\partial q_i} \right|_{q_i=0} = (1 - 2x_{ik})(\mathbf{X}^T \mathbf{X})^{-1} \left((y_i - \hat{y}_i)\mathbf{e}_i - \hat{\beta}_k \mathbf{x}_i \right)$$

Influence on the Predicted Value

The predicted value is connected to the estimated parameters by

$$\hat{y}_i = \hat{\boldsymbol{\beta}}^T \mathbf{x}_i.$$

The influence can be transferred to the influence on the predicted value. That is

$$\begin{aligned} \frac{\partial \hat{y}_i}{\partial x_{ik}} &= \frac{\partial \hat{y}_i}{\partial \hat{\boldsymbol{\beta}}} \frac{\partial \hat{\boldsymbol{\beta}}}{\partial x_{ik}} + \left. \frac{\partial \hat{y}_i}{\partial x_{ik}} \right|_{\hat{\boldsymbol{\beta}}} \\ &= \mathbf{x}_i^T (\mathbf{X}^T \mathbf{X})^{-1} \left((y_i - \hat{y}_i) \mathbf{e}_k - \hat{\beta}_k \mathbf{x}_i \right) + \hat{\beta}_k \\ &= \mathbf{x}_i^T (\mathbf{X}^T \mathbf{x})^{-1} \mathbf{e}_k (y_i - \hat{y}_i) + (1 - h_i) \hat{\beta}_k. \end{aligned}$$

Influence on Regression Characteristics

Y-influence on

- ▶ **Coefficient of determination R^2 :**

$$\frac{\partial R^2}{\partial y_i} = \frac{2}{\text{SST}} [(1 - R^2)(y_i - \bar{y}) - (y_i - \hat{y}_i)]$$

- ▶ **t-statistics** with $\mathbf{t} = s^{-1} \mathbf{D}^{-1/2} \hat{\boldsymbol{\beta}}$ where $\mathbf{D} = \text{diag}((\mathbf{X}^T \mathbf{X})^{-1})$:

$$\frac{\partial \mathbf{t}}{\partial y_i} = s^{-1} \mathbf{D}^{-1/2} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{x}_i - \frac{y_i - \hat{y}_i}{\text{RSS}} \mathbf{t}_i$$

Nonlinear Regression Models

Consider the nonlinear regression model:

$$y_i = f_i(\boldsymbol{\beta}, \mathbf{x}_i) + \epsilon_i$$

The LS estimator (LSE) of $\boldsymbol{\beta}$ is given by

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \sum_i (y_i - f_i(\boldsymbol{\beta}, \mathbf{x}_i))^2.$$

The estimating equation is given by

$$\sum_i (y_i - f_i(\boldsymbol{\beta}, \mathbf{x}_i)) \frac{\partial f_i(\boldsymbol{\beta}, \mathbf{x}_i)}{\partial \boldsymbol{\beta}} = 0.$$

Influence of the dependent variable on the LSE

The influence of y_i on the LSE $\hat{\beta}$ is

$$\frac{\partial \hat{\beta}}{\partial y_i}$$

Taking partial derivative of the estimating equation w.r.t. y_i , we have

$$\sum_j \left(\delta_{ij} - \left(\frac{\partial f_j(\hat{\beta}, \mathbf{x}_j)}{\partial \hat{\beta}} \right)^T \frac{\partial \hat{\beta}}{\partial y_i} \right) \frac{\partial f_j(\hat{\beta}, \mathbf{x}_j)}{\partial \hat{\beta}} + \sum_j (y_j - f_j(\hat{\beta}, \mathbf{x}_j)) \frac{\partial^2 f_j(\hat{\beta}, \mathbf{x}_j)}{\partial \hat{\beta}^2} \frac{\partial \hat{\beta}}{\partial y_i} = 0$$

This gives

$$\frac{\partial \hat{\beta}}{\partial y_i} = \mathbf{H}^{-1} \frac{\partial f_i(\hat{\beta}, \mathbf{x}_i)}{\partial \hat{\beta}},$$

with

$$\mathbf{H} = \sum_{j=1}^n \left[\frac{\partial f_j(\hat{\beta}, \mathbf{x}_j)}{\partial \hat{\beta}} \left(\frac{\partial f_j(\hat{\beta}, \mathbf{x}_j)}{\partial \hat{\beta}} \right)^T - (y_j - f_j(\hat{\beta}, \mathbf{x}_j)) \frac{\partial^2 f_j(\hat{\beta}, \mathbf{x}_j)}{\partial \hat{\beta}^2} \right]$$

Influence of the explanatory variable on the LSE

We can follow the same procedure to get

$$\frac{\partial \hat{\beta}}{\partial \mathbf{x}_i} = \mathbf{H}^{-1} \left[(y_i - \hat{y}_i) \frac{\partial^2 f_i(\hat{\beta}, \mathbf{x}_i)}{\partial \hat{\beta} \partial \mathbf{x}_i} - \frac{\partial f_i(\hat{\beta}, \mathbf{x}_i)}{\partial \hat{\beta}} \left(\frac{\partial f_i(\hat{\beta}, \mathbf{x}_i)}{\partial \mathbf{x}_i} \right)^T \right]$$

Influence on the predicted value

Let $\mathbf{f}(\hat{\boldsymbol{\beta}}) = (f_1(\hat{\boldsymbol{\beta}}, \mathbf{x}_1), f_2(\hat{\boldsymbol{\beta}}, \mathbf{x}_2), \dots, f_n(\hat{\boldsymbol{\beta}}, \mathbf{x}_n))^T$ be the vector of predicted values. The influence of y_i on the predicted value is given by

$$\frac{\partial \mathbf{f}(\hat{\boldsymbol{\beta}})}{\partial y_i} = \frac{\partial \mathbf{f}(\hat{\boldsymbol{\beta}})}{\partial \hat{\boldsymbol{\beta}}} \frac{\partial \hat{\boldsymbol{\beta}}}{\partial y_i} = \mathbf{GH}^{-1} \frac{\partial f_i(\hat{\boldsymbol{\beta}}, \mathbf{x}_i)}{\partial \hat{\boldsymbol{\beta}}}$$

where

$$\mathbf{G} = \frac{\partial \mathbf{f}(\hat{\boldsymbol{\beta}})}{\partial \hat{\boldsymbol{\beta}}}$$

This can be generalized to

$$\frac{\partial \mathbf{f}(\hat{\boldsymbol{\beta}})}{\partial \mathbf{y}} = \mathbf{GH}^{-1} \mathbf{G}^T,$$

which is called the **Jacobian leverage**.

Logistic Regression

Consider the logistic regression model:

$$P(y_i = 1) = \frac{e^{\boldsymbol{\beta}^T \mathbf{x}_i}}{1 + e^{\boldsymbol{\beta}^T \mathbf{x}_i}}$$

For logistic regressions, we use MLE.

The log-likelihood function is given by

$$\ell(\boldsymbol{\beta}) = \sum_{i=1}^n \left[y_i \boldsymbol{\beta}^T \mathbf{x}_i - \log(1 + e^{\boldsymbol{\beta}^T \mathbf{x}_i}) \right]$$

The score function is given by

$$\frac{\partial \ell(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = \sum_{i=1}^n y_i \mathbf{x}_i - \sum_{i=1}^n \frac{e^{\boldsymbol{\beta}^T \mathbf{x}_i}}{1 + e^{\boldsymbol{\beta}^T \mathbf{x}_i}} \mathbf{x}_i = \sum_{i=1}^n \frac{1}{1 + e^{\boldsymbol{\beta}^T \mathbf{x}_i}} \mathbf{x}_i - \sum_{i=1}^n (1 - y_i) \mathbf{x}_i$$

Influence of the covariate on the MLE

Take the partial derivative of the score function w.r.t. \mathbf{x}_i , we have

$$-(1 - y_i)\mathbf{I} + \frac{1}{1 + e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_i}}\mathbf{I} - \frac{e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_i}}{(1 + e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_i})^2}\hat{\boldsymbol{\beta}}\mathbf{x}_i^T - \sum_j \frac{e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_j}}{(1 + e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_j})^2} \frac{\partial \hat{\boldsymbol{\beta}}}{\partial \mathbf{x}_i} \mathbf{x}_j \mathbf{x}_j^T = 0$$

This gives the influence of the covariate on the MLE:

$$\frac{\partial \hat{\boldsymbol{\beta}}}{\partial \mathbf{x}_i} = \left[(y_i - \hat{p}_i)\mathbf{I} - \frac{e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_i}}{(1 + e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_i})^2}\hat{\boldsymbol{\beta}}\mathbf{x}_i^T \right] \mathbf{H}^{-1},$$

where

$$\mathbf{H} = \sum_{j=1}^n \frac{e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_j}}{(1 + e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_j})^2} \mathbf{x}_j \mathbf{x}_j^T, \quad \hat{p}_i = \frac{e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_i}}{1 + e^{\hat{\boldsymbol{\beta}}^T \mathbf{x}_i}}$$

Influence on the predicted probability

The predicted probability is given by

$$\hat{p}_i = \frac{e^{\hat{\beta}^T \mathbf{x}_i}}{1 + e^{\hat{\beta}^T \mathbf{x}_i}}$$

The influence of \mathbf{x}_i on the predicted probability is given by the chain rule:

$$\frac{\partial \hat{p}_i}{\partial \mathbf{x}_i} = \frac{\partial \hat{p}_i}{\partial \hat{\beta}} \frac{\partial \hat{\beta}}{\partial \mathbf{x}_i} + \frac{\partial \hat{p}_i}{\partial \mathbf{x}_i} \Big|_{\hat{\beta}} = \frac{e^{\hat{\beta}^T \mathbf{x}_i}}{(1 + e^{\hat{\beta}^T \mathbf{x}_i})^2} \left[\left[(y_i - \hat{p}_i) \mathbf{I} - \frac{e^{\hat{\beta}^T \mathbf{x}_i}}{(1 + e^{\hat{\beta}^T \mathbf{x}_i})^2} \hat{\beta} \mathbf{x}_i^T \right] \mathbf{H}^{-1} \mathbf{x}_i + \hat{\beta} \right]$$

Influence of measurement error

Now we consider the assumption that the covariate \mathbf{x}_i are fixed and known. We consider a broader model with measurement error in the covariate such that

$$\mathbf{x}_i = \mathbf{z}_i + \sigma \mathbf{s}_i,$$

where \mathbf{z}_i is the designed covariate, \mathbf{s}_i is the standardized measurement error, and σ is the standard deviation of the measurement error.

The model is given by

$$P(y_i = 1) = H(\boldsymbol{\gamma}^T \mathbf{u}_i + \tau \mathbf{x}_i)$$

for some probability function H .

The observed model is

$$P(y_i = 1) = \mathbb{E}_s[H(\boldsymbol{\gamma}^T \mathbf{u}_i + \tau \mathbf{z}_i + \tau \sigma \mathbf{s})]$$

The parameters is $\boldsymbol{\beta} = (\boldsymbol{\gamma}, \tau)^T$.

Influence of measurement error

The influence of the measurement error on the MLE is given by

$$\left. \frac{\partial \hat{\boldsymbol{\beta}}}{\partial \sigma^2} \right|_{\sigma^2=0} \approx -\frac{1}{\tau^2} \mathbf{H}^{-1} \left(\sum_{i=1}^n \frac{H_i'' H_i'}{H_i(1-H_i)} \begin{bmatrix} \mathbf{u}_i \\ z_i \end{bmatrix} \right)$$

with

$$\mathbf{H} = \sum_{i=1}^n \frac{H_i'^2}{H_i(1-H_i)} \begin{bmatrix} \mathbf{u}_i \\ z_i \end{bmatrix} \begin{bmatrix} \mathbf{u}_i \\ z_i \end{bmatrix}^T$$

Proof: see textbook Chapter 9.10.

Influence analysis for the LME model

Recall the LME model:

$$\mathbf{y}_i = \mathbf{X}_i\boldsymbol{\beta} + \mathbf{Z}_i\mathbf{b}_i + \boldsymbol{\epsilon}_i$$

with $\mathbf{b}_i \sim N(0, \sigma^2\mathbf{D})$ and $\boldsymbol{\epsilon}_i \sim N(0, \sigma^2\mathbf{I})$.

The MLE of $\boldsymbol{\beta}$ is given by

$$\hat{\boldsymbol{\beta}} = \mathbf{H}^{-1}\mathbf{s},$$

where

$$\mathbf{H} = \sum_{i=1}^N \mathbf{X}_i^T \mathbf{V}_i^{-1} \mathbf{X}_i, \quad \mathbf{s} = \sum_{i=1}^N \mathbf{X}_i^T \mathbf{V}_i^{-1} \mathbf{y}_i, \quad \mathbf{V}_i = \mathbf{I} + \mathbf{Z}_i \hat{\mathbf{D}} \mathbf{Z}_i^T$$

Influence analysis for the LME model

The **leverage matrix** for the LME model is defined as

$$\mathbf{P}_i = \frac{\partial \hat{\mathbf{y}}_i}{\partial \mathbf{y}_i}$$

with $\hat{\mathbf{y}}_i = \mathbf{X}_i \hat{\boldsymbol{\beta}}$.

Then we have

$$\mathbf{P}_i = \mathbf{X}_i \mathbf{H}^{-1} \mathbf{X}_i^T \mathbf{V}_i^{-1}$$

and we can verify that

$$\text{tr}(\mathbf{P}_i) = m.$$

Influence analysis for the LME model

The influence of the response variable on the MLE is

$$\frac{\partial \hat{\boldsymbol{\beta}}}{\partial \mathbf{y}_i} = \mathbf{H}^{-1} \mathbf{X}_i^T \mathbf{V}_i^{-1}$$

The influence of the covariate on the MLE is given by

$$\frac{\partial \hat{\boldsymbol{\beta}}}{\partial x_{ijk}} = \mathbf{H}^{-1} \left(\mathbf{E}_{ijk}^T \mathbf{V}_i^{-1} (\mathbf{y}_i - \hat{\mathbf{y}}_i) - \mathbf{X}_i^T \mathbf{V}_i^{-1} \mathbf{E}_{ijk} \hat{\boldsymbol{\beta}} \right)$$

where \mathbf{E}_{ijk} is an $n_i \times m$ matrix with only (j, k) -th element equal to 1.

Influence analysis for the LME model

Now we consider removing the i -th cluster from the dataset. The leave-one-out estimator is given by

$$\begin{aligned}\hat{\boldsymbol{\beta}}_{(i)} &= [\mathbf{H} - \mathbf{X}_i^T \mathbf{V}_i^{-1} \mathbf{X}_i]^{-1} [\mathbf{s} - \mathbf{X}_i^T \mathbf{V}_i^{-1} \mathbf{y}_i] \\ &= \boldsymbol{\beta} - \mathbf{H}^{-1} \mathbf{X}_i^T \mathbf{V}_i^{-1} (\mathbf{I} - \mathbf{P}_i)^{-1} (\mathbf{y}_i - \hat{\mathbf{y}}_i)\end{aligned}$$

Therefore, we can define the generalized Cook's distance for LME as

$$D_i = \frac{1}{m\hat{\sigma}^2} (\mathbf{y}_i - \hat{\mathbf{y}}_i)^T (\mathbf{I} - \mathbf{P}_i)^{-1} \mathbf{V}_i^{-1} \mathbf{X}_i \mathbf{H}^{-1} \mathbf{X}_i^T \mathbf{V}_i^{-1} (\mathbf{I} - \mathbf{P}_i)^{-1} (\mathbf{y}_i - \hat{\mathbf{y}}_i)$$