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Using diagnostic measures to detect non-MCAR processes in linear regression models with missing covariates

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Abstract

This paper presents methods to analyze and detect non-MCAR processes that lead to missing covariate values in linear regression models. First, the data situation and the problem is sketched. The next section provides an overview of the methods that deal with missing covariate values. The idea of using outlier methods to detect non-MCAR processes is described in section 3. Section 4 uses these ideas to introduce a graphical method to visualize the problem. Possible extensions conclude the presentation.

1 Data and problem

We consider the classical linear regression model

\[ y(n \times 1) = X(n \times p) \beta(p \times 1) + \epsilon(n \times 1) \]

with missing data in the \( n \times p \) covariate matrix \( X \). Reorganization of the \( n \) rows of the data matrix \( X \), the corresponding elements of the response \( y \) and the error term \( \epsilon \) leads to the following structure

\[
\begin{pmatrix}
  y_c \\
  y_{\text{mis}}
\end{pmatrix} =
\begin{pmatrix}
  X_c \\
  X_{\text{mis}}
\end{pmatrix} \beta +
\begin{pmatrix}
  \epsilon_c \\
  \epsilon_{\text{mis}}
\end{pmatrix}
\]

The index \( c \) indicates the completely observed submodel whereas the index \( \text{mis} \) corresponds to the submodel with missing values in the covariate matrix \( X_{\text{mis}} \) (note that \( y_{\text{mis}} \) is completely observed).

Using the missing data indicator matrix \( R \) introduced by (Rubin, 1976)

\[
R_{ij} = \begin{cases} 
1 & \text{if } Z_{ij} \text{ is observed} \\
0 & \text{if } Z_{ij} \text{ is missing}
\end{cases}
\]

with data \( Z_{ij} = (y_i, X_{ij}) \), the missing mechanism can be characterized by the conditional distribution \( f(R|Z, \phi) \) of \( R \) given the data \( Z \) and an unknown parameter \( \phi \). The \( n \times (p+1) \) matrix \( Z \) consists of observed data \( Z_{\text{obs}} \) and unobserved values \( Z_{\text{mis}} \).

The data are said to be missing completely at random (MCAR) if the distribution of \( R \) given \( Z \) and \( \phi \) only depends on the unknown parameter \( \phi \) for any \( Z \), i.e.

\[
f(R|Z, \phi) = f(R|\phi) \quad \forall Z.
\]

If the conditional distribution of \( R \) depends on \( Z \) only via the observed values \( Z_{\text{obs}} \) (for all \( Z_{\text{mis}}, \) i.e.

\[
f(R|Z, \phi) = f(R|Z_{\text{obs}}, \phi) \quad \forall Z_{\text{mis}},
\]

the data are called missing at random (MAR).

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The optimal estimator is the Gauss-Markov estimator $b$ applied to the data in (1):

$$b = \left( \begin{pmatrix} X_c \\ X_{\text{mis}} \end{pmatrix} \right)^t \left( \begin{pmatrix} X_c \\ X_{\text{mis}} \end{pmatrix} \right)^{-1} \left( \begin{pmatrix} X_c \\ X_{\text{mis}} \end{pmatrix} \right)^t \left( \begin{pmatrix} y_c \\ y_{\text{mis}} \end{pmatrix} \right) = (X_c^t X_c + X_{\text{mis}}^t X_{\text{mis}})^{-1} (X_c^t y_c + X_{\text{mis}}^t y_{\text{mis}}). \quad (2)$$

Due to the unknown values in $X_{\text{mis}}$, of course this estimator can not be used directly. There are a variety of methods that deal with this problem.

2 Dealing with missing values

A simple and often used method is to discard all the information available in $(y_{\text{mis}}, X_{\text{mis}})$ and to use the completely observed data in $(y_c, X_c)$ only:

$$b_c = (X_c^t X_c)^{-1} X_c^t y_c.$$ 

Using the available information in $Z$ by estimating

$$\beta = \Sigma_{xx}^{-1} \Sigma_{xy},$$

where the elements of $\Sigma_{xx}$ and $\Sigma_{xy}$ are formed by using all jointly observed pairs $x_{ij}, x_{iv}, y_i$ and $x_{ij}, y_i$ is called the available case method.

Maximum likelihood procedures address the missing data problem by factoring the joint distribution

$$f(Z, R|\theta, \xi) = f(Z|\theta) f(R|Z, \xi).$$

Integration over the missing data $Z_{\text{mis}}$ yields

$$f(Z_{\text{obs}}, R|\theta, \xi) = \int f(Z, R|\theta, \xi) dZ_{\text{mis}} = \int f(R|Z, \xi) f(Z|\theta) dZ_{\text{mis}}.$$ 

If $f(R|Z)$ depends only on the observed data $Z_{\text{obs}}$, i.e. the MAR assumption holds, we have

$$f(Z_{\text{obs}}, R|\theta, \xi) = f(R|Z_{\text{obs}}, \xi) \int f(Z|\theta) dZ_{\text{mis}} = f(R|Z_{\text{obs}}, \xi) f(Z_{\text{obs}}|\theta),$$

which is why the missing data mechanism is also called ignorable in this case.

Imputation procedures form a different approach to the problem. Here the missing values in $X_{\text{mis}}$ are replaced by new values. Having done this by some procedure, the estimator (2) with $X_{\text{mis}}$ replaced by $X_R$ with $X_R$ as described below becomes operational.

To replace the unknown values in $X_{\text{mis}}$ a variety of imputation methods exist: mean imputation or zero order regression (ZOR) replaces an unknown value $x_{ij}$ by the mean $\bar{x}_j$, either formed of the complete cases in $X_c$ or the available cases in $X_c$ and $X_{\text{mis}}$.

Conditional mean imputation or first order regression (FOR) uses auxiliary regressions to find replacements for the missing values. Regressing the covariate with missing values on the remaining covariates (with parameters estimates based on the complete cases) yields predictions of the missing values that are used as substitutes. If the response $y$ is also used in these regressions a stochastic element is introduced (see Buck (1960) or Tootenbug and Shalab (1998)).

Multiple Imputation (Rubin, 1987; Schafer, 1997) repeats the imputation step and averages the results. While a single imputation is too smooth, the differences between the individual imputation steps can be properly used to estimate the variance as the sum of the average variance within the imputed data sets and the between imputation variance. This strategy reflects the uncertainty about the imputation process which is ignored in a single imputation strategy.

By replacing a missing value by $x_R$, the model (2) becomes the mixed model

$$\begin{pmatrix} y_c \\ y_R \end{pmatrix} = \begin{pmatrix} X_c \\ X_R \end{pmatrix} \beta + \begin{pmatrix} 0 \\ \delta \end{pmatrix} + \begin{pmatrix} e_c \\ e_R \end{pmatrix},$$
where $\delta$ addresses the difference between the true but unknown values in $X_{\text{mis}}$ and their replacements in $X_R$. Using the mixed estimator (Theil and Goldberger, 1961) we have

$$
\begin{align*}
 b &= \left( \begin{pmatrix} X_c^T & X_R^T \end{pmatrix} \begin{pmatrix} X_c & X_R \end{pmatrix} \right)^{-1} \begin{pmatrix} X_c^T & X_R^T \end{pmatrix} \begin{pmatrix} y_c^T \\ y_\ast^T \end{pmatrix} \\
   &= (X_c^T X_c + X_R^T X_R)^{-1} (X_c^T y_c + X_R^T y_\ast).
\end{align*}
$$

The weighted-mixed-estimator introduced by Schaffrin and Toutenburg (1990) uses a weight $\lambda < 1$ for the values in $(y_{\text{mis}}, X_R)$

$$
\begin{align*}
 b(\lambda) &= (X_c^T X_c + \lambda X_R^T X_R)^{-1} (X_c^T y_c + \lambda X_R^T y_\ast).
\end{align*}
$$

This estimator may be interpreted as the familiar mixed estimator in the model

$$
\begin{align*}
 \left( \frac{y_c}{\sqrt{\lambda} y_\ast} \right) &= \left( \frac{X_c}{\sqrt{\lambda} X_R} \right) \beta + \left( \sqrt{\lambda} \right) \varepsilon_c.
\end{align*}
$$

### 3 MCAR diagnosis with outlier measures

Popular diagnostics to detect non-MCAR processes contain the comparison of correlation or covariance matrices, the comparison of means (\(y_c\) vs. \(y_{\text{mis}}\)) or a more general test as described by Little (????). For the situation with only one column affected by missing values Simon and Simonoff (1986) present diagnostic plots where 'envelopes' are compared.

The idea first presented by Simonoff (1988) combines the missing data problem with statistics that derive from the outlier detection field. A comparison of the values of a statistic computed with and without imputation is the comparison of the sub-samples $Z_c$ and $Z_{\text{mis}}$.

If the imputation of values can be considered appropriate under MCAR and we really have MCAR (which is the null hypothesis $H_0$), the statistics should be 'more or less' the same. If we have something other than MCAR, the statistics should reflect this by having different values.

Simonoff (1988) uses Cook's distance, which is based on the confidence ellipsoid

$$
C = \frac{(\hat{\beta}_c - \tilde{\beta}_c)(X'_c X_c)(\hat{\beta}_c - \tilde{\beta}_c)}{ps^2},
$$

the residual sum of squares $DRSS$ (Andrews and Pregibon, 1978)

$$
DRSS = \frac{(RSS_c - RSS_{\text{mis}})/(n_{\text{mis}})}{RSS_c/(n_c - n_{\text{mis}} - p + 1)},
$$

and the determinant of the $X'X$ matrix $DXX$ (Andrews and Pregibon, 1978)

$$
DXX = \frac{|X'_c X_c|}{|X'_c X_c|}.
$$

For the construction of tests the distribution of the measures under $H_0$ is needed. As this distribution also depends on the $X$ values, Monte Carlo methods are used to determine it by first computing the complete case statistics, and imputing missing values under MCAR-assumption. The generation of new response values

$$
\tilde{y}_{\text{mis}}^\text{MC} = X_{\text{mis}} \tilde{\beta} + \varepsilon_{\text{mis}}^\text{MC}
$$

with $\varepsilon_{\text{mis}}^\text{MC} \sim N(0, \sigma^2 I)$ generates a new data set where 'missing values' are drawn from using an MCAR mechanism.

After applying the imputation procedure to these data the diagnostic measures are computed. Repeating the 'data deletion' and imputation steps a null distribution of the diagnostic measure is generated. Finally the measure can be applied to the imputed original data and the resulting value can be compared to the null distribution.
4 Graphical diagnosis of the missing mechanism

Animated residual plots are presented in Cook and Weisberg (1989). In a stepwise procedure weights between 0 and 1 are used to include one case into the regression. The plots thus represent the influence of that single case. Park, Kim and Toutenburg (1992) present a similar approach to visualize the inclusion of a further variable into a regression model.

The adaption to the situation with missing data which shows a close relationship to the procedures of the preceding section is described in ?. Like in the above procedures, imputation is performed under an MCAR assumption. Having filled the gaps in $X_{\text{mis}}$, the weighted-mixed-estimator (3) is computed for certain values $\lambda \in [0, 1]$. Again the ideas is, that if we really have MCAR, there should not be any tendency in the residual plot, when stepwise including $Z_R$ in the model by increasing the weight from 0 to 1.

Figure 1 shows a small program that visualizes the following procedure:

```java
for (\lambda = 0; \lambda \leq 1; \lambda += \text{step}) {
    \text{compute regression parameters;}
    \text{compute estimated residuals;}
    \text{display residual-plot;}
}
```

![Figure 1](image)

Figure 1: Java program for visualization on computer screen. Reads data for each frame of the animation and draws the single plots of the animation. See http://www.stat.uni-muenchen.de/~andreas/

The residual plot in figure 2 shows an example of an animated plot of $\hat{y}$ (on the X-axis) versus $\epsilon$ (on the Y-axis) for a model $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$ with missing data generated by a non MAR process where $P(R_2 = 0)$ (a value $x_2$ is missing) depends on $x_2$.

An increasing $\lambda$ gives higher weight to the imputed data in the estimation of the regression parameters. The center of the residual plot in figure 2 shifts towards the origin. For $\lambda = 1$ the imputed data have the same weight as the complete data and biased estimated result. $\lambda = 0$ (the complete case estimator) on the other hand gives consistent estimates as the missing process is independent of the response $y$.

5 Possible extensions

The ideas of animated residual plots could be extended in various ways. Imagine a simultaneous plot of $\epsilon$ vs. $\hat{y}$ vs. $X_i$ in different windows where the windows are linked. By brushing selected points of the plot could be highlighted in all windows and their location or movement can be studied while the value of $\lambda$ changes.

Univariate plots $y$ vs. $X_j$ for all $j$ together with the estimated regression line $\hat{\beta}_0 + \hat{\beta}_j X_j$, where the points are static (as the imputation does not depend on the weight $\lambda$) and the estimated regression line is dynamic. Again, these plots could be linked as described above.

Creation of a null plot where missing values are created artificially by a known MCAR mechanism. This plot can be used as a means of comparison in order to have an idea of what the plot should look like under MCAR.


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Figure 2: Residual plot of $y$ (X-axis) versus $\epsilon$ (Y-axis) for a model $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$ with a non MAR process where $P(R_{ij} = 0)$ (a value $x_{ij}$ is missing) depends on $x_{ij}$. $\lambda$ from 0 (top left) to 1 (bottom right).
