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RESIDUALS IN THE GROWTH CURVE MODEL

DIETRICH VON ROSEN

Department of Mathematics, Uppsala University, Box 480, S-751 06 Uppsala, Sweden

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Abstract. Residuals for the Growth Curve model will be discussed. In univariate linear models as well as the ordinary multivariate analysis of variance model residuals are based on the difference between the observations and the mean whereas for the Growth Curve model we have three different residuals all showing various aspects useful for validating analysis. For these residuals some basic properties are established.

Key words and phrases: GMANOVA, Growth Curve model, residuals.

1. Introduction

In this paper we will discuss residuals in the Growth Curve model due to Potthoff and Roy (1964). For more details we refer to von Rosen (1994) where the results, via Edgeworth type expansions, are applied to a real data set. According to the terminology put forward in von Rosen (1989) we will refer to the model as a $MLNM(ABC)$. The reason for this notation follows from the next definition as well as from some extensions presented in von Rosen (1989).

DEFINITION 1.1. The $MLNM(ABC)$. Let $X : p\times n$, $A : p\times q$ $q \leq p$, $B : q\times k$, $C : k \times n$ $\rho(C) + p \leq n$ and $\Sigma : p \times p$ is positive definite. The columns of X are independently p-variate normally distributed with an unknown dispersion matrix Σ and $E[X] = ABC$, where A and C are known design matrices and B is an unknown parameter matrix.

In the definition as well as in the sequel $\rho(\cdot)$ denotes the rank. The $MLNM(ABC)$ is an extension of the ordinary multivariate analysis of variance model and is applicable when a linear mean structure exists within the experimental units. There exist many fields where the $MLNM(ABC)$ has been applied. In particular the model is useful for analysing short time series of repeated measurements when little knowledge about the covariance structure is available. For example, growth curves. Fundamental to all analysis with the $MLNM(ABC)$ are the interpretation of the design matrices A and C. In our setting A models the within individuals structure, i.e. the repeated measurements on each experimental unit, and C models the between individuals structure, i.e. C is the same design matrix as in univariate linear models and ordinary multivariate analysis of variance. For reviews of the model and related works see Woolson and Leeper (1980), Seber (1984) or von Rosen (1991). Maximum likelihood estimators for the parameters in the $MLNM(ABC)$ are given by (e.g. see Srivastava and Khatri (1979) or von Rosen (1989))

$$\hat{B} = (A'S^{-1}A)^{-}A'S^{-1}XC'(CC')^{-} + (A')^{o}Z_1 + A'Z_2C^{o'}, \tag{1.1}$$

where Z_1 and Z_2 are arbitrary matrices,

$$S = X(I - C'(CC')^{-}C)X' \tag{1.2}$$

and

$$\begin{aligned} n\hat{\Sigma} &= (X - A\hat{B}C)(X - A\hat{B}C)' \\ &= S + SA^{o}(A^{o'}SA^{o})^{-1}A^{o'}XC'(CC')^{-}CX'A^{o}(A^{o'}SA^{o})^{-1}A^{o'}S. \end{aligned} \tag{1.3}$$

In (1.1) and (1.3) we have used the notation A^o for any matrix of full rank which is spanning the orthogonal complement to $\mathcal{C}(A)$, i.e. $\mathcal{C}(A^o) = \mathcal{C}(A)^{\perp}$ where $\mathcal{C}(A)$ stands for the linear space generated by the columns of A (column vector space, range space). The matrix A^o is not unique but all results presented in this paper will be invariant with respect to the choice of A^o (see formula 2.4 given below). Furthermore, in (1.1)–(1.3), $^{-}$ stands for an arbitrary g-inverse in the sense of $GG^{-}G = G$. The estimator $\hat{\Sigma}$ is always unique and $\hat{B}$ is unique if A and C are of full rank. Since (1.1) is a weighted estimator with a random weight S^{-1} (1.1) is more difficult to handle than univariate least squares estimators. Furthermore, note that

$$A\hat{B}C = A(A'S^{-1}A)^{-}A'S^{-1}XC'(CC')^{-}C \tag{1.4}$$

which is always unique.

2. Residuals

In principle, when doing inference there are mainly two different strategies. One is to require as few assumptions as possible for the data, leading to so called robust methods. The other approach is to find models and then inference is based on these models together with diagnostic tools for validating the model. When considering univariate linear models many diagnostic tools are based on residuals. There exist many types of residuals, e.g. ordinary residuals, studentized residuals, external residuals, internal residuals (see Belsley *et al.* (1980), Cook and Weisberg (1982)), recursive residuals (Tobing and McGilchrist (1992)), as well as others. However, for multivariate linear models very few results exist and for the $MLNM(ABC)$, to our knowledge, any discussion of residuals does not exist. Hence, if using the $MLNM(ABC)$ in practise, it is important to fill this gap and indeed, some completely new problems arise.

In the univariate linear model, $X = \beta C + \epsilon$, the residuals are obtained if projecting X on $\mathcal{C}(C')^\perp$, i.e. $X(I - C'(CC')^- C)$. In the $MLNM(ABC)$ there are two spaces of interest, namely $\mathcal{C}_\Sigma(A)$ and $\mathcal{C}(C)$, or more precisely the tensor product of these, i.e. $\mathcal{C}(C') \otimes \mathcal{C}_\Sigma(A)$. Here $\mathcal{C}_\Sigma(A)$ means that we have an inner product which is defined by aid of Σ^{-1}, i.e. $(x, y) = x'\Sigma^{-1}y$ and $\mathcal{C}(A) = \mathcal{C}_I(A)$. Unfortunately, for the $MLNM(ABC)$, Σ is unknown, but we see that the maximum likelihood estimators, given by (1.1) and (1.3), respectively, are build up with the help of projectors where the inner product is based on S^{-1}. Hence, maximum likelihood theory tells us that we can replace Σ by S. Furthermore, from (1.4) follows that $A\hat{B}C$ is obtained with the help of the projection of X on $\mathcal{C}(C') \otimes \mathcal{C}_S(A)$. In order to study residuals according to ideas for univariate linear models we will study $(\mathcal{C}(C') \otimes \mathcal{C}_S(A))^\perp$, i.e. residuals are defined on the space which is orthogonal to the space generated by the design matrices. Typically for the $MLNM(ABC)$ is that $(\mathcal{C}(C') \otimes \mathcal{C}_S(A))^\perp$ consists of three orthogonal spaces:

$$(\mathcal{C}(C') \otimes \mathcal{C}_S(A))^\perp = \mathcal{C}(C')^\perp \otimes \mathcal{C}_S(A)^\perp \boxplus \mathcal{C}(C')^\perp \otimes \mathcal{C}_S(A) \boxplus \mathcal{C}(C') \otimes \mathcal{C}_S(A)^\perp,$$

where $\boxplus$ stands for the orthogonal sum. Hence the following residuals are obtained;

$$R_1 = SA^o(A^{o'}SA^o)^- A^{o'}X(I - C'(CC')^- C), \tag{2.1}$$

$$R_2 = A(A'S^{-1}A)^- A'S^{-1}X(I - C'(CC')^- C), \tag{2.2}$$

$$R_3 = SA^o(A^{o'}SA^o)^- A^{o'}XC'(CC')^- C, \tag{2.3}$$

where R_1 is obtained from the space $\mathcal{C}(C')^\perp \otimes \mathcal{C}_S(A)^\perp$, R_2 from $\mathcal{C}(C')^\perp \otimes \mathcal{C}_S(A)$ and R_3 from $\mathcal{C}(C') \otimes \mathcal{C}_S(A)^\perp$. If we for simplicity just will look at $R_1 + R_2$ and R_3 the interpretation is fairly clear. $R_1 + R_2 = X(I - C'(CC')^- C)$ represents the difference between the observation and $XC'(CC')^- C$ (the mean) and R_3 reflects the difference between the mean and the estimated model $A\hat{B}C$, since (2.3) is identical to $R_3 = XC'(CC')^- C - A\hat{B}C$ which follows from the fact that

$$I - A(A'S^{-1}A)^- A'S^{-1} = SA^o(A^{o'}SA^o)^- A^{o'}. \tag{2.4}$$

However, we recommend that R_1 and R_2 should be calculated separately because elements in these matrices may appear with opposite sign and of the same size and then elements in $R_1 + R_2$ will be close to zero.

Remember that $\mathcal{C}_\Sigma(A)$ represents the within individuals structure. Hence, if studing R_1 and R_2 separately we note that R_2 stands for the projection of the difference between the observation and the mean on $\mathcal{C}_S(A)$ whereas R_1 stands for the projection of the difference between the observation and the mean on $\mathcal{C}_S(A)^\perp$. This means that both R_1 and R_3 mirror the within individuals model assumption whereas R_1 and R_2 can be used to investigate the between individuals assumptions.

3. Basic properties

Unfortunately the distribution for (R_1, R_2, R_3) is difficult to obtain as well as the marginal distributions for R_i, $i = 1, 2, 3$. Therefore we will be concentrating on moment relations. These give us a possibility to understand the estimators as well as to approximate the distribution in a convenient manner. Indeed, in practise, already for the univariate linear model the complete distribution for the residuals is not always utilized. For instance, residuals are often treated as if they are independently distributed which is not the case. The most elementary properties for R_1, R_2, R_3 are presented in our first theorem and especially for graphical representations of residuals they may be important. Let $C_r[R_i]$ represent the cumulants of R_i of r-th order and in particular $C_1[R_i] = E[R_i]$ and $C_2[R_i] = D[R_i] = E[\operatorname{vec}(R_i - E[R_i])\operatorname{vec}'(R_i - E[R_i])]$. In the theorem $\overset{k}{\otimes} R_i$ stands for $\underbrace{R_i \otimes R_i \otimes \cdots \otimes R_i}_{k \text{ times}}$ and $\overset{0}{\otimes} R_i = 1$ where $\otimes$ stands for the right Kronecker product.

THEOREM 3.1. *Let R_1, R_2 and R_3, respectively be given by* (2.1), (2.2) *and* (2.3). *Then*

(i) $E[R_i] = 0$, $i = 1, 2, 3$,

(ii) $E[\overset{r}{\otimes} R_i] = 0$, $i = 1, 2, 3$ *for odd* r,

(iii) $C_r[R_i] = 0$, $i = 1, 2, 3$ *for odd* r.

PROOF. R_i, $i = 1, 2$, are odd functions in $X(I - C'(CC')^- C)$ which in turn is normally distributed with mean zero. Since the normal distribution is symmetric $E[R_i] = 0$, $i = 1, 2$. For R_3 it is noted that $XC'(CC')^- C$ is independent of S and since $E[A^{o'} XC'(CC')^- C] = 0$ we obtain that $E[R_3] = 0$. These results can immediately be generalized to cover moments of odd order, i.e. $E[\overset{r}{\otimes} R_i] = 0$, $i = 1, 2, 3$, for odd r. Furthermore, by the correspondence of moments and cumulants (iii) follows from (ii). □

One consequence of the theorem is that the distribution for the residuals are symmetric.

In the subsequent it will be convenient to rewrite R_i in a canonical form and we will use the following representation;

$$A^{o'} = T(I_{p-\rho(A)} : 0)\Gamma\Sigma^{-1/2}$$

where T is non-singular, $\Gamma' = (\Gamma_1' : \Gamma_2')\; p\times p-\rho(A) : p\times\rho(A)$ is orthogonal and $\Sigma^{1/2}$ is supposed to be symmetric. Furthermore let, $Y \sim N_{p,n}(0, I, I - C'(CC')^- C)$, $Y' = (Y_1' : Y_2')\; n-\rho(C)\times p-\rho(A) : n-\rho(C)\times\rho(A)$ and $Z \sim N_{p,n}(0, I, C'(CC')^- C)$. Observe that Z and Y are independent and that also Y_1 and Y_2 are independent. Using these definitions we obtain from (2.1), (2.2) and (2.3) canonical representations of the residuals, i.e.

$$R_1' \sim Y_1'(Y_1Y_1')^{-1}Y_1Y'\Gamma\Sigma^{1/2} = \{Y_1' : Y_1'(Y_1Y_1')^{-1}Y_1Y_2'\}\Gamma\Sigma^{1/2} \tag{3.1}$$

$$R_2' \sim (I - Y_1'(Y_1Y_1')^{-1}Y_1)Y'\Gamma\Sigma^{1/2} = (I - Y_1'(Y_1Y_1')^{-1}Y_1)Y_2'\Gamma_2\Sigma^{1/2} \tag{3.2}$$

$$R_3' \sim Z'(Y_1Y_1')^{-1}Y_1Y'\Gamma\Sigma^{1/2} = Z'\{I : (Y_1Y_1')^{-1}Y_1Y_2'\}\Gamma\Sigma^{1/2} \tag{3.3}$$

where $\sim$ stands for equality in distribution. Furthermore, for later use note that

$$\begin{aligned} \Sigma^{1/2}\Gamma_1'\Gamma_1\Sigma^{1/2} &= \Sigma - A(A'\Sigma^{-1}A)^-A' \quad \text{and} \\ \Sigma^{1/2}\Gamma_2'\Gamma_2\Sigma^{1/2} &= A(A'\Sigma^{-1}A)^-A'. \end{aligned} \tag{3.4}$$

The next theorem includes the covariance matrix between two matrices U and V which is given by $C[U,V] = E[\mathrm{vec}(U)\,\mathrm{vec}(V)'] - E[\mathrm{vec}(U)]E[\mathrm{vec}(V)']$ where the vec-operator is the operator defined by vec: $R^{n\times m} \to R^{nm}$, $xy' \to y \otimes x$ for vectors x and y of size n and m, respectively.

THEOREM 3.2. *Let* R_1, R_2 *and* R_3, *respectively be given by* (2.1), (2.2) *and* (2.3). *Then* $C[R_i, R_j] = 0$, $i \neq j$, $i,j = 1,2,3$.

PROOF. From (3.1) and (3.2) follows since Y_1 and Y_2 are independent that

$$\begin{aligned} C[R_1,R_2] &= E[\mathrm{vec}(\Sigma^{1/2}\Gamma_1'Y_1)\,\mathrm{vec}'\{\Sigma^{1/2}\Gamma_2'Y_2(I - Y_1'(Y_1Y_1')^{-1}Y_1)\}] \\ &\quad + E[\mathrm{vec}(\Sigma^{1/2}\Gamma_2'Y_2Y_1'(Y_1Y_1')^{-1}Y_1)\,\mathrm{vec}'(\Sigma^{1/2}\Gamma_2'Y_2(I - Y_1'(Y_1Y_1')^{-1}Y_1))] \\ &= 0 + E[(Y_1'(Y_1Y_1')^{-1}Y_1)(I - Y_1'(Y_1Y_1')^{-1}Y_1)] \otimes \Sigma^{1/2}\Gamma_2\Gamma_2'\Sigma^{1/2} = 0. \end{aligned}$$

We also have, because S and $XC'(CC')^-C$ are independent and $E[X] = ABC$, that

$$\begin{aligned} C[R_2,R_3] &= E[\mathrm{vec}\{A(A'S^{-1}A)^-A'S^{-1}X(I - C'(CC')^-C)\} \\ &\qquad \times E[\mathrm{vec}'\{XC'(CC')^-C\}](I \otimes A^o(A^{o\prime}SA^o)^{-1}A^{o\prime}S)] = 0. \end{aligned}$$

The proof that $C[R_1,R_3] = 0$ is identical. □

In Theorem 3.2 we have established that R_1, R_2 and R_3 are uncorrelated. It would be of advantage for the interpretation of the values of the residuals if the residuals also are independently distributed. However, the next lines show that this is not the case. If R_1 and R_2 are independent they must be normally distributed because $R_1 + R_2 = X(I - C'(CC')^-C)$ is normally distributed which is a well known characteristic of the class of normal distributions. We are going to show that R_2 is not normally distributed and from (3.2) follows that it is enough to show that $Y_2Y_1'(Y_1Y_1')^-Y_1$ is not normally distributed which also confirms that R_1 can not be normally distributed. It would indeed be very suprising if this expression is normally distributed. Put

$$H = E[\overset{2}{\otimes}\, Y_2Y_1'(Y_1Y_1')^-Y_1]$$

and if $Y_2Y_1'(Y_1Y_1')^-Y_1$ is normally distributed the fourth ordered moments are related to H in the following manner;

$$\begin{aligned} &E[\overset{4}{\otimes}\, Y_2Y_1'(Y_1Y_1')^-Y_1] \\ &\quad = \overset{2}{\otimes} H + (I_r \otimes K_{r,r} \otimes I_r)(\overset{2}{\otimes} H)(I_s \otimes K_{s,s} \otimes I_s) + K_{r,r^3}(\overset{2}{\otimes} H)K_{s^3,s} \end{aligned}$$

where $K_{u,v}$ stands for the commutation matrix (see Magnus and Neudecker (1979)), $r = p - \rho(A)$ and $s = n - \rho(C)$. However, since Y_2 is normally distributed and is independent of Y_1 this is only true if

$$E[\overset{2}{\otimes} Y_1'(Y_1Y_1')^- Y_1] = \overset{2}{\otimes} E[Y_1'(Y_1Y_1')^- Y_1]$$

which is not the case. To show that R_1 and R_3 are not independent we may note that

$$E[R_1R_1' \otimes R_3R_3'] \neq E[R_1R_1'] \otimes E[R_3R_3'].$$

Similar calculations also give that R_2 and R_3 can not be independent. However, note that R_1R_1' and R_2R_2' are independent. As already mentioned we will in this paper not obtain the exact distributions of the residuals because they are complicated. The only simple distribution property which we are able to obtain is that R_2R_2' is Wishart distributed, i.e. $W_p(A(A'\Sigma^{-1}A)^-A', n - \rho(C) - p + \rho(A))$.

In univariate linear models and the ordinary multivariate analysis of variance model the residuals are independent. Therefore it is of interest to see how the residuals R_1, R_2 and R_3 are related to the estimated mean structure $A\hat{B}C$.

THEOREM 3.3. *Let R_1, R_2 and R_3, respectively be given by* (2.1), (2.2) *and* (2.3), *and let $A\hat{B}C$ be as in* (1.4). *Then* $C[R_i, A\hat{B}C] = 0$, $i = 1, 2$, *and*

$$C[R_3, A\hat{B}C] = -\frac{p - \rho(A)}{n - \rho(C) - p + \rho(A) - 1} C'(CC')^- C \otimes A(A'\Sigma^{-1}A)^- A'$$
$$\text{if} \quad n - \rho(C) - p + \rho(A) - 1 > 0.$$

PROOF. Since $C[R_i, A\hat{B}C] = C[R_i, ABC]$, $i = 1, 2$, the first part is proved. The second part follows from a result in Grizzle and Allen (1969) concerning the dispersion matrix for $\hat{B}$ since

$$C[R_3, A\hat{B}C] = C[XC'(CC')^-C, A\hat{B}C] - D[A\hat{B}C]$$

and

$$\begin{aligned} C[XC'(CC')^-C, A\hat{B}C] &= D[XC'(CC')^-C](I \otimes E[S^{-1}A(A'S^{-1}A)^-A'] \\ &= (C'(CC')^-C \otimes \Sigma)(I \otimes \Sigma^{-1}A(A'\Sigma^{-1}A)^-A') \\ &= C'(CC')^-C \otimes A(A'\Sigma^{-1}A)^-A'. \end{aligned}$$ □

Theorem 3.3 establishes that R_i, $i = 1, 2$ and $A\hat{B}C$ are uncorrelated but in the same manner as it was shown that the residuals are not independent it can also be shown that $\hat{R}_i$, $i = 1, 2$, and $A\hat{B}C$ are not independent.

In the next theorem we are going to obtain the dispersion matrices for the residuals. These give then some ideas about the randomness among the elements in R_i and then, to some extent, can be used to identify extreme observations.

THEOREM 3.4. *Let R_1, R_2 and R_3, respectively be given by* (2.1), (2.2) *and* (2.3). *Then if* $n - \rho(C) - p + \rho(A) - 1 > 0$

(i) $D[R_1] = (I - C'(CC')^- C) \otimes \Sigma - c_1(I - C'(CC')^- C) \otimes A(A'\Sigma^{-1}A)^- A'$,
(ii) $D[R_2] = c_1(I - C'(CC')^- C) \otimes A(A'\Sigma^{-1}A)^- A'$,
(iii) $D[R_3] = C'(CC')^- C \otimes \Sigma - c_2 C'(CC')^- C \otimes A(A'\Sigma^{-1}A)^- A'$
where

$$c_1 = \frac{n - \rho(C) - p + \rho(A)}{n - \rho(C)},$$
$$c_2 = \frac{n - \rho(C) - 2(p - \rho(A)) - 1}{n - \rho(C) - p + \rho(A) - 1}.$$

PROOF. Since Y_1 and $Y_2Y_1'(Y_1Y_1')^{-1}Y_1$ are uncorrelated straightforward calculations yield

$$D[R_1] = D[\Sigma^{1/2}\Gamma_1'Y_1] + D[\Sigma^{1/2}\Gamma_2'Y_2Y_1'(Y_1Y_1')^{-1}Y_1].$$

Now,

$$D[\Sigma^{1/2}\Gamma_1'Y_1] = (I - C'(CC')^- C) \otimes \Sigma^{1/2}\Gamma_1'\Gamma_1\Sigma^{1/2}$$

and

$$D[\Sigma^{1/2}\Gamma_2'Y_2Y_1'(Y_1Y_1')^{-1}Y_1] = E[Y_1'(Y_1Y_1')^{-1}Y_1] \otimes \Sigma^{1/2}\Gamma_2'\Gamma_2\Sigma^{1/2}.$$

If using (3.4) and that

$$E[Y_1'(Y_1Y_1')^{-1}Y_1] = \frac{p - \rho(A)}{n - \rho(C)}(I - C'(CC')^- C), \tag{3.5}$$

$D[R_1]$ in (i) is established.

$D[R_2]$ in (ii) is obtained since R_1 and R_2 are uncorrelated and $R_1 + R_2 = X(I - C'(CC')^- C)$. For $D[R_3]$ in (iii) we note that

$$D[R_3] = C'(CC')^- C \otimes \{\Sigma^{1/2}\Gamma_1'\Gamma_1\Sigma^{1/2} + \Sigma^{1/2}\Gamma_2'E[Y_2Y_1'(Y_1Y_1')^{-1}(Y_1Y_1')^{-1}Y_1Y_2']\Gamma_2\Sigma^{1/2}\}$$

and some calculations together with (3.4) establishes the theorem. □

If the intention is to apply the results in Theorem 3.4 we have to estimate $D[R_i]$ $i = 1, 2, 3$. Unbiased estimators are given in the next theorem.

THEOREM 3.5. *Let* $D[R_i]$, $i = 1, 2, 3$ *be given in Theorem* 3.4. *The following estimators are unbiased.*
(i) $\hat{D}[R_1] = (I - C'(CC')^- C) \otimes \hat{\Sigma}$
$+(\frac{\rho(C)}{n}c_2 - c_1)\frac{n}{n-\rho(C)-p+\rho(A)}(I - C'(CC')^- C) \otimes A(A'\hat{\Sigma}^{-1}A)^- A'$,
(ii) $\hat{D}[R_2] = \frac{n}{n-\rho(C)}(I - C'(CC')^- C) \otimes A(A'\hat{\Sigma}^{-1}A)^- A'$,
(iii) $\hat{D}[R_3] = C'(CC')^- C \otimes \{\hat{\Sigma}$
$+(\frac{\rho(C)}{n}c_2 - c_2)\frac{n}{n-\rho(C)-p+\rho(A)}C'(CC')^- C \otimes A(A'\hat{\Sigma}^{-1}A)^- A'\}$.

PROOF. For this theorem it is utilized that

$$E[\hat{\Sigma}] = \Sigma - \frac{\rho(C)c_2}{n} A(A'\Sigma^{-1}A)^{-}A'$$

which was obtained by von Rosen (1990). Furthermore,

$$\begin{aligned} (3.6)\quad & nA(A'\hat{\Sigma}^{-1}A)^{-}A' \\ & = A(A'S^{-1}A)^{-}A' \sim W_p(A(A'\Sigma^{-1}A)^{-}A', n - \rho(C) - p + \rho(A)) \end{aligned}$$

and combining these two results verifies the theorem. □

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