Modeling Residual Covariance Structure

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Introduction

In this module, we examine the implications of linear combination theory for the modeling of the residual covariance structure in growth curve modeling. We discover that there are a number of possible forms for this covariance structure, and these forms require differing numbers of degrees of freedom to model. Consequently, there is a possibility that a more "compact" model may be able to account for our growth curve data.

A Model for Cognitive Performance

Our discussion in this section will be built around a particular example and data set"

1. Willett (1988) examined cognitive performance on a "opposites naming" task over the course of 4 weeks
2. In this time-structured data set, 35 people completed an inventory once every week
3. In addition, at wave 1, each person also completed a test of general cognitive ability (COG), which (after centering) is used as a level-2 predictor to predict both slopes and intercepts

```
> data <- read.table("opposites_pp.txt",header=T,sep=",")
> attach(data)
> options(digits=9)
```

A Model for Cognitive Performance

Denoting $X_i = COG_i - \overline{COG}$, and $T_i = TIME_i$ to simplify the notation, the standard multilevel model is

$$\begin{aligned} Y_{ij} &= \pi_{0i} + \pi_{1i} T_j + \epsilon_{ij} && (1) \\ \pi_{0i} &= \gamma_{00} + \gamma_{01} X_i + \zeta_{0i} && (2) \\ \pi_{1i} &= \gamma_{10} + \gamma_{11} X_i + \zeta_{1i} && (3) \end{aligned}$$

where

$$\epsilon_{ij} \overset{iid}{\sim} N(0, \sigma^2_\epsilon) \quad (4)$$

and

$$\begin{bmatrix} \zeta_{0i} \\ \zeta_{1i} \end{bmatrix} \overset{iid}{\sim} N\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \sigma_0^2 & \sigma_{01} \\ \sigma_{10} & \sigma_1^2 \end{bmatrix} \right) \quad (5)$$

A Model for Cognitive Performance

Combining Equations 1 – 5, we get the composite model

$$Y_{ij} = \gamma_{00} + \gamma_{10} T_j + \gamma_{01} X_i + \gamma_{11} X_i \times T_j + r_{ij} \tag{6}$$

where the composite residual r_{ij} is

$$r_{ij} = \epsilon_{ij} + \zeta_{0i} + \zeta_{1i} T_j \tag{7}$$

In using Equation 7 above, we will need to remember that, for given i and/or j, T_j is a constant while the ϵ_{ij}, ζ_{0i}, and ζ_{1i} are random variables

The Residual Vector

Suppose we were to list the Y_{ij} in order in a vector $\boldsymbol{y}$.

There would be a corresponding vector $\boldsymbol{r}$ containing the residuals.

Since these residuals are random variables, they have a multivariate distribution, and we can derive the residual variance-covariance matrix using the standard rules for linear combinations. For simplicity, suppose there were just 2 people, and therefore only 8 observations. The vector $\boldsymbol{r}$ would look like this:

The Residual Vector

$$\boldsymbol{r} = \begin{bmatrix} r_{11} \\ r_{12} \\ r_{13} \\ r_{14} \\ r_{21} \\ r_{22} \\ r_{23} \\ r_{24} \end{bmatrix} = \begin{bmatrix} \epsilon_{11} + \zeta_{01} + \zeta_{11} T_1 \\ \epsilon_{12} + \zeta_{01} + \zeta_{11} T_2 \\ \epsilon_{13} + \zeta_{01} + \zeta_{11} T_3 \\ \epsilon_{14} + \zeta_{01} + \zeta_{11} T_4 \\ \epsilon_{21} + \zeta_{02} + \zeta_{12} T_1 \\ \epsilon_{22} + \zeta_{02} + \zeta_{12} T_2 \\ \epsilon_{23} + \zeta_{02} + \zeta_{12} T_3 \\ \epsilon_{24} + \zeta_{02} + \zeta_{12} T_4 \end{bmatrix} \tag{8}$$

The Variance of a Residual

Consider the residual $r_{ij} = \epsilon_{ij} + \zeta_{0i} + \zeta_{1i} T_j$. What is its variance? To answer this question, we simply apply the heuristic rule, remembering that for a given j, T_j is a constant. We *could* begin by squaring the expression. However, recall that our beginning assumption is that every ϵ_{ij} is independent of everything, including any other ϵ. So

$$\begin{aligned}
\mathrm{Var}(r_{ij}) &= \mathrm{Var}(\epsilon_{ij}) + \mathrm{Var}(\zeta_{0i} + \zeta_{1i} T_j) \\
&= \sigma_\epsilon^2 + \mathrm{Var}(\zeta_{0i} + T_j \zeta_{1i}) \\
&= \sigma_\epsilon^2 + \mathrm{Var}(\zeta_{0i}) + \mathrm{Var}(T_j \zeta_{1i}) + 2\,\mathrm{Cov}(\zeta_{0i}, T_j \zeta_{1i}) \\
&= \sigma_\epsilon^2 + \mathrm{Var}(\zeta_{0i}) + T_j^2\,\mathrm{Var}(\zeta_{1i}) + 2\,T_j\,\mathrm{Cov}(\zeta_{0i}, \zeta_{1i}) \\
&= \sigma_\epsilon^2 + \sigma_0^2 + T_j^2 \sigma_1^2 + 2\,T_j \sigma_{01} \qquad (9)
\end{aligned}$$

The Covariance of an Individual's Residuals

Uncorrelated ϵ_{ij}

For different individuals, none of the individual constituents of the r_{ij} are correlated, so residuals across individuals must have zero covariance. However, for a given individual, the residuals *will be correlated.* Let's derive the covariance for two residuals at different times on the same individual. Again since ϵ_{ij} and $\epsilon_{ij'}$ are independent of each other and everything else, they cannot contribute to covariance, so we can simplify the calculation by eliminating them before applying the heuristic rule

$$
\begin{aligned}
\mathrm{Cov}(r_{ij}, r_{ij'}) &= \mathrm{Cov}(\zeta_{0i} + \zeta_{1i} T_j, \zeta_{0i} + \zeta_{1i} T_{j'}) \\
&= \mathrm{Cov}(\zeta_{0i}, \zeta_{0i}) + \mathrm{Cov}(\zeta_{1i} T_j, \zeta_{0i}) \\
&\quad + \mathrm{Cov}(\zeta_{0i}, \zeta_{1i} T_{j'}) + \mathrm{Cov}(\zeta_{1i} T_j, \zeta_{1i} T_{j'}) \\
&= \mathrm{Var}(\zeta_{0i}) + T_j \,\mathrm{Cov}(\zeta_{1i}, \zeta_{0i}) \\
&\quad + T_{j'} \,\mathrm{Cov}(\zeta_{0i}, \zeta_{1i}) + T_j T_{j'} \,\mathrm{Cov}(\zeta_{1i}, \zeta_{1i}) \\
&= \mathrm{Var}(\zeta_{0i}) + T_j \,\mathrm{Cov}(\zeta_{0i}, \zeta_{1i}) \\
&\quad + T_{j'} \,\mathrm{Cov}(\zeta_{0i}, \zeta_{1i}) + T_j T_{j'} \,\mathrm{Var}(\zeta_{1i}) \\
&= \sigma_0^2 + (T_j + T_{j'})\sigma_{01} + T_j T_{j'} \sigma_1^2 \qquad (10)
\end{aligned}
$$

The Covariance of an Individual's Residuals

Correlated ϵ_{ij}

So far, we have assumed that the within-subject residuals are uncorrelated across time. However, there are excellent reasons to believe that frequently this will not be the case.

So, suppose, for a given individual i, $\mathrm{Cov}(\epsilon_{ij}, \epsilon ij') \neq 0$.

What will be the new equation for $\mathrm{Cov}(r_{ij}, r_{ij'})$? (C.P.)

$$\mathrm{Cov}(r_{ij}, r_{ij'}) = \sigma_0^2 + (T_j + T_{j'})\sigma_{01} + T_j T_{j'}\sigma_1^2 + ?? \tag{11}$$

The Covariance of an Individual's Residuals

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So, suppose, for a given individual i, $\mathrm{Cov}(\epsilon_{ij}, \epsilon_{ij'}) \neq 0$.

What will be the new equation for $\mathrm{Cov}(r_{ij}, r_{ij'})$? (C.P.)

$$\mathrm{Cov}(r_{ij}, r_{ij'}) = \sigma_0^2 + (T_j + T_{j'})\sigma_{01} + T_j T_{j'}\sigma_1^2 + \mathrm{Cov}(\epsilon_{ij}, \epsilon_{ij'}) \quad (12)$$

Block Diagonal Covariance Matrix

As shown in Equations 7.9 and 7.10 on page 250 of Singer and Willett, the vector of residuals will have a covariance matrix that is typically referred to as *block diagonal*. For the first 8 observations, for example, the covariance matrix will look like this:

$$\begin{bmatrix}
\sigma^2_{r_{11}} & \sigma_{r_{11},r_{12}} & \sigma_{r_{11},r_{13}} & \sigma_{r_{11},r_{14}} & 0 & 0 & 0 & 0 \\
\sigma_{r_{12},r_{11}} & \sigma^2_{r_{12}} & \sigma_{r_{12},r_{13}} & \sigma_{r_{12},r_{14}} & 0 & 0 & 0 & 0 \\
\sigma_{r_{13},r_{11}} & \sigma_{r_{13},r_{12}} & \sigma^2_{r_{13}} & \sigma_{r_{13},r_{14}} & 0 & 0 & 0 & 0 \\
\sigma_{r_{14},r_{11}} & \sigma_{r_{14},r_{12}} & \sigma_{r_{14},r_{13}} & \sigma^2_{r_{14}} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma^2_{r_{21}} & \sigma_{r_{21},r_{22}} & \sigma_{r_{21},r_{23}} & \sigma_{r_{21},r_{24}} \\
0 & 0 & 0 & 0 & \sigma_{r_{22},r_{21}} & \sigma^2_{r_{22}} & \sigma_{r_{22},r_{23}} & \sigma_{r_{22},r_{24}} \\
0 & 0 & 0 & 0 & \sigma_{r_{23},r_{21}} & \sigma_{r_{23},r_{22}} & \sigma^2_{r_{23}} & \sigma_{r_{23},r_{24}} \\
0 & 0 & 0 & 0 & \sigma_{r_{24},r_{21}} & \sigma_{r_{24},r_{22}} & \sigma_{r_{24},r_{23}} & \sigma^2_{r_{24}}
\end{bmatrix}$$

Block Diagonal Covariance Matrix

Singer and Willett refer to the 4×4 block representing the within-subject covariance matrix of composite residuals as $\mathbf{\Sigma}_r$.

Under the assumptions of the model, the compound residuals in the mixed model have a particular structural form given by Equation 12.

The simplest version, which Singer and Willett refer to as the "standard" version, is given by Equation 10.

As we have seen, this "standard" structure is a rather complicated function of model parameters and the coded values of time.

Singer and Willett then go on to discuss other ways of *directly modeling* the covariance structure *of the composite residuals.*

Error Covariance Structure in Matrix Format

Recall how the model for the ith individual can be expressed in matrix format as

$$\begin{aligned} \boldsymbol{y}_i &= \boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{Z}_i\boldsymbol{b}_i + \boldsymbol{\epsilon}_i \\ &= \boldsymbol{X}_i\boldsymbol{\beta} + \boldsymbol{r}_i \end{aligned}$$

$$\boldsymbol{b}_i \sim N(\mathbf{0}, \boldsymbol{\Psi}), \quad \boldsymbol{\epsilon}_i \sim N(\mathbf{0}, \sigma^2\boldsymbol{\Lambda}_i) \tag{13}$$

where $\boldsymbol{X}_i$ is the fixed effects regressor matrix for the ith person, and $\boldsymbol{Z}_i$ is the random effects regressor matrix, which usually contains a subset (perhaps all) of the columns of $\boldsymbol{X}_i$. The vector $\boldsymbol{\beta}$ contains fixed effects, while $\boldsymbol{b}_i$ contains the random effects. Note that the general form has the covariance matrix of the ϵ_i as $\sigma^2\boldsymbol{\Lambda}_i$, where $\boldsymbol{\Lambda}_i$ is a correlation matrix, while the "standard assumption" has $\boldsymbol{\Lambda} = \boldsymbol{I}$.

Composite Residual Covariance Structure

From standard matrix algebra, since $\boldsymbol{r}_i = \boldsymbol{Z}_i \boldsymbol{b}_i + \boldsymbol{\epsilon}_i$, we have

$$\text{Cov}(\boldsymbol{r}_i) = \boldsymbol{Z}_i \boldsymbol{\Psi} \boldsymbol{Z}_i' + \sigma^2 \boldsymbol{\Lambda}_i \tag{14}$$

The standard assumption of uncorrelated within-subject errors (the ϵ_{ij}) gives

$$\text{Cov}(\boldsymbol{r}_i) = \boldsymbol{Z}_i \boldsymbol{\Psi} \boldsymbol{Z}_i' + \sigma^2 \boldsymbol{I} \tag{15}$$

Example Computation

For example, consider the result of fitting the model on page 247, using, as Singer and Willett did, REML.

```
> library(lme4)
> fit.1 <- lmer( OPP ~ TIME + CCOG + TIME:CCOG + (1+TIME|ID))
> fit.1

Linear mixed model fit by REML
Formula: OPP ~ TIME + CCOG + TIME:CCOG + (1 + TIME | ID)
     AIC     BIC   logLik deviance REMLdev
 1276.28 1299.82 -630.142  1266.96 1260.28
Random effects:
 Groups   Name        Variance  Std.Dev. Corr
 ID       (Intercept) 1236.4132 35.16267
          TIME         107.2492 10.35612 -0.489
 Residual              159.4771 12.62843
Number of obs: 140, groups: ID, 35

Fixed effects:
              Estimate Std. Error  t value
(Intercept) 164.374291   6.206096 26.48594
TIME         26.959981   1.993950 13.52089
CCOG         -0.113553   0.504012 -0.22530
TIME:CCOG     0.432858   0.161933  2.67306

Correlation of Fixed Effects:
          (Intr) TIME   CCOG
TIME      -0.522
CCOG       0.000  0.000
TIME:CCOG  0.000  0.000 -0.522
```

Example Computation

We can get the estimated $\mathbf{\Psi}$ with a bit more precision with the `VarCorr` function:

```
> VarCorr(fit.1)

$ID
            (Intercept)        TIME
(Intercept) 1236.413173 -178.233362
TIME        -178.233362  107.249200
attr(,"stddev")
(Intercept)        TIME
 35.1626673  10.3561190
attr(,"correlation")
             (Intercept)         TIME
(Intercept)  1.000000000 -0.489452056
TIME        -0.489452056  1.000000000

attr(,"sc")
 sigmaREML
12.6284257

> Psi <- matrix(c(1236.413173, -178.233362,-178.233362,107.2492),2,2)
```

Example Computation

Since the data are time-structured, all the $\boldsymbol{Z}_i$ are the same, i.e.,

$$\boldsymbol{Z} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \tag{16}$$

```
> Z <- matrix(c(1,1,1,1,0,1,2,3),4,2)
> sigma <- 12.6284257
> I <- diag(1,4,4)
```

Example Computation

We can compute the covariance matrix of the composite residuals in R easily as

```
> cov.r <- Z %*% Psi %*% t(Z) + sigma^2 * I
> cov.r
```

```
            [,1]        [,2]        [,3]        [,4]
[1,] 1395.890309 1058.179811  879.946449  701.713087
[2,] 1058.179811 1146.672785  916.211487  845.227325
[3,]  879.946449  916.211487 1111.953661  988.741563
[4,]  701.713087  845.227325  988.741563 1291.732937
```

For ease of comparison with Equation 7.14 on page 255 of Willett and Singer, we can round to one decimal place. There are some discrepancies.

```
> Singer.Willett.7.14 <- matrix(c(1395.9,1058.2,880,701.7,1058.2,1146.8,
+ 916.2,845.2,880,916.2,1112.3,988.8,701.7,845.2,988.8,1294.4),4,4)
> round(Singer.Willett.7.14 - cov.r,1)
```

```
     [,1] [,2] [,3] [,4]
[1,]  0.0  0.0  0.1  0.0
[2,]  0.0  0.1  0.0  0.0
[3,]  0.1  0.0  0.3  0.1
[4,]  0.0  0.0  0.1  2.7
```

The discrepancies are probably attributable to rounding differences in most cases, but careful tracing of the calculation of element (4,4) of the matrix on page 252 shows what appears to be a “digit transfer” in their rounded computation. Specifically, using the rounded values on page 252, one obtains 1292.4, rather than the printed value of 1294.4.

Which Residual Structure?

In modeling the covariance structure of residuals, one has several choices which can and should be motivated by both theoretical and practical concerns.

Let's review some of the major choices.

Fixed Effects Only

If the model has only fixed effects, then one may write

$$\boldsymbol{y}_i = \boldsymbol{X}_i \boldsymbol{\beta} + \boldsymbol{\epsilon}_i \tag{17}$$

In this case, the classic assumption is that $\mathrm{Cov}(\boldsymbol{y}_i) = \mathrm{Cov}(\boldsymbol{\epsilon}_i) = \sigma^2 \boldsymbol{I}$. A more relaxed assumption is that $\mathrm{Cov}(\boldsymbol{y}_i) = \mathrm{Cov}(\boldsymbol{\epsilon}_i) = \sigma^2 \boldsymbol{\Lambda_i}$ In either case, the definition of the "residual" is clear, it is the ϵ_i term.

Modeling the Composite Residual

If the model includes fixed and random effects, then the covariance matrix of the $\boldsymbol{y}_i$ is determined by both the random effects term $\boldsymbol{Z}_i\boldsymbol{b}_i$ *and* the error term $\boldsymbol{\epsilon}_i$, as shown above in Equation 14.

Modeling the Composite Residual

Singer and Willett present the scalar algebra equivalent of Equation 14, and call it the "standard structure" for the covariance matrix of the "composite residual" $\boldsymbol{r}_i = \boldsymbol{Z}_i \boldsymbol{b}_i + \boldsymbol{\epsilon}_i$. They then propose to go on and model other structures for the covariance matrix of $\boldsymbol{r}_i$. It is important to realize that when modeling "other structures," you have, more or less, dispensed with the random effects term, and are no longer fitting a random effects model. You are now, in fact, fitting the model of Equation 13.

Modeling the Composite Residual

This choice may be reasonable in some contexts. However, if you are comparing the "standard structure" of Equation 15 with some other structure, the models are not nested, because you have, by directly altering the covariance structure of the $\boldsymbol{r}_i$ instead of the $\boldsymbol{\epsilon}_i$, implicitly, wiped out the random effects term and simultaneously changed the model for the covariance structure of the $\boldsymbol{\epsilon}_i$.

Modeling the Error Term

In a model with both fixed and random effects, and alternative to modeling the covariance structure of the composite residual is to model the covariance structure of the $\boldsymbol{\epsilon}_i$, that is, model the structure of the matrix $\boldsymbol{\Lambda}_i$. This option is not discussed by Singer and Willett in their Chapter 7 treatment.

Choosing between the Two Residual Modeling Options

Pinheiro and Bates (2000), in their book "Mixed-Effects Models in S and S-Plus," delineate carefully between the options of

1. Dropping the random effects contribution and modeling the covariance structure of the $\boldsymbol{r}_i$, using the `gls` function, and
2. Keeping the random effects contribution and modeling the covariance structure of the $\boldsymbol{\epsilon}_i$, using the `\lme` function

Choosing between the Two Residual Modeling Options

The choice between an `lme` *model and a* `gls` *model should take into account more than just information criteria and likelihood tests. A mixed-effects model has a hierarchical structure which, in many applications, provides a more intuitive way of accounting for within-group dependency than the direct modeling of the marginal variance-covariance structure of the response in the* `gls` *approach. Furthermore, the mixed-effects estimation gives, as a byproduct, estimates for the random effects, which may be of interest in themselves. The* `gls` *model focuses on marginal inference and is more appealing when a hierarchical structure for the data is not believed to be present, or is not relevant in the analysis, and one is more interested in parameters associated with the error variance-covariance structure, as in time-series analysis and spatial statistics. (Pinheiro & Bates, 2000, pp 254–255.)*

Unstructured

This is just a general, positive-definite covariance matrix. It adds a significant number of free parameters to the fitting process, since a $p \times p$ covariance matrix has $p(p+1)/2$ non-redundant elements.

$$\begin{bmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} & \sigma_{14} \\ \sigma_{21} & \sigma_2^2 & \sigma_{23} & \sigma_{24} \\ \sigma_{31} & \sigma_{32} & \sigma_3^2 & \sigma_{34} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_4^2 \end{bmatrix} \tag{18}$$

Compound Symmetry

$$\begin{bmatrix} \sigma^2 + \sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \\ \sigma_1^2 & \sigma^2 + \sigma_1^2 & \sigma_1^2 & \sigma_1^2 \\ \sigma_1^2 & \sigma_1^2 & \sigma^2 + \sigma_1^2 & \sigma_1^2 \\ \sigma_1^2 & \sigma_1^2 & \sigma_1^2 & \sigma^2 + \sigma_1^2 \end{bmatrix} \tag{19}$$

Heterogeneous Compound Symmetry

$$\begin{bmatrix} \sigma_1^2 & \sigma_2\sigma_1\rho & \sigma_3\sigma_1\rho & \sigma_4\sigma_1\rho \\ \sigma_2\sigma_1\rho & \sigma_2^2 & \sigma_3\sigma_2\rho & \sigma_4\sigma_2\rho \\ \sigma_3\sigma_1\rho & \sigma_3\sigma_2\rho & \sigma_3^2 & \sigma_4\sigma_3\rho \\ \sigma_4\sigma_1\rho & \sigma_4\sigma_2\rho & \sigma_4\sigma_3\rho & \sigma_4^2 \end{bmatrix} \tag{20}$$

Autoregressive

$$\begin{bmatrix} \sigma^2 & \sigma^2\rho & \sigma^2\rho^2 & \sigma^2\rho^3 \\ \sigma^2\rho & \sigma^2 & \sigma^2\rho & \sigma^2\rho^2 \\ \sigma^2\rho^2 & \sigma^2\rho & \sigma^2 & \sigma^2\rho \\ \sigma^2\rho^3 & \sigma^2\rho^2 & \sigma^2\rho & \sigma^2 \end{bmatrix} \tag{21}$$

Heterogeneous Autoregressive

$$\begin{bmatrix} \sigma_1^2 & \sigma_2\sigma_1\rho & \sigma_3\sigma_1\rho^2 & \sigma_4\sigma_1\rho^3 \\ \sigma_2\sigma_1\rho & \sigma_2^2 & \sigma_3\sigma_2\rho & \sigma_4\sigma_2\rho^2 \\ \sigma_3\sigma_1\rho^2 & \sigma_3\sigma_2\rho & \sigma_3^2 & \sigma_4\sigma_3\rho \\ \sigma_4\sigma_1\rho^3 & \sigma_4\sigma_2\rho^2 & \sigma_4\sigma_3\rho & \sigma_4^2 \end{bmatrix} \tag{22}$$

Toeplitz

$$\begin{bmatrix} \sigma^2 & \sigma_1 & \sigma_2 & \sigma_3 \\ \sigma_1 & \sigma^2 & \sigma_1 & \sigma_2 \\ \sigma_2 & \sigma_1 & \sigma^2 & \sigma_1 \\ \sigma_3 & \sigma_2 & \sigma_1 & \sigma^2 \end{bmatrix} \tag{23}$$

Fixed Effects Modeling of Composite Residual Structure with R

Using the R function `gls` in the `nlme` library, we can model the covariance structure of a fixed-effects linear model. Pinheiro and Bates (2000) refer to this as the *extended linear model*, because it replaces the normal assumption that the $\boldsymbol{\epsilon}_i$ have a covariance matrix of $\sigma^2 \boldsymbol{I}$ with a more complex model. This model may assume that variances are equal, or it may allow them to be unequal. Various models for the correlation structure of the errors are supported. This option is discussed in detail by Pinheiro and Bates (2000), Section 5.4.

Mixed Effects Modeling with Nonstandard Residual Covariance Structure

The R function `lme` in the `nlme` library has a facility for modeling the covariance structure of residuals within the mixed model framework. This capability is discussed in Chapter 5 of Pinheiro and Bates (2000).