

Multivariate Linear Models with Kronecker Product Structure

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- Covariance structure of Kronecker type

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- Estimators

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The correlation may be due to time dependence, spacial dependence or some other underlying latent process which is not observable.

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For example,

- in environmental sciences: when studying catchment areas we have both spacial and temporal correlations,
- in neurosciences: when evaluating PET-image voxels, voxels are also both temporally and spacially correlated,
- in array technology: many antigens are represented on slides with observations over time, i.e. we have correlations between antigens as well over time.

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where $\mathbf{y} : pq \times 1$, $\boldsymbol{\mu} : pq \times 1$, $\boldsymbol{\Psi} : q \times q$, $\boldsymbol{\Sigma} : p \times p$, and \otimes denotes the Kronecker product.

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where $\mathbf{y} : pq \times 1$, $\boldsymbol{\mu} : pq \times 1$, $\boldsymbol{\Psi} : q \times q$, $\boldsymbol{\Sigma} : p \times p$, and \otimes denotes the Kronecker product.

Both $\boldsymbol{\Psi}$ and $\boldsymbol{\Sigma}$ are unknown but it will be supposed that they are positive definite.

Due to the Kronecker product structure, we may convert $\mathbf{y} : pq \times 1$ into a matrix $\mathbf{Y} : p \times q$ which is matrix normally distributed, i.e. $\mathbf{Y} \sim N_{p,q}(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\Psi})$, where now $\boldsymbol{\mu}$ is a $p \times q$ matrix.

Wilks (1946), Votaw (1948), Srivastava (1965), Olkin (1973), Arnold (1973), Boik (1991), Naik & Rao (2001), Chaganty & Naik (2002), Lu & Zimmerman (2005), Roy & Khattree (2005).

Covariance with Kronecker structure

We assume that we have n observations, $\mathbf{Y}_i \sim N_{p,q}(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\Psi})$, whereas in the classical case one usually has one observation matrix $\mathbf{Y} \sim N_{p,q}(\boldsymbol{\mu}, \boldsymbol{\Sigma}, \mathbf{I})$.

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The dispersion matrix of a matrix \mathbf{Y}_i is defined by a vectorized form, i.e. $D[\mathbf{Y}_i] = D[\text{vec}(\mathbf{Y}_i)]$, where vec is the usual vec-operator. In our models

$$D[\mathbf{Y}_i] = \boldsymbol{\Psi} \otimes \boldsymbol{\Sigma}.$$

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We shall exploit how the independent "matrix-observations" can be used to estimate $\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\Psi}$ with and without certain bilinear structures on $\boldsymbol{\mu}$.

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The product $\Psi \otimes \Sigma$ takes into consideration both Ψ and Σ .

Indeed, $\Psi \otimes \Sigma$ tells us that the overall covariance consists of the products of the covariances in Ψ and Σ , respectively.

Covariance with Kronecker structure

We have

$$\text{Cov}[y_{kl}, y_{rs}] = \sigma_{kr} \psi_{ls},$$

where $\mathbf{Y}_i = (y_{kl})$, $\mathbf{\Sigma} = (\sigma_{kr})$ and $\mathbf{\Psi} = (\psi_{ls})$.

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$\mathbf{\Sigma}$ may consist of the time-dependent covariances and $\mathbf{\Psi}$ takes care of the spacial correlation, or for the array data $\mathbf{\Psi}$ models the dependency between antigens and $\mathbf{\Sigma}$ represents the correlation over time.

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Note that the correlation of y_{kl} and y_{rs} equals

$$\text{corr}[y_{kl}, y_{rs}] = \frac{\sigma_{kr}}{\sqrt{\sigma_{kk}\sigma_{ll}}} \frac{\psi_{ls}}{\sqrt{\psi_{ll}\psi_{ss}}}.$$

.

Growth Curve model

Let us assume that the mean of \mathbf{Y}_i follows a multilinear model, i.e.

$$E[\mathbf{Y}_i] = \mathbf{A}\mathbf{B}\mathbf{C},$$

where $\mathbf{A} : p \times r$ and $\mathbf{C} : s \times q$ are known design matrices.

This type of mean structure was introduced by Potthoff & Roy (1964).

Under the assumption that $\mathbf{\Psi} = \mathbf{I}$ (or $\mathbf{\Psi}$ known), i.e. we have independent columns in \mathbf{Y}_i this will give us the well known Growth Curve model. For details and references connected to the model it is referred to Srivastava & Khatri (1979), Srivastava & von Rosen (1998) or Kollo & von Rosen (2005).

Growth Curve model

Observe that if the matrix $Y_i : p \times q$ is $N_{p,q}(ABC, \Sigma, \Psi)$ distributed we may form a new matrix

$$Y = (Y_1 : Y_2 : \dots : Y_n),$$

which is

$$N_{p,qn}(AB(\mathbf{1}'_n \otimes C), \Sigma, I_n \otimes \Psi),$$

where $\mathbf{1}_n$ is a vector of 1s of size n .

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- The aim is to present estimating equations for estimating B , Σ and Ψ ,
- to show how to estimate the parameters when $FBG = 0$ holds for known matrices F and G .
- based on the MLEs to consider the likelihood ratio test for testing $H_0 : FBG = 0$ versus $H_1 : FBG \neq 0$.

MLEs when Ψ is known

When Ψ is known we have a situation which is almost identical to the classical Growth Curve model setup. The main difference is that now we have n matrix observations instead of 1 , i.e. $N_{p,q}(ABC, \Sigma, \Psi)$.

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Since Ψ is positive definite, we transform the data, i.e. $Y_i = Y_i \Psi^{-1/2}$, where $\Psi^{1/2}$ is a positive definite square root of Ψ .

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Let $Y = (Y_1 : Y_2 : \dots : Y_n) : p \times qn$, then

$$Y \sim N_{p,qn}(AB(\mathbf{1}'_n \otimes C\Psi^{-1/2}), \Sigma, I).$$

MLEs when Ψ is known

From results in Srivastava & Khatri (1979) or Kollo & von Rosen (2005) it follows directly that

$$\begin{aligned} n\hat{B} &= (A'S^{-1}A)^{-1}A'S^{-1}Y(\mathbf{1}_n \otimes \Psi^{-1/2}C'(C\Psi^{-1}C')^{-1}) \\ &\quad + (A')^{\circ}Z_1 + A'Z_2C^{\circ'}, \\ S &= Y(I - n^{-1}\mathbf{1}_n\mathbf{1}_n' \otimes \Psi^{-1/2}C'(C\Psi^{-1}C')^{-1}C\Psi^{-1/2})Y', \end{aligned}$$

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where A'° and C° are any matrices which generate $\mathcal{C}(A')^\perp$ and $\mathcal{C}(C)^\perp$, i.e. the orthogonal complements of $\mathcal{C}(A')$ and $\mathcal{C}(C)$, respectively, and $\mathcal{C}(\cdot)$ denotes the column vector space.

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From results in Srivastava & Khatri (1979) or Kollo & von Rosen (2005) it follows directly that

$$\begin{aligned} n\hat{B} &= (A'S^{-1}A)^- A'S^{-1}Y(\mathbf{1}_n \otimes \Psi^{-1/2}C'(C\Psi^{-1}C')^-) \\ &\quad + (A')^\circ Z_1 + A'Z_2C^{\circ'}, \\ S &= Y(I - n^{-1}\mathbf{1}_n\mathbf{1}_n' \otimes \Psi^{-1/2}C'(C\Psi^{-1}C')^- C\Psi^{-1/2})Y', \end{aligned}$$

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Moreover, $-$ denotes an arbitrary g-inverse, and Z_1 and Z_2 are arbitrary matrices of proper size.

MLEs when Ψ is known

Furthermore,

$$\begin{aligned}nq\hat{\Sigma} &= (Y - A\hat{B}(\mathbf{1}'_n \otimes C\Psi^{-1/2}))(Y - A\hat{B}(\mathbf{1}'_n \otimes C\Psi^{-1/2}))' \\ &= S+n^{-1}SA^\circ(A^\circ' SA^\circ)^{-1}A^\circ' Y(\mathbf{1}_n\mathbf{1}'_n \otimes \Psi^{-1/2}C(C'\Psi^{-1}C)^{-1}C'\Psi^{-1/2})Y' \\ &\quad \times A^\circ(A^\circ' SA^\circ)^{-1}A^\circ' S.\end{aligned}$$

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If $\text{rank}(A)=r$ and $\text{rank}(C)=s$ then \hat{B} is uniquely estimated, i.e.

$$n\hat{B} = (A'S^{-1}A)^{-1}A'S^{-1}Y(\mathbf{1}_n \otimes \Psi^{-1/2}C'(C\Psi^{-1}C')^{-1}).$$

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Note that $\hat{\Sigma}$ is always uniquely estimated.

MLEs when Ψ is known

Turning to the restrictions $F B G = \mathbf{0}$ it is observed that these restrictions are equivalent to

$$B = (F')^\circ \theta_1 + F' \theta_2 G^{\circ'},$$

where θ_1 and θ_2 may be regarded as new parameters. From Theorem 4.1.15 in Kollo & von Rosen (2005) it follows that

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where

$$\begin{aligned} \hat{\theta}_2 = & (F A' T'_1 S_2^{-1} T_1 A F')^{-1} F A' T'_1 S_2^{-1} T_1 Y G^\circ (1_n \otimes \Psi^{-1/2} C' G^\circ) (G^{\circ' C} \Psi^{-1} C' G^\circ)^{-1} \\ & + (F A' T'_1)^\circ Z_{11} + F A' T'_1 Z_{12} (G^{\circ' C})^{\circ' \end{aligned}$$

MLEs when Ψ is known

with

$$T_1 = I - A(F')^\circ ((F')^\circ' A' S_1^{-1} A (F')^\circ)^{-1} (F')^\circ' A' S_1^{-1},$$

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with

$$S_1 = Y(I - n^{-1}\mathbf{1}_n\mathbf{1}'_n \otimes \Psi^{-1/2}C'(C\Psi^{-1}C')^{-1}C\Psi^{-1/2})Y'$$

is assumed to be positive definite,

MLEs when Ψ is known

with

$$\begin{aligned} \mathbf{S}_2 &= \mathbf{S}_1 + \mathbf{T}_1 \mathbf{Y} (n^{-1} \mathbf{1}_n \mathbf{1}_n' \otimes \Psi^{-1/2} \mathbf{C}' (\mathbf{C} \Psi^{-1} \mathbf{C}')^{-1} \mathbf{C} \Psi^{-1/2}) \\ &\times (\mathbf{I} - n^{-1} \mathbf{1}_n \mathbf{1}_n' \otimes \Psi^{-1/2} \mathbf{C}' \mathbf{G}^\circ (\mathbf{G}^{\circ'} \mathbf{C} \Psi^{-1} \mathbf{C}' \mathbf{G}^\circ)^{-1} \mathbf{G}^{\circ'} \mathbf{C} \Psi^{-1/2}) \\ &\times (n^{-1} \mathbf{1}_n \mathbf{1}_n' \otimes \Psi^{-1/2} \mathbf{C}' (\mathbf{C} \Psi^{-1} \mathbf{C}')^{-1} \mathbf{C} \Psi^{-1/2}) \mathbf{Y}' \mathbf{T}_1', \end{aligned}$$

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with

$$\begin{aligned}\hat{\theta}_1 &= (F'^{\circ'} A' S_1^{-1} A (F')^{\circ})^{-1} F'^{\circ'} A' S_1^{-1} (Y - A F' \hat{\theta}_2 G^{\circ'} C \Psi^{-1/2}) \Psi^{-1/2} C' \\ &\quad \times (C \Psi^{-1} C')^{-1} + (F'^{\circ'} A)^{\circ'} Z_{21} + F'^{\circ'} A' Z_{22} C^{\circ'},\end{aligned}$$

where Z_{ij} are arbitrary matrices,

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Furthermore,

$$nq\hat{\Sigma} = (Y - A\hat{B}(1'_n \otimes C\Psi^{-1/2}))(Y - A\hat{B}(1'_n \otimes C\Psi^{-1/2}))'.$$

Explicit estimators when Ψ is unknown

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The main idea is to produce estimators of \mathbf{B} and Σ by neglecting the dependency among columns. Thereafter the off-diagonal elements in Ψ are estimated.

Explicit estimators when Ψ is unknown

Theorem 3.1. Let $Y \sim N_{p,qn}(AB(1'_n \otimes C), \Sigma, I_n \otimes \Psi)$, where $\text{diag}(\Psi)=I$. Unbiased estimators of ABC and Σ are given by

$$\begin{aligned}nA\hat{B}C &= A(A'S^{-1}A)^{-1}A'S^{-1}Y(1_n \otimes C'(CC')^{-1}C), \\q(n-1)\hat{\Sigma} &= S = Y(1_n^\circ(1_n^\circ 1_n^\circ)^{-1}1_n^\circ \otimes I)Y'.\end{aligned}$$

Explicit estimators when Ψ is unknown

Theorem 3.2. Let $Y \sim N_{p,qn}(AB(\mathbf{1}'_n \otimes C), \Sigma, I_n \otimes \Psi)$, where $\text{diag}(\Psi)=I$. A consistent estimator of the unknown elements in Ψ is given by

$$\begin{aligned} \hat{\psi}_{kl} = n^{-1} \text{tr}(\hat{\Sigma}^{-1}(Y(I \otimes e_k) - A\hat{B}(\mathbf{1}'_n \otimes e_k)) \\ \times (Y(I \otimes e_l) - A\hat{B}(\mathbf{1}'_n \otimes e_l))'), \quad k \neq l, \end{aligned}$$

where

$$\begin{aligned} A\hat{B}e_k &= n^{-1}A(A'S^{-1}A)^{-1}A'S^{-1}Y(\mathbf{1}_n \otimes C'(CC')^{-1}e_k), \\ \hat{\Sigma} &= (qn)^{-1}S \end{aligned}$$

and S is given in Theorem 3.1.

Explicit estimators when Ψ is unknown

Theorem 3.3. Let $Y \sim N_{p,qn}(AB(\mathbf{1}'_n \otimes C), \Sigma, I_n \Psi)$, where $\text{diag}(\Psi)=I$ and $FBG = 0$. Unbiased estimators of ABC and Σ

$$\begin{aligned}\widehat{ABC} &= A(F')^\circ \hat{\theta}_1 C + AF' \hat{\theta}_2 G^{\circ'} C, \\ q(n-1) \hat{\Sigma} &= S = Y(\mathbf{1}_n^\circ (\mathbf{1}_n^{\circ'} \mathbf{1}_n^\circ)^{-1} \mathbf{1}_n^{\circ'} \otimes I) Y',\end{aligned}$$

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$$T_1 = I - A(F')^\circ ((F')^\circ A' S^{-1} A(F')^\circ)^{-1} (F')^\circ A' S^{-1},$$

$$\begin{aligned}n \hat{\theta}_1 &= ((F')^\circ A' S^{-1} A(F')^\circ)^{-1} F'^{\circ'} A' S^{-1} (Y - AF' \hat{\theta}_2 G^\circ C \Psi^{-1/2}) \Psi^{-1/2} C' \\ &\quad \times (C \Psi^{-1} C')^{-1} + (F'^{\circ'} A)^\circ Z_{21} + F'^{\circ'} A' Z_{22} C^\circ,\end{aligned}$$

where Z_{ij} are arbitrary matrices.

MLEs of B , Σ and Ψ

The aim is to find maximum likelihood estimators of the parameters in the model

$$Y \sim N_{p,qn}(AB(\mathbf{1}'_n \otimes C), \Sigma, I_n \otimes \Psi).$$

We assume that the uniqueness condition $\psi_{qq} = 1$ holds.

The other diagonal elements of Ψ will be positive but unknown (earlier we assumed $\text{diag}(\Psi) = bI$).

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First we study the following model

$$Y \sim N_{p,qn}(\mu(\mathbf{1}'_n \otimes I), \Sigma, I \otimes \Psi).$$

and thereafter the model with $E[Y] = AB(\mathbf{1}'_n \otimes C)$.

MLEs of B , Σ and Ψ

The likelihood equals

$$L = c |\Sigma|^{-1/2qn} |\Psi|^{-1/2np} e^{-\frac{1}{2} \text{tr}\{\Sigma^{-1}(\mathbf{Y} - \boldsymbol{\mu}(\mathbf{1}'_n \otimes \mathbf{I}_q))(\mathbf{I} \otimes \Psi)^{-1}(\mathbf{Y} - \boldsymbol{\mu}(\mathbf{1}'_n \otimes \mathbf{I}_q))'\}},$$

where c is a proportionality constant which does not depend on the parameters.

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The MLE of the mean equals

$$\hat{\boldsymbol{\mu}} = n^{-1} \mathbf{Y} (\mathbf{1}_n \otimes \mathbf{I}_q)$$

MLEs of B , Σ and Ψ

The MLE of Σ equals

$$nq\hat{\Sigma} = Y(\mathbf{1}_n^o(\mathbf{1}_n^{o'}\mathbf{1}_n^o)\mathbf{1}_n^{o'} \otimes \Psi)Y'.$$

MLEs of B , Σ and Ψ

The MLE of Σ equals

$$nq\hat{\Sigma} = Y(\mathbf{1}_n^o(\mathbf{1}_n^{o'}\mathbf{1}_n^o)\mathbf{1}_n^{o'} \otimes \Psi)Y'.$$

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The idea is to condition with respect to columns $\mathbf{y}_{i1}, \dots, \mathbf{y}_{iq}$. Put

$$\mathbf{Z}_{ik} = (\mathbf{y}_{ik} : \mathbf{y}_{ik+1} : \dots : \mathbf{y}_{iq})$$

and let f_{Y_i} denote the density function for Y_i . Then,

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$$f_{Y_i} = \prod_{k=2}^q (f_{\mathbf{y}_{ik-1} | \mathbf{z}_{ik}}) f_{\mathbf{y}_{iq}}.$$

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The conditional distributions are normal with parameters

$$\mathbf{B}^k = (\Psi_{22}^k)^{-1} \Psi_{21}^k$$

$$\psi_{1\bullet 2}^k = \psi_{11}^k - \Psi_{12}^k (\Psi_{22}^k)^{-1} \Psi_{21}^k,$$

where

$$\Psi^k = (0 : \mathbf{I}_t) \Psi \begin{pmatrix} 0 \\ \mathbf{I}_t \end{pmatrix}, \quad t = q - k - 2,$$

$$\Psi^k = \begin{pmatrix} \psi_{11}^k & \Psi_{12}^k \\ \Psi_{21}^k & \Psi_{22}^k \end{pmatrix}, \quad \begin{pmatrix} 1 \times 1 & 1 \times t - 1 \\ t - 1 \times 1 & t - 1 \times t - 1 \end{pmatrix}$$

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The parameters $\{B^k, \Psi_{1\bullet 2}^k\}$ are in one-to-one correspondence with Ψ if $\psi_{qq} = 1$.

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The parameters $\{B^k, \Psi_{1\bullet 2}^k\}$ are in one-to-one correspondence with Ψ if $\psi_{qq} = 1$. Estimation equations are given by

$$\begin{aligned} \hat{B}^k &= \left(\sum_{i=1}^n (z_{ik} - \mu_2^k)' \Sigma^{-1} (z_{ik} - \mu_2^k) \right)^{-1} \sum_{i=1}^n (z_{ik} - \mu_2^k)' \Sigma^{-1} (x_{k-1} - \mu_1^k), \\ k &= 2, 3, \dots, q, \\ np \hat{\Psi}_{1\bullet 2}^k &= \text{tr} \left\{ \Sigma^{-1} \left(y_{k-1} - \left(\mu_1^k + (z_k - (\mathbf{1}'_n \otimes \mu_2^k)) (\mathbf{I}_n \otimes \hat{B}^k) \right) \right) \right. \\ &\quad \left. \times \left(y_{k-1} - \left(\mu_1^k + (z_k - (\mathbf{1}'_n \otimes \mu_2^k)) (\mathbf{I}_n \otimes \hat{B}^k) \right) \right)' \right\}. \end{aligned}$$

where

$$\mu^k = \mu \begin{pmatrix} 0 \\ \mathbf{I}_t \end{pmatrix}$$

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Estimation equations when $\psi_{qq} = 1$; Summary.

$$\boldsymbol{\mu} = n^{-1} \mathbf{Y} (\mathbf{1}_n \otimes \mathbf{I}_q),$$

$$nq\Sigma = \mathbf{Y} (\mathbf{1}_n^\circ (\mathbf{1}_n^\circ \mathbf{1}_n^\circ)^{-1} \mathbf{1}_n^\circ \otimes \Psi^{-1}) \mathbf{Y}',$$

$$\begin{aligned} & B^k \\ &= \left(\sum_{i=1}^n (\mathbf{z}_{ik} - \boldsymbol{\mu}_2^k)' \Sigma^{-1} (\mathbf{z}_{ik} - \boldsymbol{\mu}_2^k) \right)^{-1} \sum_{i=1}^n (\mathbf{z}_{ik} - \boldsymbol{\mu}_2^k)' \Sigma^{-1} (\mathbf{x}_{k-1} - \boldsymbol{\mu}_1^k), \end{aligned}$$

$$np\Psi_{1\bullet 2}^k = \text{tr} \left\{ \Sigma^{-1} (\mathbf{y}_{k-1} - (\boldsymbol{\mu}_1^k + (\mathbf{z}_k - (\mathbf{1}_n' \otimes \boldsymbol{\mu}_2^k)) (\mathbf{I}_n \otimes B^k))) \right\},$$

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Estimation equations when $\psi_{qq} = 1$ can also be obtained when $\mu = \mathbf{ABC}$. In this case we replace the equation concerning μ by an equation for \mathbf{B} which is obtained from a ML-approach where Ψ is known:

$$n\hat{\mathbf{B}} = (\mathbf{A}'\mathbf{S}^{-1}\mathbf{A})^{-1}\mathbf{A}'\mathbf{S}^{-1}\mathbf{Y}(\mathbf{1}_n \otimes \Psi^{-1/2}\mathbf{C}'(\mathbf{C}\Psi^{-1}\mathbf{C}')^{-1}).$$

$$n_q\hat{\Sigma} = (\mathbf{Y} - \mathbf{A}\hat{\mathbf{B}}(\mathbf{1}'_n \otimes \mathbf{C}\Psi^{-1/2}))(\mathbf{Y} - \mathbf{A}\hat{\mathbf{B}}(\mathbf{1}'_n \otimes \mathbf{C}\Psi^{-1/2}))'$$

Thank you!