

Web-Supplement for:  
**Streamlined Variational Inference for  
Higher Level Group-Specific Curve Models**

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## S.1 Derivation of Result 1

Straightforward algebra can be used to verify that

$$C^T R_{\text{BLUP}}^{-1} C + D_{\text{BLUP}} = B^T B \quad \text{and} \quad C^T R_{\text{BLUP}}^{-1} \mathbf{y} = B^T \mathbf{b}$$

where  $B$  and  $\mathbf{b}$  have sparse forms (2.9) with non-zero sub-blocks equal to

$$\mathbf{b}_i \equiv \begin{bmatrix} \sigma_\varepsilon^{-1} \mathbf{y}_i \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad B_i \equiv \begin{bmatrix} \sigma_\varepsilon^{-1} \mathbf{X}_i & \sigma_\varepsilon^{-1} \mathbf{Z}_{\text{gbl},i} \\ \mathbf{O} & m^{-1/2} \sigma_{\text{gbl}}^{-1} \mathbf{I}_{K_{\text{gbl}}} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix} \quad \text{and} \quad \dot{B}_i \equiv \begin{bmatrix} \sigma_\varepsilon^{-1} \mathbf{X}_i & \sigma_\varepsilon^{-1} \mathbf{Z}_{\text{grp},i} \\ \mathbf{O} & \mathbf{O} \\ \Sigma^{-1/2} & \mathbf{O} \\ \mathbf{O} & \sigma_{\text{grp}}^{-1} \mathbf{I}_{K_{\text{grp}}} \end{bmatrix}.$$

Therefore, in view of (2.6),

$$\begin{bmatrix} \hat{\beta} \\ \hat{\mathbf{u}} \end{bmatrix} = (B^T B)^{-1} B^T \mathbf{b} \quad \text{and} \quad \text{Cov} \left( \begin{bmatrix} \hat{\beta} \\ \hat{\mathbf{u}} - \mathbf{u} \end{bmatrix} \right) = (B^T B)^{-1}.$$

The sub-blocks of

$$\text{Cov} \left( \begin{bmatrix} \hat{\beta} \\ \hat{\mathbf{u}} - \mathbf{u} \end{bmatrix} \right)$$

listed in (2.7) correspond to the non- $\times$  sub-blocks of  $A^{-1} = (B^T B)^{-1}$  where  $A^{-1}$  is given by (2.10). The result follows immediately.

## S.2 Derivation of Algorithm 1

Algorithm 1 is simply a proceduralization of Result 1.

## S.3 The Inverse G-Wishart and Inverse $\chi^2$ Distributions

The Inverse G-Wishart corresponds to the matrix inverses of random matrices that have a *G-Wishart* distribution (e.g. Atay-Kayis & Massam, 2005). For any positive integer  $d$ , let  $G$  be an undirected graph with  $d$  nodes labeled  $1, \dots, d$  and set  $E$  consisting of sets of pairs of nodes that are connected by an edge. We say that the symmetric  $d \times d$  matrix  $M$  respects  $G$  if

$$M_{ij} = 0 \quad \text{for all} \quad \{i, j\} \notin E.$$

A  $d \times d$  random matrix  $X$  has an Inverse G-Wishart distribution with graph  $G$  and parameters  $\xi > 0$  and symmetric  $d \times d$  matrix  $\Lambda$ , written

$$X \sim \text{Inverse-G-Wishart}(G, \xi, \Lambda)$$

if and only if the density function of  $\mathbf{X}$  satisfies

$$p(\mathbf{X}) \propto |\mathbf{X}|^{-(\xi+2)/2} \exp\{-\frac{1}{2}\text{tr}(\mathbf{\Lambda} \mathbf{X}^{-1})\}$$

over arguments  $\mathbf{X}$  such that  $\mathbf{X}$  is symmetric and positive definite and  $\mathbf{X}^{-1}$  respects  $G$ . Two important special cases are

$$G = G_{\text{full}} \equiv \text{totally connected } d\text{-node graph,}$$

for which the Inverse G-Wishart distribution coincides with the ordinary Inverse Wishart distribution, and

$$G = G_{\text{diag}} \equiv \text{totally disconnected } d\text{-node graph,}$$

for which the Inverse G-Wishart distribution coincides with a product of independent Inverse Chi-Squared random variables. The subscripts of  $G_{\text{full}}$  and  $G_{\text{diag}}$  reflect the fact that  $\mathbf{X}^{-1}$  is a full matrix and  $\mathbf{X}^{-1}$  is a diagonal matrix in each special case.

The  $G = G_{\text{full}}$  case corresponds to the ordinary Inverse Wishart distribution. However, with message passing in mind, we will work with the more general Inverse G-Wishart family throughout this article.

In the  $d = 1$  special case the graph  $G = G_{\text{full}} = G_{\text{diag}}$  and the Inverse G-Wishart distribution reduces to the Inverse Chi-Squared distributions. We write

$$x \sim \text{Inverse-}\chi^2(\xi, \lambda)$$

for this Inverse-G-Wishart( $G_{\text{diag}}, \xi, \lambda$ ) special case with  $d = 1$  and  $\lambda > 0$  scalar.

## S.4 Derivation of Result 2

It is straightforward to verify that the  $\mu_{q(\beta, \mathbf{u})}$  and  $\Sigma_{q(\beta, \mathbf{u})}$  updates, given at (2.12), may be written as

$$\mu_{q(\beta, \mathbf{u})} \leftarrow (\mathbf{B}^T \mathbf{B})^{-1} \mathbf{B}^T \mathbf{b} \quad \text{and} \quad \Sigma_{q(\beta, \mathbf{u})} \leftarrow (\mathbf{B}^T \mathbf{B})^{-1}$$

where  $\mathbf{B}$  and  $\mathbf{b}$  have the forms (2.9) with

$$\mathbf{b}_i \equiv \begin{bmatrix} \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{y}_i \\ m^{-1/2} \Sigma_\beta^{-1/2} \mu_\beta \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{B}_i \equiv \begin{bmatrix} \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{X}_i & \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{Z}_{\text{gbl}, i} \\ m^{-1/2} \Sigma_\beta^{-1/2} & \mathbf{O} \\ \mathbf{O} & m^{-1/2} \mu_{q(1/\sigma_{\text{gbl}}^2)}^{1/2} \mathbf{I}_{K_{\text{gbl}}} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix}$$

and

$$\dot{\mathbf{B}}_i \equiv \begin{bmatrix} \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{X}_i & \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{Z}_{\text{grp}, i} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{M}_{q(\Sigma^{-1})}^{1/2} & \mathbf{O} \\ \mathbf{O} & \mu_{q(1/\sigma_{\text{grp}}^2)}^{1/2} \mathbf{I}_{K_{\text{grp}}} \end{bmatrix}.$$

Result 2 immediately follows from Theorem 2 of Nolan & Wand (2018).

## S.5 Derivation of Algorithm 2

We provide expressions for the  $q$ -densities for mean field variational Bayesian inference for the parameters in (2.10), with product density restriction (2.11). Arguments analogous to those given in, for example, Appendix C of Wand & Ormerod (2011) lead to:

$q(\boldsymbol{\beta}, \mathbf{u})$  is a  $N(\boldsymbol{\mu}_{q(\boldsymbol{\beta}, \mathbf{u})}, \boldsymbol{\Sigma}_{q(\boldsymbol{\beta}, \mathbf{u})})$  density function

where

$$\boldsymbol{\Sigma}_{q(\boldsymbol{\beta}, \mathbf{u})} = (\mathbf{C}^T \mathbf{R}_{\text{MFVB}}^{-1} \mathbf{C} + \mathbf{D}_{\text{MFVB}})^{-1} \quad \text{and} \quad \boldsymbol{\mu}_{q(\boldsymbol{\beta}, \mathbf{u})} = \boldsymbol{\Sigma}_{q(\boldsymbol{\beta}, \mathbf{u})} (\mathbf{C}^T \mathbf{R}_{\text{MFVB}}^{-1} \mathbf{y} + \mathbf{o}_{\text{MFVB}})$$

with  $\mathbf{R}_{\text{MFVB}}$ ,  $\mathbf{D}_{\text{MFVB}}$  and  $\mathbf{o}_{\text{MFVB}}$  defined via (2.13),

$q(\sigma_\varepsilon^2)$  is an Inverse- $\chi^2(\xi_{q(\sigma_\varepsilon^2)}, \lambda_{q(\sigma_\varepsilon^2)})$  density function

where  $\xi_{q(\sigma_\varepsilon^2)} = \nu_\varepsilon + \sum_{i=1}^m n_i$  and

$$\begin{aligned} \lambda_{q(\sigma_\varepsilon^2)} &= \mu_{q(1/a_\varepsilon)} + \sum_{i=1}^m E_q \left\{ \left\| \mathbf{y}_i - \mathbf{C}_{\text{gbl},i} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \mathbf{C}_{\text{grp},i} \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} \right\|^2 \right\} \\ &= \mu_{q(1/a_\varepsilon)} + \sum_{i=1}^m \left[ \left\| E_q \left( \mathbf{y}_i - \mathbf{C}_{\text{gbl},i} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \mathbf{C}_{\text{grp},i} \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} \right) \right\|^2 \right. \\ &\quad \left. + \text{tr} \left\{ \text{Cov}_q \left( \mathbf{C}_{\text{gbl},i} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl},i} \end{bmatrix} + \mathbf{C}_{\text{grp},i} \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} \right) \right\} \right] \\ &= \mu_{q(1/a_\varepsilon)} + \sum_{i=1}^m \left\{ \left\| E_q \left( \mathbf{y}_i - \mathbf{C}_{\text{gbl},i} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \mathbf{C}_{\text{grp},i} \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} \right) \right\|^2 \right. \\ &\quad \left. + \text{tr}(\mathbf{C}_{\text{gbl},i}^T \mathbf{C}_{\text{gbl},i} \boldsymbol{\Sigma}_{q(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})}) + \text{tr}(\mathbf{C}_{\text{grp},i}^T \mathbf{C}_{\text{grp},i} \boldsymbol{\Sigma}_{q(\mathbf{u}_{\text{lin},i}, \mathbf{u}_{\text{grp},i})}) \right. \\ &\quad \left. + 2 \text{tr} \left[ \mathbf{C}_{\text{grp},i}^T \mathbf{C}_{\text{gbl},i} E_q \left\{ \left( \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{q(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})} \right) \times \right. \right. \right. \\ &\quad \left. \left. \left. \left( \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} - \boldsymbol{\mu}_{q(\mathbf{u}_{\text{lin},i}, \mathbf{u}_{\text{grp},i})} \right)^T \right\} \right] \right\} \end{aligned}$$

where  $\mathbf{C}_{\text{gbl},i} \equiv [\mathbf{X}_i \mathbf{Z}_{\text{gbl},i}]$ ,  $\mathbf{C}_{\text{grp},i} \equiv [\mathbf{X}_i \mathbf{Z}_{\text{grp},i}]$ , and with reciprocal moment  $\mu_{q(1/\sigma_\varepsilon^2)} = \xi_{q(\sigma_\varepsilon^2)} / \lambda_{q(\sigma_\varepsilon^2)}$ ,

$q(\sigma_{\text{gbl}}^2)$  is an Inverse- $\chi^2(\xi_{q(\sigma_{\text{gbl}}^2)}, \lambda_{q(\sigma_{\text{gbl}}^2)})$  density function

where  $\xi_{q(\sigma_{\text{gbl}}^2)} = \nu_{\text{gbl}} + K_{\text{gbl}}$  and

$$\lambda_{q(\sigma_{\text{gbl}}^2)} = \mu_{q(1/a_{\text{gbl}})} + \|\boldsymbol{\mu}_{q(\mathbf{u}_{\text{gbl}})}\|^2 + \text{tr}(\boldsymbol{\Sigma}_{q(\mathbf{u}_{\text{gbl}})}),$$

with reciprocal moment  $\mu_{q(1/\sigma_{\text{gbl}}^2)} = \xi_{q(\sigma_{\text{gbl}}^2)} / \lambda_{q(\sigma_{\text{gbl}}^2)}$ ,

$q(\sigma_{\text{grp}}^2)$  is an Inverse- $\chi^2(\xi_{q(\sigma_{\text{grp}}^2)}, \lambda_{q(\sigma_{\text{grp}}^2)})$  density function

where  $\xi_{q(\sigma_{\text{grp}}^2)} = \nu_{\text{grp}} + mK_{\text{grp}}$  and

$$\lambda_{q(\sigma_{\text{grp}}^2)} = \mu_{q(1/a_{\text{grp}})} + \sum_{i=1}^m \left\{ \|\boldsymbol{\mu}_{q(\mathbf{u}_{\text{grp},i})}\|^2 + \text{tr}(\boldsymbol{\Sigma}_{q(\mathbf{u}_{\text{grp},i})}) \right\},$$

with reciprocal moment  $\mu_{q(1/\sigma_{\text{grp}}^2)} = \xi_{q(\sigma_{\text{grp}}^2)}/\lambda_{q(\sigma_{\text{grp}}^2)}$ ,

$q(\Sigma)$  is an Inverse-G-Wishart ( $G_{\text{full}}, \xi_{q(\Sigma)}, \Lambda_{q(\Sigma)}$ ) density function

where  $\xi_{q(\Sigma)} = \nu_{\Sigma} + 2 + m$

$$\Lambda_{q(\Sigma)} = M_{q(\mathbf{A}_{\Sigma}^{-1})} + \sum_{i=1}^m \left( \boldsymbol{\mu}_{q(\mathbf{u}_{\text{in},i})} \boldsymbol{\mu}_{q(\mathbf{u}_{\text{in},i})}^T + \Sigma_{q(\mathbf{u}_{\text{in},i})} \right),$$

with inverse moment  $M_{q(\Sigma^{-1})} = (\xi_{q(\Sigma)} - 1) \Lambda_{q(\Sigma)}^{-1}$ ,

$q(a_{\varepsilon})$  is an Inverse- $\chi^2(\xi_{q(a_{\varepsilon})}, \lambda_{q(a_{\varepsilon})})$  density function

where  $\xi_{q(a_{\varepsilon})} = \nu_{\varepsilon} + 1$ ,

$$\lambda_{q(a_{\varepsilon})} = \mu_{q(1/\sigma_{\varepsilon}^2)} + 1/(\nu_{\varepsilon} s_{\varepsilon}^2)$$

with reciprocal moment  $\mu_{q(1/a_{\varepsilon})} = \xi_{q(a_{\varepsilon})}/\lambda_{q(a_{\varepsilon})}$ ,

$q(a_{\text{gbl}})$  is an Inverse- $\chi^2(\xi_{q(a_{\text{gbl}})}, \lambda_{q(a_{\text{gbl}})})$  density function

where  $\xi_{q(a_{\text{gbl}})} = \nu_{\text{gbl}} + 1$ ,

$$\lambda_{q(a_{\text{gbl}})} = \mu_{q(1/\sigma_{\text{gbl}}^2)} + 1/(\nu_{\text{gbl}} s_{\text{gbl}}^2)$$

with reciprocal moment  $\mu_{q(1/a_{\text{gbl}})} = \xi_{q(a_{\text{gbl}})}/\lambda_{q(a_{\text{gbl}})}$ ,

$q(a_{\text{grp}})$  is an Inverse- $\chi^2(\xi_{q(a_{\text{grp}})}, \lambda_{q(a_{\text{grp}})})$  density function

where  $\xi_{q(a_{\text{grp}})} = \nu_{\text{grp}} + 1$ ,

$$\lambda_{q(a_{\text{grp}})} = \mu_{q(1/\sigma_{\text{grp}}^2)} + 1/(\nu_{\text{grp}} s_{\text{grp}}^2)$$

with reciprocal moment  $\mu_{q(1/a_{\text{grp}})} = \xi_{q(a_{\text{grp}})}/\lambda_{q(a_{\text{grp}})}$  and

$q(\mathbf{A}_{\Sigma})$  is an Inverse-G-Wishart ( $G_{\text{diag}}, \xi_{q(\mathbf{A}_{\Sigma})}, \Lambda_{q(\mathbf{A}_{\Sigma})}$ ) density function

where  $\xi_{q(\mathbf{A}_{\Sigma})} = \nu_{\Sigma} + 2$ ,

$$\Lambda_{q(\mathbf{A}_{\Sigma})} = \text{diag}\{\text{diagonal}(M_{q(\Sigma^{-1})})\} + \Lambda_{\mathbf{A}_{\Sigma}}$$

with inverse moment  $M_{q(\mathbf{A}_{\Sigma}^{-1})} = \xi_{q(\mathbf{A}_{\Sigma})} \Lambda_{q(\mathbf{A}_{\Sigma})}^{-1}$ .

## S.6 Approximate Marginal Log-Likelihood for Two-Level Models

The expression for the lower bound on the marginal log-likelihood for Algorithm 2 is

$$\begin{aligned}
\log \underline{\mathbf{p}}(\mathbf{y}; \mathbf{q}) = & \\
& -\frac{1}{2} \log(\pi) \sum_{i=1}^m n_i - \frac{1}{2} \log |\boldsymbol{\Sigma}_\beta| - \frac{1}{2} \text{tr} \left( \boldsymbol{\Sigma}_\beta^{-1} \left\{ \left( \boldsymbol{\mu}_{\mathbf{q}(\beta)} - \boldsymbol{\mu}_\beta \right) \left( \boldsymbol{\mu}_{\mathbf{q}(\beta)} - \boldsymbol{\mu}_\beta \right)^T + \boldsymbol{\Sigma}_{\mathbf{q}(\beta)} \right\} \right) \\
& - \frac{1}{2} \text{tr} \left( \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}^{-1})} \left\{ \sum_{i=1}^m \left( \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i})} \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i})}^T + \boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{lin},i})} \right) \right\} \right) + \frac{1}{2} \{2 + K_{\text{gbl}} + m(2 + K_{\text{grp}})\} \\
& - \frac{1}{2} \mu_{\mathbf{q}(1/\sigma_\varepsilon^2)} \left\{ \|\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{gbl}})}\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{gbl}})}) \right\} - \frac{1}{2} \mu_{\mathbf{q}(1/\sigma_{\text{grp}}^2)} \sum_{i=1}^m \left\{ \|\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{grp},i})}\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{grp},i)})} \right\} \\
& + \frac{1}{2} \log |\boldsymbol{\Sigma}_\beta| + \{\nu_\Sigma + m + 1 + \frac{1}{2}(\nu_\varepsilon + \nu_{\text{gbl}} + K_{\text{gbl}} + \nu_{\text{grp}} + mK_{\text{grp}})\} \log(2) - \log \Gamma\left(\frac{\nu_\varepsilon}{2}\right) \\
& - \frac{1}{2} \mu_{\mathbf{q}(1/a_\varepsilon)} \mu_{\mathbf{q}(1/\sigma_\varepsilon^2)} - \frac{1}{2} \xi_{\mathbf{q}(\sigma_\varepsilon^2)} \log(\lambda_{\mathbf{q}(\sigma_\varepsilon^2)}) + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(\sigma_\varepsilon^2)})\} + \frac{1}{2} \lambda_{\mathbf{q}(\sigma_\varepsilon^2)} \mu_{\mathbf{q}(1/\sigma_\varepsilon^2)} - \frac{1}{2} \log(\nu_\varepsilon s_\varepsilon^2) \\
& - 3 \log\{\Gamma(\frac{1}{2})\} - \frac{1}{2\nu_\varepsilon s_\varepsilon^2} \mu_{\mathbf{q}(1/a_\varepsilon)} - \frac{1}{2} \xi_{\mathbf{q}(a_\varepsilon)} \log(\lambda_{\mathbf{q}(a_\varepsilon)}) + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(a_\varepsilon)})\} + \frac{1}{2} \lambda_{\mathbf{q}(a_\varepsilon)} \mu_{\mathbf{q}(1/a_\varepsilon)} \\
& - \log \Gamma\left(\frac{\nu_{\text{gbl}}}{2}\right) - \frac{1}{2} \mu_{\mathbf{q}(1/a_{\text{gbl}})} \mu_{\mathbf{q}(1/\sigma_{\text{gbl}}^2)} - \frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{gbl}}^2)} \log(\lambda_{\mathbf{q}(\sigma_{\text{gbl}}^2)}) + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{gbl}}^2)})\} - \frac{1}{2} \log(\nu_{\text{gbl}} s_{\text{gbl}}^2) \\
& + \frac{1}{2} \lambda_{\mathbf{q}(\sigma_{\text{gbl}}^2)} \mu_{\mathbf{q}(1/\sigma_{\text{gbl}}^2)} - \{1/(2\nu_{\text{gbl}} s_{\text{gbl}}^2)\} \mu_{\mathbf{q}(1/a_{\text{gbl}})} - \frac{1}{2} \xi_{\mathbf{q}(a_{\text{gbl}})} \log(\lambda_{\mathbf{q}(a_{\text{gbl}})}) - \frac{1}{2} \mu_{\mathbf{q}(1/a_{\text{grp}})} \mu_{\mathbf{q}(1/\sigma_{\text{grp}}^2)} \\
& + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(a_{\text{gbl}})})\} + \frac{1}{2} \lambda_{\mathbf{q}(a_{\text{gbl}})} \mu_{\mathbf{q}(1/a_{\text{gbl}})} - \log \Gamma\left(\frac{\nu_{\text{grp}}}{2}\right) + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{grp}}^2)})\} - \frac{1}{2} \log(\nu_{\text{grp}} s_{\text{grp}}^2) \\
& - \frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{grp}}^2)} \log(\lambda_{\mathbf{q}(\sigma_{\text{grp}}^2)}) + \frac{1}{2} \lambda_{\mathbf{q}(\sigma_{\text{grp}}^2)} \mu_{\mathbf{q}(1/\sigma_{\text{grp}}^2)} - \{1/(2\nu_{\text{grp}} s_{\text{grp}}^2)\} \mu_{\mathbf{q}(1/a_{\text{grp}})} - \frac{1}{2} \xi_{\mathbf{q}(a_{\text{grp}})} \log(\lambda_{\mathbf{q}(a_{\text{grp}})}) \\
& + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(a_{\text{grp}})})\} + \frac{1}{2} \lambda_{\mathbf{q}(a_{\text{grp}})} \mu_{\mathbf{q}(1/a_{\text{grp}})} - \frac{1}{2} \text{tr}(\mathbf{M}_{\mathbf{q}(\mathbf{A}_\Sigma^{-1})} \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}^{-1})}) + \frac{1}{2} \text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma})} \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}^{-1})}) \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(\xi_{\mathbf{q}(\mathbf{A}_\Sigma)} + 2 - j)\right) - \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(\nu_\Sigma + 4 - j)\right) - \frac{1}{2}(\xi_{\mathbf{q}(\boldsymbol{\Sigma})} - 1) \log |\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma})}| \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(\xi_{\mathbf{q}(\boldsymbol{\Sigma})} + 2 - j)\right) - \frac{1}{2} \sum_{j=1}^2 1/(\nu_\Sigma s_{\Sigma,j}^2) \left( \mathbf{M}_{\mathbf{q}(\mathbf{A}_\Sigma^{-1})} \right)_{jj} - \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(3 - j)\right) \\
& - \frac{1}{2}(\xi_{\mathbf{q}(\mathbf{A}_\Sigma)} - 1) \log |\boldsymbol{\Lambda}_{\mathbf{q}(\mathbf{A}_\Sigma)}| + \frac{1}{2} \text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}(\mathbf{A}_\Sigma)} \mathbf{M}_{\mathbf{q}(\mathbf{A}_\Sigma^{-1})}) \\
& - \frac{1}{2} \mu_{\mathbf{q}(1/\sigma_\varepsilon^2)} \sum_{i=1}^m \left\{ \left\| E_{\mathbf{q}} \left( \mathbf{y}_i - \mathbf{C}_{\text{gbl},i} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl},i} \end{bmatrix} - \mathbf{C}_{\text{grp},i} \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} \right) \right\|^2 \right. \\
& \quad + \text{tr}(\mathbf{C}_{\text{gbl},i}^T \mathbf{C}_{\text{gbl},i} \boldsymbol{\Sigma}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})}) + \text{tr}(\mathbf{C}_{\text{grp},i}^T \mathbf{C}_{\text{grp},i} \boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}, \mathbf{u}_{\text{grp},i})}) \\
& \quad \left. + 2 \text{tr} \left[ \mathbf{C}_{\text{grp},i}^T \mathbf{C}_{\text{gbl},i} E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})} \right) \times \right. \right. \right. \\
& \quad \quad \left. \left. \left( \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}, \mathbf{u}_{\text{grp},i})} \right)^T \right\} \right] \right\}. \tag{S.1}
\end{aligned}$$

*Derivation:* The lower-bound on the marginal log-likelihood is achieved through the following expression:

$$\begin{aligned}
\log \underline{\mathbf{p}}(\mathbf{y}; \mathbf{q}) = & E_{\mathbf{q}}\{\log \mathbf{p}(\mathbf{y}, \boldsymbol{\beta}, \mathbf{u}, \sigma_\varepsilon^2, a_\varepsilon, \sigma_{\text{gbl}}^2, a_{\text{gbl}}, \sigma_{\text{grp}}^2, a_{\text{grp}}, \boldsymbol{\Sigma}, \mathbf{A}_\Sigma) \\
& - \log \mathbf{q}^*(\boldsymbol{\beta}, \mathbf{u}, \sigma_\varepsilon^2, a_\varepsilon, \sigma_{\text{gbl}}^2, a_{\text{gbl}}, \sigma_{\text{grp}}^2, a_{\text{grp}}, \boldsymbol{\Sigma}, \mathbf{A}_\Sigma)\}
\end{aligned}$$

$$\begin{aligned}
&= E_q\{\log \mathbf{p}(\mathbf{y} \mid \boldsymbol{\beta}, \mathbf{u}, \sigma_\varepsilon^2)\} \\
&\quad + E_q\{\log \mathbf{p}(\boldsymbol{\beta}, \mathbf{u} \mid \sigma_{\text{gbl}}^2, \sigma_{\text{grp}}^2, \boldsymbol{\Sigma})\} - E_q\{\log \mathbf{q}^*(\boldsymbol{\beta}, \mathbf{u})\} \\
&\quad + E_q\{\log \mathbf{p}(\sigma_\varepsilon^2 \mid a_\varepsilon)\} - E_q\{\log \mathbf{q}^*(\sigma_\varepsilon^2)\} + E_q\{\log \mathbf{p}(a_\varepsilon)\} - E_q\{\log \mathbf{q}^*(a_\varepsilon)\} \\
&\quad + E_q\{\log \mathbf{p}(\sigma_{\text{gbl}}^2 \mid a_{\text{gbl}})\} - E_q\{\log \mathbf{q}^*(\sigma_{\text{gbl}}^2)\} + E_q\{\log \mathbf{p}(a_{\text{gbl}})\} - E_q\{\log \mathbf{q}^*(a_{\text{gbl}})\} \\
&\quad + E_q\{\log \mathbf{p}(\sigma_{\text{grp}}^2 \mid a_{\text{grp}})\} - E_q\{\log \mathbf{q}^*(\sigma_{\text{grp}}^2)\} + E_q\{\log \mathbf{p}(a_{\text{grp}})\} - E_q\{\log \mathbf{q}^*(a_{\text{grp}})\} \\
&\quad + E_q\{\log \mathbf{p}(\boldsymbol{\Sigma} \mid \mathbf{A}_\Sigma)\} - E_q\{\log \mathbf{q}^*(\boldsymbol{\Sigma})\} + E_q\{\log \mathbf{p}(\mathbf{A}_\Sigma)\} - E_q\{\log \mathbf{q}^*(\mathbf{A}_\Sigma)\}.
\end{aligned}$$

First we note that

$$\log \mathbf{p}(\mathbf{y} \mid \boldsymbol{\beta}, \mathbf{u}, \sigma_\varepsilon^2) = -\frac{1}{2} \log(2\pi) \sum_{i=1}^m n_i - \frac{1}{2} \log(\sigma_\varepsilon^2) \sum_{i=1}^m n_i - \frac{1}{2\sigma_\varepsilon^2} \sum_{i=1}^m \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\mathbf{u}\|^2$$

where

$$\begin{aligned}
&\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\mathbf{u}\|^2 \\
&= \left\| \begin{bmatrix} \mathbf{y}_1 \\ \vdots \\ \mathbf{y}_m \end{bmatrix} - \begin{bmatrix} \mathbf{X}_1 \\ \vdots \\ \mathbf{X}_m \end{bmatrix} \boldsymbol{\beta} - \begin{bmatrix} \mathbf{Z}_{\text{gbl},1} \\ \vdots \\ \mathbf{Z}_{\text{gbl},m} \end{bmatrix} \mathbf{u}_{\text{gbl}} - \text{blockdiag}(\mathbf{Z}_{\text{grp},i})_{1 \leq i \leq m} \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix}_{1 \leq i \leq m} \right\|^2 \\
&= \sum_{i=1}^m \|\mathbf{y}_i - \mathbf{X}_i \boldsymbol{\beta} - \mathbf{Z}_{\text{gbl},i} \mathbf{u}_{\text{gbl},i} - \mathbf{X}_i \mathbf{u}_{\text{lin},i} - \mathbf{Z}_{\text{grp},i} \mathbf{u}_{\text{grp},i}\|^2 \\
&= \sum_{i=1}^m \left\| \mathbf{y}_i - \mathbf{C}_{\text{gbl},i} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl},i} \end{bmatrix} - \mathbf{C}_{\text{grp},i} \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} \right\|^2
\end{aligned}$$

and

$$\mathbf{C}_{\text{gbl},i} \equiv [\mathbf{X}_i \mathbf{Z}_{\text{gbl},i}], \quad \mathbf{C}_{\text{grp},i} \equiv [\mathbf{X}_i \mathbf{Z}_{\text{grp},i}].$$

Therefore,

$$\begin{aligned}
&E_q\{\log \mathbf{p}(\mathbf{y} \mid \boldsymbol{\beta}, \mathbf{u}, \sigma_\varepsilon^2)\} \\
&= -\frac{1}{2} \log(2\pi) \sum_{i=1}^m n_i - \frac{1}{2} E_q\{\log(\sigma_\varepsilon^2)\} \sum_{i=1}^m n_i \\
&\quad - \frac{1}{2} \mu_{\mathbf{q}(1/\sigma_\varepsilon^2)} \sum_{i=1}^m \left\{ \left\| E_q \left( \mathbf{y}_i - \mathbf{C}_{\text{gbl},i} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl},i} \end{bmatrix} - \mathbf{C}_{\text{grp},i} \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} \right) \right\|^2 \right. \\
&\quad \left. + \text{tr}(\mathbf{C}_{\text{gbl},i}^T \mathbf{C}_{\text{gbl},i} \boldsymbol{\Sigma}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})}) + \text{tr}(\mathbf{C}_{\text{grp},i}^T \mathbf{C}_{\text{grp},i} \boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}, \mathbf{u}_{\text{grp},i})}) \right. \\
&\quad \left. + 2 \text{tr} \left[ \mathbf{C}_{\text{grp},i}^T \mathbf{C}_{\text{gbl},i} E_q \left\{ \left( \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})} \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},i} \\ \mathbf{u}_{\text{grp},i} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}, \mathbf{u}_{\text{grp},i})} \right)^T \right\} \right] \right\}
\end{aligned}$$

The remainder of the expectations in (S.4) are expressed as:

$$\begin{aligned}
E_q\{\log \mathbf{p}(\boldsymbol{\beta}, \mathbf{u} \mid \sigma_{\text{gbl}}^2, \sigma_{\text{grp}}^2, \boldsymbol{\Sigma})\} &= -\frac{1}{2} \{2 + K_{\text{gbl}} + m(2 + K_{\text{grp}})\} \log(2\pi) - \frac{1}{2} \log |\boldsymbol{\Sigma} \boldsymbol{\beta}| \\
&\quad - \frac{K_{\text{gbl}}}{2} E_q\{\log(\sigma_{\text{gbl}}^2)\} - \frac{m}{2} E_q\{\log |\boldsymbol{\Sigma}|\} - \frac{mK_{\text{grp}}}{2} E_q\{\log(\sigma_{\text{grp}}^2)\} \\
&\quad - \frac{1}{2} \text{tr} \left( \boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} \left\{ \left( \boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta})} - \boldsymbol{\mu}_{\boldsymbol{\beta}} \right) \left( \boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta})} - \boldsymbol{\mu}_{\boldsymbol{\beta}} \right)^T + \boldsymbol{\Sigma}_{\mathbf{q}(\boldsymbol{\beta})} \right\} \right) \\
&\quad - \frac{1}{2} \mu_{\mathbf{q}(1/\sigma_{\text{gbl}}^2)} \left\{ \|\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{gbl}})}\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{gbl}})}) \right\} \\
&\quad - \frac{1}{2} \text{tr} \left( \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}^{-1})} \left\{ \sum_{i=1}^m \left( \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i})} \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i})}^T + \boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{lin},i})} \right) \right\} \right) \\
&\quad - \frac{1}{2} \mu_{\mathbf{q}(1/\sigma_{\text{grp}}^2)} \sum_{i=1}^m \left\{ \|\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{grp},i})}\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{grp},i)})} \right\}
\end{aligned}$$

$$\begin{aligned}
E_{\mathbf{q}}\{\log \mathbf{q}^*(\boldsymbol{\beta}, \mathbf{u})\} &= -\frac{1}{2}\{2 + K_{\text{gbl}} + m(2 + K_{\text{grp}})\} - \frac{1}{2}\{2 + K_{\text{gbl}} + m(2 + K_{\text{grp}})\} \log(2\pi) \\
&\quad - \frac{1}{2} \log |\boldsymbol{\Sigma}_{\boldsymbol{\beta}}| \\
E_{\mathbf{q}}\{\log \mathbf{p}(\sigma_{\varepsilon}^2 | a_{\varepsilon})\} &= -\frac{1}{2}\nu_{\varepsilon} E_{\mathbf{q}}\{\log(2a_{\varepsilon})\} - \log \Gamma(\nu_{\varepsilon}/2) - (\frac{1}{2}\nu_{\varepsilon} + 1)E_{\mathbf{q}}\{\log(\sigma_{\varepsilon}^2)\} \\
&\quad - \frac{1}{2}\mu_{\mathbf{q}}(1/a_{\varepsilon})\mu_{\mathbf{q}}(1/\sigma_{\varepsilon}^2) \\
E_{\mathbf{q}}\{\log \mathbf{q}^*(\sigma_{\varepsilon}^2)\} &= \frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\varepsilon}^2) \log(\lambda_{\mathbf{q}}(\sigma_{\varepsilon}^2)/2) - \log\{\Gamma(\frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\varepsilon}^2))\} - (\frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\varepsilon}^2) + 1)E_{\mathbf{q}}\{\log(\sigma_{\varepsilon}^2)\} \\
&\quad - \frac{1}{2}\lambda_{\mathbf{q}}(\sigma_{\varepsilon}^2)\mu_{\mathbf{q}}(1/\sigma_{\varepsilon}^2) \\
E_{\mathbf{q}}\{\log \mathbf{p}(a_{\varepsilon})\} &= -\frac{1}{2} \log(2\nu_{\varepsilon}s_{\varepsilon}^2) - \log\{\Gamma(\frac{1}{2})\} - (\frac{1}{2} + 1)E_{\mathbf{q}}\{\log(a_{\varepsilon})\} \\
&\quad - \{1/(2\nu_{\varepsilon}s_{\varepsilon}^2)\}\mu_{\mathbf{q}}(1/a_{\varepsilon}) \\
E_{\mathbf{q}}\{\log \mathbf{q}^*(a_{\varepsilon})\} &= \frac{1}{2}\xi_{\mathbf{q}}(a_{\varepsilon}) \log(\lambda_{\mathbf{q}}(a_{\varepsilon})/2) - \log\{\Gamma(\frac{1}{2}\xi_{\mathbf{q}}(a_{\varepsilon}))\} - (\frac{1}{2}\xi_{\mathbf{q}}(a_{\varepsilon}) + 1)E_{\mathbf{q}}\{\log(a_{\varepsilon})\} \\
&\quad - \frac{1}{2}\lambda_{\mathbf{q}}(a_{\varepsilon})\mu_{\mathbf{q}}(1/a_{\varepsilon}) \\
E_{\mathbf{q}}\{\log \mathbf{p}(\sigma_{\text{gbl}}^2 | a_{\text{gbl}})\} &= -\frac{1}{2}\nu_{\text{gbl}} E_{\mathbf{q}}\{\log(2a_{\text{gbl}})\} - \log \Gamma(\nu_{\text{gbl}}/2) - (\frac{1}{2}\nu_{\text{gbl}} + 1)E_{\mathbf{q}}\{\log(\sigma_{\text{gbl}}^2)\} \\
&\quad - \frac{1}{2}\mu_{\mathbf{q}}(1/a_{\text{gbl}})\mu_{\mathbf{q}}(1/\sigma_{\text{gbl}}^2) \\
E_{\mathbf{q}}\{\log \mathbf{q}^*(\sigma_{\text{gbl}}^2)\} &= \frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{gbl}}^2) \log(\lambda_{\mathbf{q}}(\sigma_{\text{gbl}}^2)/2) - \log\{\Gamma(\frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{gbl}}^2))\} - (\frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{gbl}}^2) + 1)E_{\mathbf{q}}\{\log(\sigma_{\text{gbl}}^2)\} \\
&\quad - \frac{1}{2}\lambda_{\mathbf{q}}(\sigma_{\text{gbl}}^2)\mu_{\mathbf{q}}(1/\sigma_{\text{gbl}}^2) \\
E_{\mathbf{q}}\{\log \mathbf{p}(a_{\text{gbl}})\} &= -\frac{1}{2} \log(2\nu_{\text{gbl}}s_{\text{gbl}}^2) - \log\{\Gamma(\frac{1}{2})\} - (\frac{1}{2} + 1)E_{\mathbf{q}}\{\log(a_{\text{gbl}})\} \\
&\quad - \{1/(2\nu_{\text{gbl}}s_{\text{gbl}}^2)\}\mu_{\mathbf{q}}(1/a_{\text{gbl}}) \\
E_{\mathbf{q}}\{\log \mathbf{q}^*(a_{\text{gbl}})\} &= \frac{1}{2}\xi_{\mathbf{q}}(a_{\text{gbl}}) \log(\lambda_{\mathbf{q}}(a_{\text{gbl}})/2) - \log\{\Gamma(\frac{1}{2}\xi_{\mathbf{q}}(a_{\text{gbl}}))\} - (\frac{1}{2}\xi_{\mathbf{q}}(a_{\text{gbl}}) + 1)E_{\mathbf{q}}\{\log(a_{\text{gbl}})\} \\
&\quad - \frac{1}{2}\lambda_{\mathbf{q}}(a_{\text{gbl}})\mu_{\mathbf{q}}(1/a_{\text{gbl}}) \\
E_{\mathbf{q}}\{\log \mathbf{p}(\sigma_{\text{grp}}^2 | a_{\text{grp}})\} &= -\frac{1}{2}\nu_{\text{grp}} E_{\mathbf{q}}\{\log(2a_{\text{grp}})\} - \log \Gamma(\nu_{\text{grp}}/2) - (\frac{1}{2}\nu_{\text{grp}} + 1)E_{\mathbf{q}}\{\log(\sigma_{\text{grp}}^2)\} \\
&\quad - \frac{1}{2}\mu_{\mathbf{q}}(1/a_{\text{grp}})\mu_{\mathbf{q}}(1/\sigma_{\text{grp}}^2) \\
E_{\mathbf{q}}\{\log \mathbf{q}^*(\sigma_{\text{grp}}^2)\} &= \frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{grp}}^2) \log(\lambda_{\mathbf{q}}(\sigma_{\text{grp}}^2)/2) - \log\{\Gamma(\frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{grp}}^2))\} - (\frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{grp}}^2) + 1)E_{\mathbf{q}}\{\log(\sigma_{\text{grp}}^2)\} \\
&\quad - \frac{1}{2}\lambda_{\mathbf{q}}(\sigma_{\text{grp}}^2)\mu_{\mathbf{q}}(1/\sigma_{\text{grp}}^2) \\
E_{\mathbf{q}}\{\log \mathbf{p}(a_{\text{grp}})\} &= -\frac{1}{2} \log(2\nu_{\text{grp}}s_{\text{grp}}^2) - \log\{\Gamma(\frac{1}{2})\} - (\frac{1}{2} + 1)E_{\mathbf{q}}\{\log(a_{\text{grp}})\} \\
&\quad - \{1/(2\nu_{\text{grp}}s_{\text{grp}}^2)\}\mu_{\mathbf{q}}(1/a_{\text{grp}}) \\
E_{\mathbf{q}}\{\log \mathbf{q}^*(a_{\text{grp}})\} &= \frac{1}{2}\xi_{\mathbf{q}}(a_{\text{grp}}) \log(\lambda_{\mathbf{q}}(a_{\text{grp}})/2) - \log\{\Gamma(\frac{1}{2}\xi_{\mathbf{q}}(a_{\text{grp}}))\} - (\frac{1}{2}\xi_{\mathbf{q}}(a_{\text{grp}}) + 1)E_{\mathbf{q}}\{\log(a_{\text{grp}})\} \\
&\quad - \frac{1}{2}\lambda_{\mathbf{q}}(a_{\text{grp}})\mu_{\mathbf{q}}(1/a_{\text{grp}}) \\
E_{\mathbf{q}}[\log\{\mathbf{p}(\boldsymbol{\Sigma} | \mathbf{A}_{\boldsymbol{\Sigma}})\}] &= -\frac{1}{2}(\nu_{\boldsymbol{\Sigma}} + 1)E_{\mathbf{q}}\{\log |\mathbf{A}_{\boldsymbol{\Sigma}}|\} - \frac{1}{2}(\nu_{\boldsymbol{\Sigma}} + 4)E_{\mathbf{q}}\{\log |\boldsymbol{\Sigma}|\} - \frac{1}{2} \log(\pi) \\
&\quad - \frac{1}{2} \text{tr}(\mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}}^{-1})} \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}^{-1})}) - (\nu_{\boldsymbol{\Sigma}} + 3) \log(2) - \sum_{j=1}^2 \log \Gamma(\frac{1}{2}(\nu_{\boldsymbol{\Sigma}} + 4 - j)) \\
E_{\mathbf{q}}[\log\{\mathbf{q}(\boldsymbol{\Sigma})\}] &= \frac{1}{2}(\xi_{\mathbf{q}}(\boldsymbol{\Sigma}) - 1) \log |\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma})}| - \frac{1}{2}(\xi_{\mathbf{q}}(\boldsymbol{\Sigma}) + 2)E_{\mathbf{q}}\{\log |\boldsymbol{\Sigma}|\} - \frac{1}{2} \text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma})} \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}^{-1})}) \\
&\quad - (\xi_{\mathbf{q}}(\boldsymbol{\Sigma}) + 1) \log(2) - \frac{1}{2} \log(\pi) - \sum_{j=1}^2 \log \Gamma(\frac{1}{2}(\xi_{\mathbf{q}}(\boldsymbol{\Sigma}) + 2 - j)) \\
E_{\mathbf{q}}[\log\{\mathbf{p}(\mathbf{A}_{\boldsymbol{\Sigma}})\}] &= -\frac{3}{2}E_{\mathbf{q}}\{\log |\mathbf{A}_{\boldsymbol{\Sigma}}|\} - \frac{1}{2} \sum_{j=1}^2 1/(\nu_{\boldsymbol{\Sigma}} s_{\boldsymbol{\Sigma}, j}^2) \left( \mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}}^{-1})} \right)_{jj} - 2 \log(2) - \frac{1}{2} \log(\pi) \\
&\quad - \sum_{j=1}^2 \log \Gamma(\frac{1}{2}(3 - j)) \\
E_{\mathbf{q}}[\log\{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}})\}] &= \frac{1}{2}(\xi_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}}) - 1) \log |\boldsymbol{\Lambda}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}})}| - \frac{1}{2}(\xi_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}}) + 2)E_{\mathbf{q}}\{\log |\mathbf{A}_{\boldsymbol{\Sigma}}|\} - \frac{1}{2} \text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}})} \mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}}^{-1})}) \\
&\quad - (\xi_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}}) + 1) \log(2) - \frac{1}{2} \log(\pi) - \sum_{j=1}^2 \log \Gamma(\frac{1}{2}(\xi_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}}) + 2 - j))
\end{aligned}$$

In the summation of each of these  $\log \mathbf{p}(\mathbf{y}; \mathbf{q})$  terms, note that the coefficient of  $E_{\mathbf{q}}\{\log(\sigma_{\varepsilon}^2)\}$  is

$$-\frac{1}{2} \sum_{i=1}^m n_i - \frac{1}{2}\nu_{\varepsilon} - 1 + \frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\varepsilon}^2) + 1 = -\frac{1}{2} \sum_{i=1}^m n_i - \frac{1}{2}\nu_{\varepsilon} - 1 + \frac{1}{2}(\nu_{\varepsilon} + \sum_{i=1}^m n_i) + 1 = 0.$$

The coefficient of  $E_q\{\log(\sigma_{\text{gbl}}^2)\}$  is

$$-\frac{1}{2}K_{\text{gbl}} - \frac{1}{2}\nu_{\text{gbl}} - 1 + \frac{1}{2}\xi_{\text{q}}(\sigma_{\text{gbl}}^2) + 1 = -\frac{1}{2}K_{\text{gbl}} - \frac{1}{2}\nu_{\text{gbl}} - 1 + \frac{1}{2}(\nu_{\text{gbl}} + K_{\text{gbl}}) + 1 = 0.$$

The coefficient of  $E_q\{\log(\sigma_{\text{grp}}^2)\}$  is

$$-\frac{1}{2}mK_{\text{grp}} - \frac{1}{2}\nu_{\text{grp}} - 1 + \frac{1}{2}\xi_{\text{q}}(\sigma_{\text{grp}}^2) + 1 = -\frac{1}{2}mK_{\text{grp}} - \frac{1}{2}\nu_{\text{grp}} - 1 + \frac{1}{2}(\nu_{\text{grp}} + mK_{\text{grp}}) + 1 = 0.$$

The coefficient of  $E_q\{\log|\Sigma|\}$  is

$$-\frac{m}{2} - \frac{1}{2}(\nu_{\Sigma} + 4) + \frac{1}{2}(\xi_{\text{q}}(\Sigma) + 2) = -\frac{1}{2}(m + \nu_{\Sigma} + 4) + \frac{1}{2}(m + \nu_{\Sigma} + 4) = 0.$$

The coefficient of  $E_q\{\log(a_{\varepsilon})\}$  is

$$-\frac{1}{2}\nu_{\varepsilon} - \frac{1}{2} - 1 + \frac{1}{2}\xi_{\text{q}}(a_{\varepsilon}) + 1 = -\frac{1}{2}\nu_{\varepsilon} - \frac{1}{2} - 1 + \frac{1}{2}(\nu_{\varepsilon} + 1) + 1 = 0.$$

The coefficient of  $E_q\{\log(a_{\text{gbl}})\}$  is

$$-\frac{1}{2}\nu_{\text{gbl}} - \frac{1}{2} - 1 + \frac{1}{2}\xi_{\text{q}}(a_{\text{gbl}}) + 1 = -\frac{1}{2}\nu_{\text{gbl}} - \frac{1}{2} - 1 + \frac{1}{2}(\nu_{\text{gbl}} + 1) + 1 = 0.$$

The coefficient of  $E_q\{\log(a_{\text{grp}})\}$  is

$$-\frac{1}{2}\nu_{\text{grp}} - \frac{1}{2} - 1 + \frac{1}{2}\xi_{\text{q}}(a_{\text{grp}}) + 1 = -\frac{1}{2}\nu_{\text{grp}} - \frac{1}{2} - 1 + \frac{1}{2}(\nu_{\text{grp}} + 1) + 1 = 0.$$

The coefficient of  $E_q\{\log|\mathbf{A}_{\Sigma}|\}$  is

$$-\frac{1}{2}(\nu_{\Sigma} + 1) - \frac{3}{2} + \frac{1}{2}(\xi_{\text{q}}(\mathbf{A}_{\Sigma}) + 2) = -\frac{1}{2}(\nu_{\Sigma} + 2) + \frac{1}{2}(\nu_{\Sigma} + 2) = 0.$$

Therefore, these terms can be dropped and the approximate marginal log-likelihood expression in (S.1) results.

## S.7 Derivation of Result 3

If  $B$  and  $b$  have the same forms given by equation (7) in Nolan & Wand (2018) with

$$\mathbf{b}_{ij} \equiv \begin{bmatrix} \sigma_{\varepsilon}^{-1} \mathbf{y}_{ij} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{B}_{ij} \equiv \begin{bmatrix} \sigma_{\varepsilon}^{-1} \mathbf{X}_{ij} & \sigma_{\varepsilon}^{-1} \mathbf{Z}_{\text{gbl},ij} \\ \mathbf{O} & (\sum_{i=1}^m n_i)^{-1/2} \sigma_{\text{gbl}}^{-1} \mathbf{I}_{K_{\text{gbl}}} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix},$$

$$\dot{\mathbf{B}}_{ij} \equiv \begin{bmatrix} \sigma_{\varepsilon}^{-1} \mathbf{X}_{ij} & \sigma_{\varepsilon}^{-1} \mathbf{Z}_{\text{grp},ij}^g \\ \mathbf{O} & \mathbf{O} \\ n_i^{-1/2} \Sigma_g^{-1/2} & \mathbf{O} \\ \mathbf{O} & n_i^{-1/2} \sigma_{\text{grp},g}^{-1} \mathbf{I}_{K_{\text{grp}}^g} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix} \quad \text{and} \quad \ddot{\mathbf{B}}_{ij} \equiv \begin{bmatrix} \sigma_{\varepsilon}^{-1} \mathbf{X}_{ij} & \sigma_{\varepsilon}^{-1} \mathbf{Z}_{\text{grp},ij}^h \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \Sigma_h^{-1/2} & \mathbf{O} \\ \mathbf{O} & \sigma_{\text{grp},h}^{-1} \mathbf{I}_{K_{\text{grp}}^h} \end{bmatrix},$$

then straightforward algebra leads to

$$\mathbf{B}^T \mathbf{B} = \mathbf{C}^T \mathbf{R}_{\text{BLUP}}^{-1} \mathbf{C} + \mathbf{D}_{\text{BLUP}} \quad \text{and} \quad \mathbf{B}^T \mathbf{b} = \mathbf{C}^T \mathbf{R}_{\text{BLUP}}^{-1} \mathbf{y}$$



where

$$C \equiv [\mathbf{X} \ \mathbf{Z}], \quad D_{\text{BLUP}} \equiv \begin{bmatrix} \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{G}^{-1} \end{bmatrix} \quad \text{and} \quad \mathbf{R}_{\text{BLUP}} \equiv \sigma_\varepsilon^2 \mathbf{I}, \quad (\text{S.2})$$

and  $\mathbf{G}$  as defined in (3.3). The remainder of the derivation of Result 3 is analogous to that of Result 1.

## S.8 Derivation of Algorithm 3

Algorithm 3 is simply a proceduralization of Result 3.

## S.9 Derivation of Result 4

It is straightforward to verify that the  $\mu_{q(\beta, \mathbf{u})}$  and  $\Sigma_{q(\beta, \mathbf{u})}$  updates, given at (2.12) but with  $D_{\text{MFVB}}$  as given in (3.6), may be written as

$$\mu_{q(\beta, \mathbf{u})} \longleftarrow (\mathbf{B}^T \mathbf{B})^{-1} \mathbf{B}^T \mathbf{b} \quad \text{and} \quad \Sigma_{q(\beta, \mathbf{u})} \longleftarrow (\mathbf{B}^T \mathbf{B})^{-1}$$

where  $\mathbf{B}$  and  $\mathbf{b}$  have the forms given by equation (7) in Nolan & Wand (2018) with

$$\mathbf{b}_{ij} \equiv \begin{bmatrix} \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{y}_{ij} \\ (\sum_{i=1}^m n_i)^{-1/2} \Sigma_\beta^{-1/2} \mu_\beta \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{B}_{ij} \equiv \begin{bmatrix} \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{X}_{ij} & \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{Z}_{\text{gbl}, ij} \\ (\sum_{i=1}^m n_i)^{-1/2} \Sigma_\beta^{-1/2} & \mathbf{O} \\ \mathbf{O} & (\sum_{i=1}^m n_i)^{-1/2} \mu_{q(1/\sigma_{\text{gbl}}^2)}^{1/2} \mathbf{I}_{K_{\text{gbl}}} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix},$$

$$\dot{\mathbf{B}}_{ij} \equiv \begin{bmatrix} \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{X}_{ij} & \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{Z}_{\text{grp}, ij}^g \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ n_i^{-1/2} M_{q(\Sigma_g^{-1})}^{1/2} & \mathbf{O} \\ \mathbf{O} & n_i^{-1/2} \mu_{q(1/\sigma_{\text{grp}, g}^2)}^{1/2} \mathbf{I}_{K_{\text{grp}}^g} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix} \quad \text{and} \quad \ddot{\mathbf{B}}_{ij} \equiv \begin{bmatrix} \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{X}_{ij} & \mu_{q(1/\sigma_\varepsilon^2)}^{1/2} \mathbf{Z}_{\text{grp}, ij}^h \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ M_{q(\Sigma_h^{-1})}^{1/2} & \mathbf{O} \\ \mathbf{O} & \mu_{q(1/\sigma_{\text{grp}, h}^2)}^{1/2} \mathbf{I}_{K_{\text{grp}}^h} \end{bmatrix}.$$

Result 4 immediately follows from Theorem 4 of Nolan & Wand (2018).

## S.10 Derivation of Algorithm 4

Algorithm 4 relies on expressions for the  $q$ -densities for mean field variational Bayesian inference for the parameters in (3.4) with product density restriction (3.5). We have

$$q(\beta, \mathbf{u}) \text{ is a } N(\mu_{q(\beta, \mathbf{u})}, \Sigma_{q(\beta, \mathbf{u})}) \text{ density function}$$

where

$$\Sigma_{q(\beta, \mathbf{u})} = (\mathbf{C}^T \mathbf{R}_{\text{MFVB}}^{-1} \mathbf{C} + D_{\text{MFVB}})^{-1} \quad \text{and} \quad \mu_{q(\beta, \mathbf{u})} = \Sigma_{q(\beta, \mathbf{u})} (\mathbf{C}^T \mathbf{R}_{\text{MFVB}}^{-1} \mathbf{y} + \mathbf{o}_{\text{MFVB}})$$

with  $\mathbf{R}_{\text{MFVB}} \equiv \mu_{\mathbf{q}(1/\sigma_\varepsilon^2)}^{-1} \mathbf{I}$ ,  $\mathbf{o}_{\text{MFVB}} \equiv \begin{bmatrix} \boldsymbol{\Sigma}_\beta^{-1} \boldsymbol{\mu}_\beta \\ \mathbf{0} \end{bmatrix}$  and  $D_{\text{MFVB}}$  as given in (3.3),

$\mathbf{q}(\sigma_\varepsilon^2)$  is an Inverse- $\chi^2$  ( $\xi_{\mathbf{q}(\sigma_\varepsilon^2)}$ ,  $\lambda_{\mathbf{q}(\sigma_\varepsilon^2)}$ ) density function

where  $\xi_{\mathbf{q}(\sigma_\varepsilon^2)} = \nu_\varepsilon + \sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij}$  and

$$\begin{aligned} \lambda_{\mathbf{q}(\sigma_\varepsilon^2)} &= \mu_{\mathbf{q}(1/a_\varepsilon)} + \sum_{i=1}^m \sum_{j=1}^{n_i} E_{\mathbf{q}} \left\{ \left\| \mathbf{y}_{ij} - \mathbf{C}_{\text{gbl},ij} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^g \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^h \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} \right\|^2 \right\} \\ &= \mu_{\mathbf{q}(1/a_\varepsilon)} + \sum_{i=1}^m \sum_{j=1}^{n_i} \left[ \left\| E_{\mathbf{q}} \left( \mathbf{y}_{ij} - \mathbf{C}_{\text{gbl},ij} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^g \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^h \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} \right) \right\|^2 \right. \\ &\quad \left. + \text{tr} \left\{ \text{Cov}_{\mathbf{q}} \left( \mathbf{C}_{\text{gbl},ij} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} + \mathbf{C}_{\text{grp},ij}^g \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} + \mathbf{C}_{\text{grp},ij}^h \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} \right) \right\} \right] \\ &= \mu_{\mathbf{q}(1/a_\varepsilon)} + \sum_{i=1}^m \sum_{j=1}^{n_i} \left\{ \left\| E_{\mathbf{q}} \left( \mathbf{y}_{ij} - \mathbf{C}_{\text{gbl},ij} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^g \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^h \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} \right) \right\|^2 \right. \\ &\quad + \text{tr}(\mathbf{C}_{\text{gbl},ij}^T \mathbf{C}_{\text{gbl},ij} \boldsymbol{\Sigma}_{\mathbf{q}}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})) + \text{tr}((\mathbf{C}_{\text{grp},ij}^g)^T \mathbf{C}_{\text{grp},ij}^g \boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g)) + \text{tr}((\mathbf{C}_{\text{grp},ij}^h)^T \mathbf{C}_{\text{grp},ij}^h \boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h)) \\ &\quad + 2 \text{tr} \left[ (\mathbf{C}_{\text{grp},ij}^g)^T \mathbf{C}_{\text{gbl},ij} E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}}) \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g) \right)^T \right\} \right] \\ &\quad + 2 \text{tr} \left[ (\mathbf{C}_{\text{grp},ij}^h)^T \mathbf{C}_{\text{gbl},ij} E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}}) \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h) \right)^T \right\} \right] \\ &\quad \left. + 2 \text{tr} \left[ (\mathbf{C}_{\text{grp},ij}^g)^T \mathbf{C}_{\text{grp},ij}^h E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g) \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h) \right)^T \right\} \right] \right\} \end{aligned}$$

where  $\mathbf{C}_{\text{gbl},ij} \equiv [\mathbf{X}_{ij} \mathbf{Z}_{\text{gbl},ij}]$ ,  $\mathbf{C}_{\text{grp},ij}^g \equiv [\mathbf{X}_{ij} \mathbf{Z}_{\text{grp},ij}^g]$ ,  $\mathbf{C}_{\text{grp},ij}^h \equiv [\mathbf{X}_{ij} \mathbf{Z}_{\text{grp},ij}^h]$  and with reciprocal moment  $\mu_{\mathbf{q}(1/\sigma_\varepsilon^2)} = \xi_{\mathbf{q}(\sigma_\varepsilon^2)} / \lambda_{\mathbf{q}(\sigma_\varepsilon^2)}$ ,

$\mathbf{q}(\sigma_{\text{gbl}}^2)$  is an Inverse- $\chi^2$  ( $\xi_{\mathbf{q}(\sigma_{\text{gbl}}^2)}$ ,  $\lambda_{\mathbf{q}(\sigma_{\text{gbl}}^2)}$ ) density function

where  $\xi_{\mathbf{q}(\sigma_{\text{gbl}}^2)} = \nu_{\text{gbl}} + K_{\text{gbl}}$  and

$$\lambda_{\mathbf{q}(\sigma_{\text{gbl}}^2)} = \mu_{\mathbf{q}(1/a_{\text{gbl}})} + \|\boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{gbl}})\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{gbl}})),$$

with reciprocal moment  $\mu_{\mathbf{q}(1/\sigma_{\text{gbl}}^2)} = \xi_{\mathbf{q}(\sigma_{\text{gbl}}^2)} / \lambda_{\mathbf{q}(\sigma_{\text{gbl}}^2)}$ ,

$\mathbf{q}(\sigma_{\text{grp},g}^2)$  is an Inverse- $\chi^2$  ( $\xi_{\mathbf{q}(\sigma_{\text{grp},g}^2)}$ ,  $\lambda_{\mathbf{q}(\sigma_{\text{grp},g}^2)}$ ) density function

where  $\xi_{\mathbf{q}(\sigma_{\text{grp},g}^2)} = \nu_{\text{grp},g} + mK_{\text{grp}}^g$  and

$$\lambda_{\mathbf{q}(\sigma_{\text{grp},g}^2)} = \mu_{\mathbf{q}(1/a_{\text{grp},g})} + \sum_{i=1}^m \left\{ \|\boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{grp},i}^g)\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{grp},i}^g)) \right\},$$

with reciprocal moment  $\mu_{q(1/\sigma_{\text{grp},g}^2)} = \xi_{q(\sigma_{\text{grp},g}^2)}/\lambda_{q(\sigma_{\text{grp},g}^2)}$ ,

$q(\Sigma_g)$  is an Inverse-G-Wishart  $(G_{\text{full}}, \xi_{q(\Sigma_g)}, \Lambda_{q(\Sigma_g)})$  density function

where  $\xi_{q(\Sigma_g)} = \nu_{\Sigma_g} + 2 + m$  and

$$\Lambda_{q(\Sigma_g)} = M_{q(\mathbf{A}_{\Sigma_g}^{-1})} + \sum_{i=1}^m \left( \boldsymbol{\mu}_{q(\mathbf{u}_{\text{lin},i}^g)} \boldsymbol{\mu}_{q(\mathbf{u}_{\text{lin},i}^g)}^T + \Sigma_{q(\mathbf{u}_{\text{lin},i}^g)} \right),$$

with inverse moment  $M_{q(\Sigma_g^{-1})} = (\xi_{q(\Sigma_g)} - 1) \Lambda_{q(\Sigma_g)}^{-1}$ ,

$q(\sigma_{\text{grp},h}^2)$  is an Inverse- $\chi^2$   $(\xi_{q(\sigma_{\text{grp},h}^2)}, \lambda_{q(\sigma_{\text{grp},h}^2)})$  density function

where  $\xi_{q(\sigma_{\text{grp},h}^2)} = \nu_{\text{grp},h} + K_{\text{grp}}^h \sum_{i=1}^m n_i$  and

$$\lambda_{q(\sigma_{\text{grp},h}^2)} = \mu_{q(1/a_{\text{grp},h})} + \sum_{i=1}^m \sum_{j=1}^{n_i} \left\{ \|\boldsymbol{\mu}_{q(\mathbf{u}_{\text{grp},ij}^h)}\|^2 + \text{tr} \left( \Sigma_{q(\mathbf{u}_{\text{grp},ij}^h)} \right) \right\},$$

with reciprocal moment  $\mu_{q(1/\sigma_{\text{grp},h}^2)} = \xi_{q(\sigma_{\text{grp},h}^2)}/\lambda_{q(\sigma_{\text{grp},h}^2)}$ ,

$q(\Sigma_h)$  is an Inverse-G-Wishart  $(G_{\text{full}}, \xi_{q(\Sigma_h)}, \Lambda_{q(\Sigma_h)})$  density function

where  $\xi_{q(\Sigma_h)} = \nu_{\Sigma_h} + 2 + \sum_{i=1}^m n_i$  and

$$\Lambda_{q(\Sigma_h)} = M_{q(\mathbf{A}_{\Sigma_h}^{-1})} + \sum_{i=1}^m \sum_{j=1}^{n_i} \left( \boldsymbol{\mu}_{q(\mathbf{u}_{\text{lin},ij}^h)} \boldsymbol{\mu}_{q(\mathbf{u}_{\text{lin},ij}^h)}^T + \Sigma_{q(\mathbf{u}_{\text{lin},ij}^h)} \right),$$

with inverse moment  $M_{q(\Sigma_h^{-1})} = (\xi_{q(\Sigma_h)} - 1) \Lambda_{q(\Sigma_h)}^{-1}$ ,

$q(a_\varepsilon)$  is an Inverse- $\chi^2$   $(\xi_{q(a_\varepsilon)}, \lambda_{q(a_\varepsilon)})$  density function

where  $\xi_{q(a_\varepsilon)} = \nu_\varepsilon + 1$ ,

$$\lambda_{q(a_\varepsilon)} = \mu_{q(1/\sigma_\varepsilon^2)} + 1/(\nu_\varepsilon s_\varepsilon^2)$$

with reciprocal moment  $\mu_{q(1/a_\varepsilon)} = \xi_{q(a_\varepsilon)}/\lambda_{q(a_\varepsilon)}$ ,

$q(a_{\text{gbl}})$  is an Inverse- $\chi^2$   $(\xi_{q(a_{\text{gbl}})}, \lambda_{q(a_{\text{gbl}})})$  density function

where  $\xi_{q(a_{\text{gbl}})} = \nu_{\text{gbl}} + 1$ ,

$$\lambda_{q(a_{\text{gbl}})} = \mu_{q(1/\sigma_{\text{gbl}}^2)} + 1/(\nu_{\text{gbl}} s_{\text{gbl}}^2)$$

with reciprocal moment  $\mu_{q(1/a_{\text{gbl}})} = \xi_{q(a_{\text{gbl}})}/\lambda_{q(a_{\text{gbl}})}$ ,

$q(a_{\text{grp},g})$  is an Inverse- $\chi^2$   $(\xi_{q(a_{\text{grp},g})}, \lambda_{q(a_{\text{grp},g})})$  density function

where  $\xi_{q(a_{\text{grp},g})} = \nu_{\text{grp},g} + 1$ ,

$$\lambda_{q(a_{\text{grp},g})} = \mu_{q(1/\sigma_{\text{grp},g}^2)} + 1/(\nu_{\text{grp},g} s_{\text{grp},g}^2)$$

with reciprocal moment  $\mu_{q(1/a_{\text{grp},g})} = \xi_{q(a_{\text{grp},g})}/\lambda_{q(a_{\text{grp},g})}$  and

$q(\mathbf{A}_{\Sigma_g})$  is an Inverse-G-Wishart  $(G_{\text{diag}}, \xi_{q(\mathbf{A}_{\Sigma_g})}, \Lambda_{q(\mathbf{A}_{\Sigma_g})})$  density function

where  $\xi_{q(\mathbf{A}_{\Sigma_g})} = \nu_{\Sigma_g} + 2$ ,

$$\Lambda_{q(\mathbf{A}_{\Sigma_g})} = \text{diag} \{ \text{diagonal}(M_{q(\Sigma_g^{-1})}) \} + \Lambda_{\mathbf{A}_{\Sigma_g}}$$

with inverse moment  $M_{\mathbf{q}(\mathbf{A}_{\Sigma_g}^{-1})} = \xi_{\mathbf{q}(\mathbf{A}_{\Sigma_g})} \mathbf{\Lambda}_{\mathbf{q}(\mathbf{A}_{\Sigma_g})}^{-1}$ ,

$\mathbf{q}(a_{\text{grp}, h})$  is an Inverse- $\chi^2(\xi_{\mathbf{q}(a_{\text{grp}, h})}, \lambda_{\mathbf{q}(a_{\text{grp}, h})})$  density function

where  $\xi_{\mathbf{q}(a_{\text{grp}, h})} = \nu_{\text{grp}, h} + 1$ ,

$$\lambda_{\mathbf{q}(a_{\text{grp}, h})} = \mu_{\mathbf{q}(1/\sigma_{\text{grp}, h}^2)} + 1/(\nu_{\text{grp}, h} \xi_{\mathbf{q}(a_{\text{grp}, h})}^2)$$

with reciprocal moment  $\mu_{\mathbf{q}(1/a_{\text{grp}, h})} = \xi_{\mathbf{q}(a_{\text{grp}, h})} / \lambda_{\mathbf{q}(a_{\text{grp}, h})}$  and

$\mathbf{q}(\mathbf{A}_{\Sigma_h})$  is an Inverse-G-Wishart  $(G_{\text{diag}}, \xi_{\mathbf{q}(\mathbf{A}_{\Sigma_h})}, \mathbf{\Lambda}_{\mathbf{q}(\mathbf{A}_{\Sigma_h})})$  density function

where  $\xi_{\mathbf{q}(\mathbf{A}_{\Sigma_h})} = \nu_{\Sigma_h} + 2$

$$\mathbf{\Lambda}_{\mathbf{q}(\mathbf{A}_{\Sigma_h})} = \text{diag}\{\text{diagonal}(M_{\mathbf{q}(\Sigma_h^{-1})})\} + \mathbf{\Lambda}_{\mathbf{A}_{\Sigma_h}}$$

with inverse moment  $M_{\mathbf{q}(\mathbf{A}_{\Sigma_h}^{-1})} = \xi_{\mathbf{q}(\mathbf{A}_{\Sigma_h})} \mathbf{\Lambda}_{\mathbf{q}(\mathbf{A}_{\Sigma_h})}^{-1}$ .

## S.11 Approximate Marginal Log-Likelihood for Three-Level Models

$$\begin{aligned}
& \log \underline{p}(\mathbf{y}; \mathbf{q}) = \\
& -\frac{1}{2} \left\{ \sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij} + 4 \right\} \log(\pi) + \frac{1}{2} \left\{ 2 + K_{\text{gbl}} + m(2 + K_{\text{grp}}) + \sum_{i=1}^m n_i(2 + K_{\text{grp}}^h) \right\} \\
& -\frac{1}{2} \left( \sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij} + \nu_\varepsilon + \nu_{\text{gbl}} + \nu_{\text{grp},g} + \nu_{\text{grp},h} \right) \log(2) + \left( 2 + m + \sum_{i=1}^m n_i + \nu_{\Sigma_g} + \nu_{\Sigma_h} \right) \log(2) \\
& -\frac{1}{2} \text{tr} \left( \Sigma_\beta^{-1} \left\{ \left( \boldsymbol{\mu}_{\mathbf{q}(\beta)} - \boldsymbol{\mu}_\beta \right) \left( \boldsymbol{\mu}_{\mathbf{q}(\beta)} - \boldsymbol{\mu}_\beta \right)^T + \Sigma_{\mathbf{q}(\beta)} \right\} \right) - \frac{1}{2} \log |\Sigma_\beta| + \frac{1}{2} \log |\Sigma_{\mathbf{q}(\beta, \mathbf{u})}| \\
& -\frac{1}{2} \text{tr} \left( \mathbf{M}_{\mathbf{q}(\Sigma_g^{-1})} \sum_{i=1}^m \left( \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}^g)} \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}^g)}^T + \Sigma_{\mathbf{q}(\mathbf{u}_{\text{lin},i}^g)} \right) \right) - \frac{1}{2} \mu_{\mathbf{q}(1/\sigma_{\text{grp},h}^2)} \sum_{i=1}^m \sum_{j=1}^{n_i} \left\{ \|\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{grp},ij}^h)}\|^2 + \text{tr}(\Sigma_{\mathbf{q}(\mathbf{u}_{\text{grp},ij}^h)}) \right\} \\
& -\frac{1}{2} \text{tr} \left( \mathbf{M}_{\mathbf{q}(\Sigma_h^{-1})} \sum_{i=1}^m \sum_{j=1}^{n_i} \left( \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h)} \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h)}^T + \Sigma_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h)} \right) \right) - \frac{1}{2} \mu_{\mathbf{q}(1/\sigma_{\text{gbl}}^2)} \left\{ \|\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{gbl}})}\|^2 + \text{tr}(\Sigma_{\mathbf{q}(\mathbf{u}_{\text{gbl}})}) \right\} \\
& -\frac{1}{2} \mu_{\mathbf{q}(1/\sigma_{\text{grp},g}^2)} \sum_{i=1}^m \left\{ \|\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{grp},i}^g)}\|^2 + \text{tr}(\Sigma_{\mathbf{q}(\mathbf{u}_{\text{grp},i}^g)}) \right\} - \log \Gamma\left(\frac{\nu_\varepsilon}{2}\right) - \frac{1}{2} \mu_{\mathbf{q}(1/a_\varepsilon)} \mu_{\mathbf{q}(1/\sigma_\varepsilon^2)} \\
& -\frac{1}{2} \xi_{\mathbf{q}(\sigma_\varepsilon^2)} \log(\lambda_{\mathbf{q}(\sigma_\varepsilon^2)}) + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(\sigma_\varepsilon^2)})\} + \frac{1}{2} \lambda_{\mathbf{q}(\sigma_\varepsilon^2)} \mu_{\mathbf{q}(1/\sigma_\varepsilon^2)} - \frac{1}{2} \log(\nu_\varepsilon s_\varepsilon^2) - \frac{1}{2\nu_\varepsilon s_\varepsilon^2} \mu_{\mathbf{q}(1/a_\varepsilon)} - \frac{1}{2} \xi_{\mathbf{q}(a_\varepsilon)} \log(\lambda_{\mathbf{q}(a_\varepsilon)}) \\
& + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(a_\varepsilon)})\} + \frac{1}{2} \lambda_{\mathbf{q}(a_\varepsilon)} \mu_{\mathbf{q}(1/a_\varepsilon)} - \log \Gamma\left(\frac{\nu_{\text{gbl}}}{2}\right) - \frac{1}{2} \mu_{\mathbf{q}(1/a_{\text{gbl}})} \mu_{\mathbf{q}(1/\sigma_{\text{gbl}}^2)} - \frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{gbl}}^2)} \log(\lambda_{\mathbf{q}(\sigma_{\text{gbl}}^2)}) \\
& + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{gbl}}^2)})\} - \frac{1}{2} \log(\nu_{\text{gbl}} s_{\text{gbl}}^2) + \frac{1}{2} \lambda_{\mathbf{q}(\sigma_{\text{gbl}}^2)} \mu_{\mathbf{q}(1/\sigma_{\text{gbl}}^2)} - \{1/(2\nu_{\text{gbl}} s_{\text{gbl}}^2)\} \mu_{\mathbf{q}(1/a_{\text{gbl}})} - \frac{1}{2} \xi_{\mathbf{q}(a_{\text{gbl}})} \log(\lambda_{\mathbf{q}(a_{\text{gbl}})}) \\
& + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(a_{\text{gbl}})})\} + \frac{1}{2} \lambda_{\mathbf{q}(a_{\text{gbl}})} \mu_{\mathbf{q}(1/a_{\text{gbl}})} - \frac{1}{2} \mu_{\mathbf{q}(1/a_{\text{grp},g})} \mu_{\mathbf{q}(1/\sigma_{\text{grp},g}^2)} - \log \Gamma\left(\frac{\nu_{\text{grp},g}}{2}\right) + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{grp},g}^2)})\} \\
& -\frac{1}{2} \log(\nu_{\text{grp},g} s_{\text{grp},g}^2) - \frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{grp},g}^2)} \log(\lambda_{\mathbf{q}(\sigma_{\text{grp},g}^2)}) + \frac{1}{2} \lambda_{\mathbf{q}(\sigma_{\text{grp},g}^2)} \mu_{\mathbf{q}(1/\sigma_{\text{grp},g}^2)} - \{1/(2\nu_{\text{grp},g} s_{\text{grp},g}^2)\} \mu_{\mathbf{q}(1/a_{\text{grp},g})} \\
& -\frac{1}{2} \xi_{\mathbf{q}(a_{\text{grp},g})} \log(\lambda_{\mathbf{q}(a_{\text{grp},g})}) + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(a_{\text{grp},g})})\} + \frac{1}{2} \lambda_{\mathbf{q}(a_{\text{grp},g})} \mu_{\mathbf{q}(1/a_{\text{grp},g})} - \frac{1}{2} \mu_{\mathbf{q}(1/a_{\text{grp},h})} \mu_{\mathbf{q}(1/\sigma_{\text{grp},h}^2)} \\
& -\log \Gamma\left(\frac{\nu_{\text{grp},h}}{2}\right) + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{grp},h}^2)})\} - \frac{1}{2} \log(\nu_{\text{grp},h} s_{\text{grp},h}^2) - \frac{1}{2} \xi_{\mathbf{q}(\sigma_{\text{grp},h}^2)} \log(\lambda_{\mathbf{q}(\sigma_{\text{grp},h}^2)}) + \frac{1}{2} \lambda_{\mathbf{q}(\sigma_{\text{grp},h}^2)} \mu_{\mathbf{q}(1/\sigma_{\text{grp},h}^2)} \\
& -\{1/(2\nu_{\text{grp},h} s_{\text{grp},h}^2)\} \mu_{\mathbf{q}(1/a_{\text{grp},h})} - \frac{1}{2} \xi_{\mathbf{q}(a_{\text{grp},h})} \log(\lambda_{\mathbf{q}(a_{\text{grp},h})}) + \log\{\Gamma(\frac{1}{2} \xi_{\mathbf{q}(a_{\text{grp},h})})\} + \frac{1}{2} \lambda_{\mathbf{q}(a_{\text{grp},h})} \mu_{\mathbf{q}(1/a_{\text{grp},h})} \\
& -\frac{1}{2} \text{tr}(\mathbf{M}_{\mathbf{q}(\mathbf{A}_{\Sigma_g}^{-1})} \mathbf{M}_{\mathbf{q}(\Sigma_g^{-1})}) + \frac{1}{2} \text{tr}(\mathbf{A}_{\mathbf{q}(\Sigma_g)} \mathbf{M}_{\mathbf{q}(\Sigma_g^{-1})}) - \frac{1}{2} \text{tr}(\mathbf{M}_{\mathbf{q}(\mathbf{A}_{\Sigma_h}^{-1})} \mathbf{M}_{\mathbf{q}(\Sigma_h^{-1})}) + \frac{1}{2} \text{tr}(\mathbf{A}_{\mathbf{q}(\Sigma_h)} \mathbf{M}_{\mathbf{q}(\Sigma_h^{-1})}) \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(\xi_{\mathbf{q}(\mathbf{A}_{\Sigma_g})} + 2 - j)\right) - \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(\nu_{\Sigma_g} + 4 - j)\right) - \frac{1}{2}(\xi_{\mathbf{q}(\Sigma_g)} - 1) \log |\mathbf{A}_{\mathbf{q}(\Sigma_g)}| \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(\xi_{\mathbf{q}(\Sigma_g)} + 2 - j)\right) - \frac{1}{2} \sum_{j=1}^2 1/(\nu_{\Sigma_g} s_{\Sigma_g,j}^2) \left( \mathbf{M}_{\mathbf{q}(\mathbf{A}_{\Sigma_g}^{-1})} \right)_{jj} - \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(3 - j)\right) \\
& -\frac{1}{2}(\xi_{\mathbf{q}(\mathbf{A}_{\Sigma_g})} - 1) \log |\mathbf{A}_{\mathbf{q}(\mathbf{A}_{\Sigma_g})}| + \frac{1}{2} \text{tr}(\mathbf{A}_{\mathbf{q}(\mathbf{A}_{\Sigma_g})} \mathbf{M}_{\mathbf{q}(\mathbf{A}_{\Sigma_g}^{-1})}) \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(\xi_{\mathbf{q}(\mathbf{A}_{\Sigma_h})} + 2 - j)\right) - \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(\nu_{\Sigma_h} + 4 - j)\right) - \frac{1}{2}(\xi_{\mathbf{q}(\Sigma_h)} - 1) \log |\mathbf{A}_{\mathbf{q}(\Sigma_h)}| \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(\xi_{\mathbf{q}(\Sigma_h)} + 2 - j)\right) - \frac{1}{2} \sum_{j=1}^2 1/(\nu_{\Sigma_h} s_{\Sigma_h,j}^2) \left( \mathbf{M}_{\mathbf{q}(\mathbf{A}_{\Sigma_h}^{-1})} \right)_{jj} - \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2}(3 - j)\right)
\end{aligned} \tag{S.3}$$

$$\begin{aligned}
& -\frac{1}{2}(\xi_{\mathbf{q}(\mathbf{A}_{\Sigma_h})} - 1) \log |\mathbf{\Lambda}_{\mathbf{q}(\mathbf{A}_{\Sigma_h})}| + \frac{1}{2} \text{tr}(\mathbf{\Lambda}_{\mathbf{q}(\mathbf{A}_{\Sigma_h})} \mathbf{M}_{\mathbf{q}(\mathbf{A}_{\Sigma_h}^{-1})}) \\
& -\frac{1}{2} \mu_{\mathbf{q}(1/\sigma_\varepsilon^2)} \sum_{i=1}^m \sum_{j=1}^{n_i} \left\{ \left\| E_{\mathbf{q}} \left( \mathbf{y}_{ij} - \mathbf{C}_{\text{gbl},ij} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl},i} \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^g \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^h \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} \right) \right\|^2 \\
& + \text{tr} \left( \mathbf{C}_{\text{gbl},ij}^T \mathbf{C}_{\text{gbl},ij} \boldsymbol{\Sigma}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})} \right) + \text{tr} \left( \mathbf{C}_{\text{grp},ij}^g{}^T \mathbf{C}_{\text{grp},ij}^g \boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g)} \right) \\
& + \text{tr} \left( \mathbf{C}_{\text{grp},ij}^h{}^T \mathbf{C}_{\text{grp},ij}^h \boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h)} \right) \\
& + 2 \text{tr} \left[ \mathbf{C}_{\text{grp},ij}^g{}^T \mathbf{C}_{\text{gbl},ij} E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})} \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g)} \right) \right\}^T \right] \\
& + 2 \text{tr} \left[ \mathbf{C}_{\text{grp},ij}^h{}^T \mathbf{C}_{\text{gbl},ij} E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})} \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h)} \right) \right\}^T \right] \\
& + 2 \text{tr} \left[ \mathbf{C}_{\text{grp},ij}^g{}^T \mathbf{C}_{\text{grp},ij}^h E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g)} \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h)} \right) \right\}^T \right] \left. \right\}.
\end{aligned}$$

*Derivation:* The lower bound on the marginal log-likelihood is achieved through the following expression:

$$\begin{aligned}
\log \underline{\mathbf{p}}(\mathbf{y}; \mathbf{q}) &= E_{\mathbf{q}} \{ \log \mathbf{p}(\mathbf{y}, \boldsymbol{\beta}, \mathbf{u}, \sigma_\varepsilon^2, a_\varepsilon, \sigma_{\text{gbl}}^2, a_{\text{gbl}}, \sigma_{\text{grp},g}^2, \boldsymbol{\Sigma}_g, a_{\text{grp},g}, \mathbf{A}_{\Sigma_g}, \sigma_{\text{grp},h}^2, \boldsymbol{\Sigma}_h, a_{\text{grp},h}, \mathbf{A}_{\Sigma_h}) \\
&\quad - \log \mathbf{q}^*(\boldsymbol{\beta}, \mathbf{u}, \sigma_\varepsilon^2, a_\varepsilon, \sigma_{\text{gbl}}^2, a_{\text{gbl}}, \sigma_{\text{grp},g}^2, \boldsymbol{\Sigma}_g, a_{\text{grp},g}, \mathbf{A}_{\Sigma_g}, \sigma_{\text{grp},h}^2, \boldsymbol{\Sigma}_h, a_{\text{grp},h}, \mathbf{A}_{\Sigma_h}) \} \\
&= E_{\mathbf{q}} \{ \log \mathbf{p}(\mathbf{y} | \boldsymbol{\beta}, \mathbf{u}, \sigma_\varepsilon^2) \} \\
&\quad + E_{\mathbf{q}} \{ \log \mathbf{p}(\boldsymbol{\beta}, \mathbf{u} | \sigma_{\text{gbl}}^2, \sigma_{\text{grp},g}^2, \boldsymbol{\Sigma}_g, \sigma_{\text{grp},h}^2, \boldsymbol{\Sigma}_h) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(\boldsymbol{\beta}, \mathbf{u}) \} \\
&\quad + E_{\mathbf{q}} \{ \log \mathbf{p}(\sigma_\varepsilon^2 | a_\varepsilon) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(\sigma_\varepsilon^2) \} + E_{\mathbf{q}} \{ \log \mathbf{p}(a_\varepsilon) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(a_\varepsilon) \} \\
&\quad + E_{\mathbf{q}} \{ \log \mathbf{p}(\sigma_{\text{gbl}}^2 | a_{\text{gbl}}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(\sigma_{\text{gbl}}^2) \} + E_{\mathbf{q}} \{ \log \mathbf{p}(a_{\text{gbl}}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(a_{\text{gbl}}) \} \\
&\quad + E_{\mathbf{q}} \{ \log \mathbf{p}(\sigma_{\text{grp},g}^2 | a_{\text{grp},g}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(\sigma_{\text{grp},g}^2) \} + E_{\mathbf{q}} \{ \log \mathbf{p}(a_{\text{grp},g}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(a_{\text{grp},g}) \} \\
&\quad + E_{\mathbf{q}} \{ \log \mathbf{p}(\boldsymbol{\Sigma}_g | \mathbf{A}_{\Sigma_g}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(\boldsymbol{\Sigma}_g) \} + E_{\mathbf{q}} \{ \log \mathbf{p}(\mathbf{A}_{\Sigma_g}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(\mathbf{A}_{\Sigma_g}) \} \\
&\quad + E_{\mathbf{q}} \{ \log \mathbf{p}(\sigma_{\text{grp},h}^2 | a_{\text{grp},h}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(\sigma_{\text{grp},h}^2) \} + E_{\mathbf{q}} \{ \log \mathbf{p}(a_{\text{grp},h}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(a_{\text{grp},h}) \} \\
&\quad + E_{\mathbf{q}} \{ \log \mathbf{p}(\boldsymbol{\Sigma}_h | \mathbf{A}_{\Sigma_h}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(\boldsymbol{\Sigma}_h) \} + E_{\mathbf{q}} \{ \log \mathbf{p}(\mathbf{A}_{\Sigma_h}) \} - E_{\mathbf{q}} \{ \log \mathbf{q}^*(\mathbf{A}_{\Sigma_h}) \}.
\end{aligned} \tag{S.4}$$

First we note that

$$\log \mathbf{p}(\mathbf{y} | \boldsymbol{\beta}, \mathbf{u}, \sigma_\varepsilon^2) = -\frac{1}{2} \log(2\pi) \sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij} - \frac{1}{2} \log(\sigma_\varepsilon^2) \sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij} - \frac{1}{2\sigma_\varepsilon^2} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\mathbf{u}\|^2$$

where

$$\begin{aligned}
& \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{Z}\mathbf{u}\|^2 \\
&= \sum_{i=1}^m \sum_{j=1}^{n_i} \|\mathbf{y}_{ij} - \mathbf{X}_{ij}\boldsymbol{\beta} - \mathbf{Z}_{\text{gbl},ij} \mathbf{u}_{\text{gbl},i} - \mathbf{X}_{ij} \mathbf{u}_{\text{lin},i}^g - \mathbf{Z}_{\text{grp},ij}^g \mathbf{u}_{\text{grp},i}^g - \mathbf{X}_{ij} \mathbf{u}_{\text{lin},ij}^h - \mathbf{Z}_{\text{grp},ij}^h \mathbf{u}_{\text{grp},ij}^h\|^2 \\
&= \sum_{i=1}^m \sum_{j=1}^{n_i} \left\| \mathbf{y}_{ij} - \mathbf{C}_{\text{gbl},ij} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl},i} \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^g \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^h \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} \right\|^2
\end{aligned}$$

and

$$\mathbf{C}_{\text{gbl},ij} \equiv [\mathbf{X}_{ij} \mathbf{Z}_{\text{gbl},ij}], \quad \mathbf{C}_{\text{grp},ij}^g \equiv [\mathbf{X}_{ij} \mathbf{Z}_{\text{grp},ij}^g], \quad \mathbf{C}_{\text{grp},ij}^h \equiv [\mathbf{X}_{ij} \mathbf{Z}_{\text{grp},ij}^h].$$

Therefore,

$$\begin{aligned}
& E_{\mathbf{q}}\{\log \mathbf{p}(\mathbf{y} \mid \boldsymbol{\beta}, \mathbf{u}, \sigma_{\varepsilon}^2)\} \\
&= -\frac{1}{2} \log(2\pi) \sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij} - \frac{1}{2} E_{\mathbf{q}}\{\log(\sigma_{\varepsilon}^2)\} \sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij} \\
&\quad - \frac{1}{2} \mu_{\mathbf{q}}(1/\sigma_{\varepsilon}^2) \sum_{i=1}^m \sum_{j=1}^{n_i} \left\{ \left\| E_{\mathbf{q}} \left( \mathbf{y}_{ij} - \mathbf{C}_{\text{gbl},ij} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl},i} \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^g \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^h \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} \right) \right\|^2 \right. \\
&\quad \left. + \text{tr} \left( \mathbf{C}_{\text{gbl},ij}^T \mathbf{C}_{\text{gbl},ij} \boldsymbol{\Sigma}_{\mathbf{q}}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}}) \right) + \text{tr} \left( \mathbf{C}_{\text{grp},ij}^{g,T} \mathbf{C}_{\text{grp},ij}^g \boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g) \right) \right. \\
&\quad \left. + \text{tr} \left( \mathbf{C}_{\text{grp},ij}^{h,T} \mathbf{C}_{\text{grp},ij}^h \boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h) \right) \right. \\
&\quad \left. + 2 \text{tr} \left[ \mathbf{C}_{\text{grp},ij}^{g,T} \mathbf{C}_{\text{gbl},ij} E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}}) \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g) \right)^T \right\} \right] \right. \\
&\quad \left. + 2 \text{tr} \left[ \mathbf{C}_{\text{grp},ij}^{h,T} \mathbf{C}_{\text{gbl},ij} E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}}) \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h) \right)^T \right\} \right] \right. \\
&\quad \left. + 2 \text{tr} \left[ \mathbf{C}_{\text{grp},ij}^{g,T} \mathbf{C}_{\text{grp},ij}^h E_{\mathbf{q}} \left\{ \left( \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g) \right) \left( \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h) \right)^T \right\} \right] \right\}
\end{aligned}$$

The remainder of the expectations in (S.4) are expressed as:

$$\begin{aligned}
& E_{\mathbf{q}}\{\log \mathbf{p}(\boldsymbol{\beta}, \mathbf{u} \mid \sigma_{\text{gbl}}^2, \sigma_{\text{grp},g}^2, \boldsymbol{\Sigma}_g, \sigma_{\text{grp},h}^2, \boldsymbol{\Sigma}_h)\} \\
&= -\frac{1}{2} \{2 + K_{\text{gbl}} + m(2 + K_{\text{grp}}^g) + (2 + K_{\text{grp}}^h) \sum_{i=1}^m n_i\} \log(2\pi) - \frac{1}{2} \log |\boldsymbol{\Sigma}_{\boldsymbol{\beta}}| - \frac{1}{2} K_{\text{gbl}} E_{\mathbf{q}}\{\log(\sigma_{\text{gbl}}^2)\} \\
&\quad - \frac{1}{2} m (E_{\mathbf{q}}\{\log |\boldsymbol{\Sigma}_g|\} - K_{\text{grp}}^g E_{\mathbf{q}}\{\log(\sigma_{\text{grp},g}^2)\}) - \frac{1}{2} (E_{\mathbf{q}}\{\log |\boldsymbol{\Sigma}_h|\} - K_{\text{grp}}^h E_{\mathbf{q}}\{\log(\sigma_{\text{grp},h}^2)\}) \sum_{i=1}^m n_i \\
&\quad - \frac{1}{2} \mu_{\mathbf{q}}(1/\sigma_{\text{gbl}}^2) \left\{ \|\boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{gbl}})\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{gbl}})) \right\} - \frac{1}{2} \mu_{\mathbf{q}}(1/\sigma_{\text{grp},g}^2) \sum_{i=1}^m \left\{ \|\boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{grp},i}^g)\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{grp},i}^g)) \right\} \\
&\quad - \frac{1}{2} \mu_{\mathbf{q}}(1/\sigma_{\text{grp},h}^2) \sum_{i=1}^m \sum_{j=1}^{n_i} \left\{ \|\boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{grp},ij}^h)\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{grp},ij}^h)) \right\} \\
&\quad - \frac{1}{2} \text{tr} \left( \boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} \left\{ \left( \boldsymbol{\mu}_{\mathbf{q}}(\boldsymbol{\beta}) - \boldsymbol{\mu}_{\boldsymbol{\beta}} \right) \left( \boldsymbol{\mu}_{\mathbf{q}}(\boldsymbol{\beta}) - \boldsymbol{\mu}_{\boldsymbol{\beta}} \right)^T + \boldsymbol{\Sigma}_{\mathbf{q}}(\boldsymbol{\beta}) \right\} \right) \\
&\quad - \frac{1}{2} \text{tr} \left( \mathbf{M}_{\mathbf{q}}(\boldsymbol{\Sigma}_g^{-1}) \left\{ \sum_{i=1}^m \left( \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},i}^g) \boldsymbol{\mu}_{\mathbf{q}}^T(\mathbf{u}_{\text{lin},i}^g) + \boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{lin},i}^g) \right) \right\} \right) \\
&\quad - \frac{1}{2} \text{tr} \left( \mathbf{M}_{\mathbf{q}}(\boldsymbol{\Sigma}_h^{-1}) \left\{ \sum_{i=1}^m \sum_{j=1}^{n_i} \left( \boldsymbol{\mu}_{\mathbf{q}}(\mathbf{u}_{\text{lin},ij}^h) \boldsymbol{\mu}_{\mathbf{q}}^T(\mathbf{u}_{\text{lin},ij}^h) + \boldsymbol{\Sigma}_{\mathbf{q}}(\mathbf{u}_{\text{lin},ij}^h) \right) \right\} \right), \\
& E_{\mathbf{q}}\{\log \mathbf{q}^*(\boldsymbol{\beta}, \mathbf{u})\} = -\frac{1}{2} \left\{ 2 + K_{\text{gbl}} + m(2 + K_{\text{grp}}^g) + (2 + K_{\text{grp}}^h) \sum_{i=1}^m n_i \right\} \{1 + \log(2\pi)\} \\
&\quad - \frac{1}{2} \log |\boldsymbol{\Sigma}_{\mathbf{q}}(\boldsymbol{\beta}, \mathbf{u})|,
\end{aligned}$$

Expressions for  $E_{\mathbf{q}}\{\log \mathbf{p}(\sigma_{\varepsilon}^2 \mid a_{\varepsilon})\}$ ,  $E_{\mathbf{q}}\{\log \mathbf{q}^*(\sigma_{\varepsilon}^2)\}$ ,  $E_{\mathbf{q}}\{\log \mathbf{p}(a_{\varepsilon})\}$ ,  $E_{\mathbf{q}}\{\log \mathbf{q}^*(a_{\varepsilon})\}$ ,  $E_{\mathbf{q}}\{\log \mathbf{p}(\sigma_{\text{gbl}}^2 \mid a_{\text{gbl}})\}$ ,  $E_{\mathbf{q}}\{\log \mathbf{q}^*(\sigma_{\text{gbl}}^2)\}$ ,  $E_{\mathbf{q}}\{\log \mathbf{p}(a_{\text{gbl}})\}$  and  $E_{\mathbf{q}}\{\log \mathbf{q}^*(a_{\text{gbl}})\}$  follow the same form as shown from the derivations in the two-level case.

Following on, we have

$$\begin{aligned}
E_{\mathbf{q}}\{\log \mathbf{p}(\sigma_{\text{grp},g}^2 \mid a_{\text{grp},g})\} &= -\frac{1}{2} \nu_{\text{grp},g} E_{\mathbf{q}}\{\log(2a_{\text{grp},g})\} - \log \Gamma(\nu_{\text{grp},g}/2) - (\frac{1}{2} \nu_{\text{grp},g} + 1) E_{\mathbf{q}}\{\log(\sigma_{\text{grp},g}^2)\} \\
&\quad - \frac{1}{2} \mu_{\mathbf{q}}(1/a_{\text{grp},g}) \mu_{\mathbf{q}}(1/\sigma_{\text{grp},g}^2),
\end{aligned}$$

$$\begin{aligned}
E_q\{\log \mathbf{q}^*(\sigma_{\text{grp},g}^2)\} &= \frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{grp},g}^2) \log(\lambda_{\mathbf{q}}(\sigma_{\text{grp},g}^2)/2) - \log\{\Gamma(\frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{grp},g}^2))\} - (\frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{grp},g}^2) + 1)E_q\{\log(\sigma_{\text{grp},g}^2)\} \\
&\quad - \frac{1}{2}\lambda_{\mathbf{q}}(\sigma_{\text{grp},g}^2)\mu_{\mathbf{q}}(1/\sigma_{\text{grp},g}^2), \\
E_q\{\log \mathbf{p}(a_{\text{grp},g})\} &= -\frac{1}{2}\log(2\nu_{\text{grp},g}s_{\text{grp},g}^2) - \log\{\Gamma(\frac{1}{2})\} - (\frac{1}{2} + 1)E_q\{\log(a_{\text{grp},g})\} \\
&\quad - \{1/(2\nu_{\text{grp},g}s_{\text{grp},g}^2)\}\mu_{\mathbf{q}}(1/a_{\text{grp},g}), \\
E_q\{\log \mathbf{q}^*(a_{\text{grp},g})\} &= \frac{1}{2}\xi_{\mathbf{q}}(a_{\text{grp},g}) \log(\lambda_{\mathbf{q}}(a_{\text{grp},g})/2) - \log\{\Gamma(\frac{1}{2}\xi_{\mathbf{q}}(a_{\text{grp},g}))\} - (\frac{1}{2}\xi_{\mathbf{q}}(a_{\text{grp},g}) + 1)E_q\{\log(a_{\text{grp},g})\} \\
&\quad - \frac{1}{2}\lambda_{\mathbf{q}}(a_{\text{grp},g})\mu_{\mathbf{q}}(1/a_{\text{grp},g}), \\
E_q[\log\{\mathbf{p}(\boldsymbol{\Sigma}_g|\mathbf{A}_{\boldsymbol{\Sigma}_g})\}] &= -\frac{1}{2}(\nu_{\boldsymbol{\Sigma}_g} + 1)E_q\{\log|\mathbf{A}_{\boldsymbol{\Sigma}_g}|\} - \frac{1}{2}(\nu_{\boldsymbol{\Sigma}_g} + 4)E_q\{\log|\boldsymbol{\Sigma}_g|\} - \frac{1}{2}\log(\pi) \\
&\quad - \frac{1}{2}\text{tr}(\mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_g}^{-1})}\mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}_g^{-1})}) - (\nu_{\boldsymbol{\Sigma}_g} + 3)\log(2) - \sum_{j=1}^2 \log\Gamma(\frac{1}{2}(\nu_{\boldsymbol{\Sigma}_g} + 4 - j)), \\
E_q[\log\{\mathbf{q}^*(\boldsymbol{\Sigma}_g)\}] &= \frac{1}{2}(\xi_{\mathbf{q}}(\boldsymbol{\Sigma}_g) - 1)\log|\boldsymbol{\Lambda}_{\mathbf{q}}(\boldsymbol{\Sigma}_g)| - \frac{1}{2}(\xi_{\mathbf{q}}(\boldsymbol{\Sigma}_g) + 2)E_q\{\log|\boldsymbol{\Sigma}_g|\} - \frac{1}{2}\text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}}(\boldsymbol{\Sigma}_g)\mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}_g^{-1})}) \\
&\quad - (\xi_{\mathbf{q}}(\boldsymbol{\Sigma}_g) + 1)\log(2) - \frac{1}{2}\log(\pi) - \sum_{j=1}^2 \log\Gamma(\frac{1}{2}(\xi_{\mathbf{q}}(\boldsymbol{\Sigma}_g) + 2 - j)), \\
E_q[\log\{\mathbf{p}(\mathbf{A}_{\boldsymbol{\Sigma}_g})\}] &= -\frac{3}{2}E_q\{\log|\mathbf{A}_{\boldsymbol{\Sigma}_g}|\} - \frac{1}{2}\sum_{j=1}^2 1/(\nu_{\boldsymbol{\Sigma}_g}s_{\boldsymbol{\Sigma}_g,j}^2) \left(\mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_g}^{-1})}\right)_{jj} - 2\log(2) \\
&\quad - \frac{1}{2}\log(\pi) - \sum_{j=1}^2 \log\Gamma(\frac{1}{2}(3 - j)),
\end{aligned}$$

and

$$\begin{aligned}
E_q[\log\{\mathbf{q}^*(\mathbf{A}_{\boldsymbol{\Sigma}_g})\}] &= \frac{1}{2}(\xi_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}_g}) - 1)\log|\boldsymbol{\Lambda}_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}_g})| - \frac{1}{2}(\xi_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}_g}) + 2)E_q\{\log|\mathbf{A}_{\boldsymbol{\Sigma}_g}|\} \\
&\quad - \frac{1}{2}\text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}_g})\mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_g}^{-1})}) - (\xi_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}_g}) + 1)\log(2) - \frac{1}{2}\log(\pi) \\
&\quad - \sum_{j=1}^2 \log\Gamma(\frac{1}{2}(\xi_{\mathbf{q}}(\mathbf{A}_{\boldsymbol{\Sigma}_g}) + 2 - j)).
\end{aligned}$$

In addition, the expressions for  $E_q\{\log \mathbf{p}(\sigma_{\text{grp},h}^2 | a_{\text{grp},h})\}$ ,  $E_q\{\log \mathbf{q}^*(\sigma_{\text{grp},h}^2)\}$ ,  $E_q\{\log \mathbf{p}(a_{\text{grp},h})\}$ ,  $E_q\{\log \mathbf{q}^*(a_{\text{grp},h})\}$ ,  $E_q[\log\{\mathbf{p}(\boldsymbol{\Sigma}|\mathbf{A}_{\boldsymbol{\Sigma}_h})\}]$ ,  $E_q[\log\{\mathbf{q}(\boldsymbol{\Sigma}_h)\}]$ ,  $E_q[\log\{\mathbf{p}(\mathbf{A}_{\boldsymbol{\Sigma}_h})\}]$ ,  $E_q[\log\{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_h})\}]$ , are similar to the ones shown above.

In the summation of each of these  $\log \mathbf{p}(\mathbf{y}; \mathbf{q})$  terms, note that the coefficient of  $E_q\{\log(\sigma_\varepsilon^2)\}$  is

$$-\frac{1}{2}\sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij} - \frac{1}{2}\nu_\varepsilon - 1 + \frac{1}{2}\xi_{\mathbf{q}}(\sigma_\varepsilon^2) + 1 = -\frac{1}{2}\sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij} - \frac{1}{2}\nu_\varepsilon - 1 + \frac{1}{2}(\nu_\varepsilon + \sum_{i=1}^m \sum_{j=1}^{n_i} o_{ij}) + 1 = 0.$$

The coefficient of  $E_q\{\log(\sigma_{\text{gbl}}^2)\}$  is

$$-\frac{1}{2}K_{\text{gbl}} - \frac{1}{2}\nu_{\text{gbl}} - 1 + \frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{gbl}}^2) + 1 = -\frac{1}{2}K_{\text{gbl}} - \frac{1}{2}\nu_{\text{gbl}} - 1 + \frac{1}{2}(\nu_{\text{gbl}} + K_{\text{gbl}}) + 1 = 0.$$

The coefficient of  $E_q\{\log(\sigma_{\text{grp},g}^2)\}$  is

$$-\frac{1}{2}mK_{\text{grp}}^g - \frac{1}{2}\nu_{\text{grp},g} - 1 + \frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{grp},g}^2) + 1 = -\frac{1}{2}mK_{\text{grp}}^g - \frac{1}{2}\nu_{\text{grp},g} - 1 + \frac{1}{2}(\nu_{\text{grp},g} + mK_{\text{grp}}^g) + 1 = 0.$$

The coefficient of  $E_q\{\log(\sigma_{\text{grp},h}^2)\}$  is

$$-\frac{1}{2}K_{\text{grp}}^h \sum_{i=1}^m n_i - \frac{1}{2}\nu_{\text{grp},h} - 1 + \frac{1}{2}\xi_{\mathbf{q}}(\sigma_{\text{grp},h}^2) + 1 = -\frac{1}{2}K_{\text{grp}}^h \sum_{i=1}^m n_i - \frac{1}{2}\nu_{\text{grp},h} - 1 + \frac{1}{2}\left(\nu_{\text{grp},h} + K_{\text{grp}}^h \sum_{i=1}^m n_i\right) + 1 = 0.$$

The coefficient of  $E_q\{\log|\boldsymbol{\Sigma}_g|\}$  is

$$-\frac{m}{2} - \frac{1}{2}(\nu_{\boldsymbol{\Sigma}_g} + 4) + \frac{1}{2}(\xi_{\mathbf{q}}(\boldsymbol{\Sigma}_g) + 2) = -\frac{1}{2}(m + \nu_{\boldsymbol{\Sigma}_g} + 4) + \frac{1}{2}(m + \nu_{\boldsymbol{\Sigma}_g} + 4) = 0.$$

The coefficient of  $E_q\{\log|\boldsymbol{\Sigma}_h|\}$  is

$$-\frac{1}{2}\sum_{i=1}^m n_i - \frac{1}{2}(\nu_{\boldsymbol{\Sigma}_h} + 4) + \frac{1}{2}(\xi_{\mathbf{q}}(\boldsymbol{\Sigma}_h) + 2) = -\frac{1}{2}\left(\sum_{i=1}^m n_i + \nu_{\boldsymbol{\Sigma}_h} + 4\right) + \frac{1}{2}\left(\sum_{i=1}^m n_i + \nu_{\boldsymbol{\Sigma}_h} + 4\right) = 0.$$



The coefficient of  $E_q\{\log(a_\varepsilon)\}$  is

$$-\frac{1}{2}\nu_\varepsilon - \frac{1}{2} - 1 + \frac{1}{2}\xi_{q(a_\varepsilon)} + 1 = -\frac{1}{2}\nu_\varepsilon - \frac{1}{2} - 1 + \frac{1}{2}(\nu_\varepsilon + 1) + 1 = 0.$$

The coefficient of  $E_q\{\log(a_{\text{gbl}})\}$  is

$$-\frac{1}{2}\nu_{\text{gbl}} - \frac{1}{2} - 1 + \frac{1}{2}\xi_{q(a_{\text{gbl}})} + 1 = -\frac{1}{2}\nu_{\text{gbl}} - \frac{1}{2} - 1 + \frac{1}{2}(\nu_{\text{gbl}} + 1) + 1 = 0.$$

The coefficient of  $E_q\{\log(a_{\text{grp},g})\}$  is

$$-\frac{1}{2}\nu_{\text{grp},g} - \frac{1}{2} - 1 + \frac{1}{2}\xi_{q(a_{\text{grp},g})} + 1 = -\frac{1}{2}\nu_{\text{grp},g} - \frac{1}{2} - 1 + \frac{1}{2}(\nu_{\text{grp},g} + 1) + 1 = 0.$$

The coefficient of  $E_q\{\log(a_{\text{grp},h})\}$  is

$$-\frac{1}{2}\nu_{\text{grp},h} - \frac{1}{2} - 1 + \frac{1}{2}\xi_{q(a_{\text{grp},h})} + 1 = -\frac{1}{2}\nu_{\text{grp},h} - \frac{1}{2} - 1 + \frac{1}{2}(\nu_{\text{grp},h} + 1) + 1 = 0.$$

The coefficient of  $E_q\{\log|\mathbf{A}_{\Sigma_g}|\}$  is

$$-\frac{1}{2}(\nu_{\Sigma_g} + 1) - \frac{3}{2} + \frac{1}{2}(\xi_{q(\mathbf{A}_{\Sigma_g})} + 2) = -\frac{1}{2}(\nu_{\Sigma_g} + 2) + \frac{1}{2}(\nu_{\Sigma_g} + 2) = 0.$$

The coefficient of  $E_q\{\log|\mathbf{A}_{\Sigma_h}|\}$  is

$$-\frac{1}{2}(\nu_{\Sigma_h} + 1) - \frac{3}{2} + \frac{1}{2}(\xi_{q(\mathbf{A}_{\Sigma_h})} + 2) = -\frac{1}{2}(\nu_{\Sigma_h} + 2) + \frac{1}{2}(\nu_{\Sigma_h} + 2) = 0.$$

Therefore these terms can be dropped and the cancellations led by the above expectations lead to the lower bound expression in (S.3).

## S.12 The SOLVETWOLEVELSPARSELEASTSQUARES Algorithm

The SOLVETWOLEVELSPARSELEASTSQUARES is listed in Nolan *et al.* (2018) and based on Theorem 2 of Nolan & Wand (2018). Given its centrality to Algorithms 1 and 2 we list it again here. The algorithm solves a sparse version of the the least squares problem:

$$\min_x \|\mathbf{b} - \mathbf{B}\mathbf{x}\|^2$$

which has solution  $\mathbf{x} = \mathbf{A}^{-1}\mathbf{B}^T\mathbf{b}$  where  $\mathbf{A} = \mathbf{B}^T\mathbf{B}$  where  $\mathbf{B}$  and  $\mathbf{b}$  have the following structure:

$$\mathbf{B} \equiv \begin{bmatrix} \mathbf{B}_1 & \dot{\mathbf{B}}_1 & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{B}_2 & \mathbf{O} & \dot{\mathbf{B}}_2 & \cdots & \mathbf{O} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{B}_m & \mathbf{O} & \mathbf{O} & \cdots & \dot{\mathbf{B}}_m \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_m \end{bmatrix}. \quad (\text{S.5})$$

The sub-matrices corresponding to the non-zero blocks of  $\mathbf{x}$  and  $\mathbf{A}$  are labelled according to:

$$\mathbf{x} \equiv \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_{2,1} \\ \mathbf{x}_{2,2} \\ \vdots \\ \mathbf{x}_{2,m} \end{bmatrix} \quad \text{and} \quad \mathbf{A}^{-1} = \begin{bmatrix} \mathbf{A}^{11} & \mathbf{A}^{12,1} & \mathbf{A}^{12,2} & \cdots & \mathbf{A}^{12,m} \\ \mathbf{A}^{12,1T} & \mathbf{A}^{22,1} & \times & \cdots & \times \\ \mathbf{A}^{12,2T} & \times & \mathbf{A}^{22,2} & \cdots & \times \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{A}^{12,mT} & \times & \times & \cdots & \mathbf{A}^{22,m} \end{bmatrix} \quad (\text{S.6})$$

with  $\times$  denoting sub-blocks that are not of interest. The SOLVETWOLEVELSPARSELEASTSQUARES algorithm is given in Algorithm S.1.

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**Algorithm S.1** SOLVETWOLEVELSPARSELEASTSQUARES *for solving the two-level sparse matrix least squares problem: minimise  $\|\mathbf{b} - \mathbf{B}\mathbf{x}\|^2$  in  $\mathbf{x}$  and sub-blocks of  $\mathbf{A}^{-1}$  corresponding to the non-zero sub-blocks of  $\mathbf{A} = \mathbf{B}^T \mathbf{B}$ . The sub-block notation is given by (S.5) and (S.6).*

---

Inputs:  $\{(\mathbf{b}_i(\tilde{n}_i \times 1), \mathbf{B}_i(\tilde{n}_i \times p), \dot{\mathbf{B}}_i(\tilde{n}_i \times q)) : 1 \leq i \leq m\}$

$\omega_3 \leftarrow \text{NULL}$  ;  $\Omega_4 \leftarrow \text{NULL}$

For  $i = 1, \dots, m$ :

Decompose  $\dot{\mathbf{B}}_i = \mathbf{Q}_i \begin{bmatrix} \mathbf{R}_i \\ \mathbf{0} \end{bmatrix}$  such that  $\mathbf{Q}_i^{-1} = \mathbf{Q}_i^T$  and  $\mathbf{R}_i$  is upper-triangular.

$\mathbf{c}_{0i} \leftarrow \mathbf{Q}_i^T \mathbf{b}_i$  ;  $\mathbf{C}_{0i} \leftarrow \mathbf{Q}_i^T \mathbf{B}_i$

$\mathbf{c}_{1i} \leftarrow$  first  $q$  rows of  $\mathbf{c}_{0i}$  ;  $\mathbf{c}_{2i} \leftarrow$  remaining rows of  $\mathbf{c}_{0i}$  ;  $\omega_3 \leftarrow \begin{bmatrix} \omega_3 \\ \mathbf{c}_{2i} \end{bmatrix}$

$\mathbf{C}_{1i} \leftarrow$  first  $q$  rows of  $\mathbf{C}_{0i}$  ;  $\mathbf{C}_{2i} \leftarrow$  remaining rows of  $\mathbf{C}_{0i}$  ;  $\Omega_4 \leftarrow \begin{bmatrix} \Omega_4 \\ \mathbf{C}_{2i} \end{bmatrix}$

Decompose  $\Omega_4 = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$  such that  $\mathbf{Q}^{-1} = \mathbf{Q}^T$  and  $\mathbf{R}$  is upper-triangular.

$\mathbf{c} \leftarrow$  first  $p$  rows of  $\mathbf{Q}^T \omega_3$  ;  $\mathbf{x}_1 \leftarrow \mathbf{R}^{-1} \mathbf{c}$  ;  $\mathbf{A}^{11} \leftarrow \mathbf{R}^{-1} \mathbf{R}^{-T}$

For  $i = 1, \dots, m$ :

$\mathbf{x}_{2,i} \leftarrow \mathbf{R}_i^{-1}(\mathbf{c}_{1i} - \mathbf{C}_{1i} \mathbf{x}_1)$  ;  $\mathbf{A}^{12,i} \leftarrow -\mathbf{A}^{11}(\mathbf{R}_i^{-1} \mathbf{C}_{1i})^T$

$\mathbf{A}^{22,i} \leftarrow \mathbf{R}_i^{-1}(\mathbf{R}_i^{-T} - \mathbf{C}_{1i} \mathbf{A}^{12,i})$

Output:  $(\mathbf{x}_1, \mathbf{A}^{11}, \{(\mathbf{x}_{2,i}, \mathbf{A}^{22,i}, \mathbf{A}^{12,i}) : 1 \leq i \leq m\})$

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### S.13 The SOLVETHREELEVELSPARSELEASTSQUARES Algorithm

The SOLVETHREELEVELSPARSELEASTSQUARES, listed in Nolan *et al.* (2018) is a proceduralization of Theorem 4 of Nolan & Wand (2018). Since it is central to Algorithms 3 and 4 we list it here. The SOLVETHREELEVELSPARSELEASTSQUARES algorithm is concerned with solving the sparse three-level version of

$$\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{B}\mathbf{x}\|^2$$

with the solution  $\mathbf{x} = \mathbf{A}^{-1}\mathbf{B}^T\mathbf{b}$  where  $\mathbf{A} = \mathbf{B}^T\mathbf{B}$  where  $\mathbf{B}$  and  $\mathbf{b}$  have the following structure:

$$\mathbf{B} \equiv \left[ \begin{array}{c} \text{stack}_{1 \leq i \leq m} \left\{ \text{stack}_{1 \leq j \leq n_i} (\mathbf{B}_{ij}) \right\} \mid \text{blockdiag}_{1 \leq i \leq m} \left\{ \left[ \begin{array}{c} \text{stack}_{1 \leq j \leq n_i} (\dot{\mathbf{B}}_{ij}) \mid \text{blockdiag}_{1 \leq j \leq n_i} (\ddot{\mathbf{B}}_{ij}) \end{array} \right] \right\} \end{array} \right] \quad (\text{S.7})$$

and

$$\mathbf{b} \equiv \text{stack}_{1 \leq i \leq m} \left\{ \text{stack}_{1 \leq j \leq n_i} (\mathbf{b}_{ij}) \right\}. \quad (\text{S.8})$$

The three-level sparse matrix inverse problem involves determination of all sub-blocks of  $\mathbf{x}$  and the sub-blocks of  $\mathbf{A}^{-1}$  corresponding to the non-zero sub-blocks of  $\mathbf{A}$ . Our notation for these sub-blocks is illustrated by

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_{2,1} \\ \mathbf{x}_{2,11} \\ \mathbf{x}_{2,12} \\ \mathbf{x}_{2,2} \\ \mathbf{x}_{2,21} \\ \mathbf{x}_{2,22} \\ \mathbf{x}_{2,23} \end{bmatrix} \quad (\text{S.9})$$

$$\text{and } \mathbf{A}^{-1} = \begin{bmatrix} \mathbf{A}^{11} & \mathbf{A}^{12,1} & \mathbf{A}^{12,11} & \mathbf{A}^{12,12} & \mathbf{A}^{12,2} & \mathbf{A}^{12,21} & \mathbf{A}^{12,22} & \mathbf{A}^{12,23} \\ \mathbf{A}^{12,1T} & \mathbf{A}^{22,1} & \mathbf{A}^{12,1,1} & \mathbf{A}^{12,1,2} & \times & \times & \times & \times \\ \mathbf{A}^{12,11T} & \mathbf{A}^{12,1,1T} & \mathbf{A}^{22,11} & \times & \times & \times & \times & \times \\ \mathbf{A}^{12,12T} & \mathbf{A}^{12,1,2T} & \times & \mathbf{A}^{22,12} & \times & \times & \times & \times \\ \mathbf{A}^{12,2T} & \times & \times & \times & \mathbf{A}^{22,2} & \mathbf{A}^{12,2,1} & \mathbf{A}^{12,2,2} & \mathbf{A}^{12,2,3} \\ \mathbf{A}^{12,21T} & \times & \times & \times & \mathbf{A}^{12,2,1T} & \mathbf{A}^{22,21} & \times & \times \\ \mathbf{A}^{12,22T} & \times & \times & \times & \mathbf{A}^{12,2,2T} & \times & \mathbf{A}^{22,22} & \times \\ \mathbf{A}^{12,23T} & \times & \times & \times & \mathbf{A}^{12,2,3T} & \times & \times & \mathbf{A}^{22,23} \end{bmatrix}$$

for the  $m = 2$ ,  $n_1 = 2$  and  $n_2 = 3$  case. The  $\times$  symbol denotes sub-blocks that are not of interest. The SOLVETHREELEVELSPARSELEASTSQUARES algorithm is given in Algorithm S.2.

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**Algorithm S.2** SOLVETHREELLEVELSPARSELEASTSQUARES for solving the three-level sparse matrix least squares problem: minimise  $\|\mathbf{b} - \mathbf{B}\mathbf{x}\|^2$  in  $\mathbf{x}$  and sub-blocks of  $\mathbf{A}^{-1}$  corresponding to the non-zero sub-blocks of  $\mathbf{A} = \mathbf{B}^T\mathbf{B}$ . The sub-block notation is given by (S.7), (S.8) and (S.9).

---

Inputs:  $\{(\mathbf{b}_{ij}(\tilde{o}_{ij} \times 1), \mathbf{B}_{ij}(\tilde{o}_{ij} \times p), \dot{\mathbf{B}}_{ij}(\tilde{o}_{ij} \times q_1), \ddot{\mathbf{B}}_{ij}(\tilde{o}_{ij} \times q_2)) : 1 \leq i \leq m, 1 \leq j \leq n_i\}$

$\omega_7 \leftarrow \text{NULL}$  ;  $\Omega_8 \leftarrow \text{NULL}$

For  $i = 1, \dots, m$ :

$\omega_9 \leftarrow \text{NULL}$  ;  $\Omega_{10} \leftarrow \text{NULL}$  ;  $\Omega_{11} \leftarrow \text{NULL}$

For  $j = 1, \dots, n_i$ :

Decompose  $\ddot{\mathbf{B}}_{ij} = \mathbf{Q}_{ij} \begin{bmatrix} \mathbf{R}_{ij} \\ \mathbf{0} \end{bmatrix}$  such that  $\mathbf{Q}_{ij}^{-1} = \mathbf{Q}_{ij}^T$  and  $\mathbf{R}_{ij}$  is upper-triangular.

$d_{0ij} \leftarrow \mathbf{Q}_{ij}^T \mathbf{b}_{ij}$  ;  $D_{0ij} \leftarrow \mathbf{Q}_{ij}^T \mathbf{B}_{ij}$  ;  $\dot{D}_{0ij} \leftarrow \mathbf{Q}_{ij}^T \dot{\mathbf{B}}_{ij}$

$d_{1ij} \leftarrow$  1st  $q_2$  rows of  $d_{0ij}$  ;  $d_{2ij} \leftarrow$  remaining rows of  $d_{0ij}$  ;  $\omega_9 \leftarrow \begin{bmatrix} \omega_9 \\ d_{2ij} \end{bmatrix}$

$D_{1ij} \leftarrow$  1st  $q_2$  rows of  $D_{0ij}$  ;  $D_{2ij} \leftarrow$  remaining rows of  $D_{0ij}$  ;  $\Omega_{10} \leftarrow \begin{bmatrix} \Omega_{10} \\ D_{2ij} \end{bmatrix}$

$\dot{D}_{1ij} \leftarrow$  1st  $q_2$  rows of  $\dot{D}_{0ij}$  ;  $\dot{D}_{2ij} \leftarrow$  remaining rows of  $\dot{D}_{0ij}$  ;  $\Omega_{11} \leftarrow \begin{bmatrix} \Omega_{11} \\ \dot{D}_{2ij} \end{bmatrix}$

Decompose  $\Omega_{11} = \mathbf{Q}_i \begin{bmatrix} \mathbf{R}_i \\ \mathbf{0} \end{bmatrix}$  such that  $\mathbf{Q}_i^{-1} = \mathbf{Q}_i^T$  and  $\mathbf{R}_i$  is upper-triangular.

$c_{0i} \leftarrow \mathbf{Q}_i^T \omega_9$  ;  $C_{0i} \leftarrow \mathbf{Q}_i^T \Omega_{10}$

$c_{1i} \leftarrow$  1st  $q_1$  rows of  $c_{0i}$  ;  $c_{2i} \leftarrow$  remaining rows of  $c_{0i}$  ;  $\omega_7 \leftarrow \begin{bmatrix} \omega_7 \\ c_{2i} \end{bmatrix}$

$C_{1i} \leftarrow$  1st  $q_1$  rows of  $C_{0i}$  ;  $C_{2i} \leftarrow$  remaining rows of  $C_{0i}$  ;  $\Omega_8 \leftarrow \begin{bmatrix} \Omega_8 \\ C_{2i} \end{bmatrix}$

Decompose  $\Omega_8 = \mathbf{Q} \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix}$  so that  $\mathbf{Q}^{-1} = \mathbf{Q}^T$  and  $\mathbf{R}$  is upper-triangular.

$\mathbf{c} \leftarrow$  first  $p$  rows of  $\mathbf{Q}^T \omega_7$  ;  $\mathbf{x}_1 \leftarrow \mathbf{R}^{-1} \mathbf{c}$  ;  $\mathbf{A}^{11} \leftarrow \mathbf{R}^{-1} \mathbf{R}^{-T}$

For  $i = 1, \dots, m$ :

$\mathbf{x}_{2,i} \leftarrow \mathbf{R}_i^{-1}(\mathbf{c}_{1i} - \mathbf{C}_{1i} \mathbf{x}_1)$  ;  $\mathbf{A}^{12,i} \leftarrow -\mathbf{A}^{11}(\mathbf{R}_i^{-1} \mathbf{C}_{1i})^T$

$\mathbf{A}^{22,i} \leftarrow \mathbf{R}_i^{-1}(\mathbf{R}_i^{-T} - \mathbf{C}_{1i} \mathbf{A}^{12,i})$

For  $j = 1, \dots, n_i$ :

$\mathbf{x}_{2,ij} \leftarrow \mathbf{R}_{ij}^{-1}(d_{1ij} - D_{1ij} \mathbf{x}_1 - \dot{D}_{1ij} \mathbf{x}_{2,i})$

$\mathbf{A}^{12,ij} \leftarrow -\left\{ \mathbf{R}_{ij}^{-1}(D_{1ij} \mathbf{A}^{11} + \dot{D}_{1ij} \mathbf{A}^{12,iT}) \right\}^T$

$\mathbf{A}^{12,i,j} \leftarrow -\left\{ \mathbf{R}_{ij}^{-1}(D_{1ij} \mathbf{A}^{12,i} + \dot{D}_{1ij} \mathbf{A}^{22,i}) \right\}^T$

$\mathbf{A}^{22,ij} \leftarrow \mathbf{R}_{ij}^{-1}(\mathbf{R}_{ij}^{-T} - D_{1ij} \mathbf{A}^{12,ij} - \dot{D}_{1ij} \mathbf{A}^{12,i,j})$

Output:  $\left( \mathbf{x}_1, \mathbf{A}^{11}, \{(\mathbf{x}_{2,i}, \mathbf{A}^{22,i}, \mathbf{A}^{12,i}) : 1 \leq i \leq m\} \right)$   
 $\{(\mathbf{x}_{2,ij}, \mathbf{A}^{22,ij}, \mathbf{A}^{12,ij}, \mathbf{A}^{12,i,j}) : 1 \leq i \leq m, 1 \leq j \leq n_i\}$

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