

Supplementary materials for:
**Streamlined Variational Inference for
Higher Level Group-Specific Curve Models**

BY M. MENICTAS¹, T.H. NOLAN^{1,3}, D.G. SIMPSON² AND M.P. WAND^{1,3}

*University of Technology Sydney¹, University of Illinois² and the
Australian Research Council Centre of Excellence for Mathematical and Statistical Frontiers³*

S.1 Derivation of Result 1

Straightforward algebra can be used to verify that

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

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

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

Therefore, in view of (2.6),

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

The sub-blocks of

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

listed in (2.7) correspond to the non- \times sub-blocks of $\mathbf{A}^{-1} = (\mathbf{B}^T \mathbf{B})^{-1}$ where \mathbf{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 χ^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 \mathbf{M} respects G if

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

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

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

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

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

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_{full} and G_{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 $\boldsymbol{\mu}_{q(\beta, u)}$ and $\boldsymbol{\Sigma}_{q(\beta, u)}$ updates, given at (2.12), may be written as

$$\boldsymbol{\mu}_{q(\beta, u)} \longleftarrow (\mathbf{B}^T \mathbf{B})^{-1} \mathbf{B}^T \mathbf{b} \quad \text{and} \quad \boldsymbol{\Sigma}_{q(\beta, u)} \longleftarrow (\mathbf{B}^T \mathbf{B})^{-1}$$

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

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

and

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

Result 2 immediately follows from Theorem 2.3 of Nolan & Wand (2020).

S.5 Derivation of Algorithm 2

We provide expressions for the \mathbf{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:

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

where

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\Lambda_{q(\Sigma)} = M_{q(A_{\Sigma}^{-1})} + \sum_{i=1}^m \left(\mu_{q(u_{\text{lin},i})} \mu_{q(u_{\text{lin},i})}^T + \Sigma_{q(u_{\text{lin},i})} \right),$$

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

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

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

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

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

$q(a_{\text{grp}})$ 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

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

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

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

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

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\{ (\boldsymbol{\mu}_{\mathbf{q}(\beta)} - \boldsymbol{\mu}_{\beta}) (\boldsymbol{\mu}_{\mathbf{q}(\beta)} - \boldsymbol{\mu}_{\beta})^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 (\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) + \frac{1}{2} \{2 + K_{\text{gbl}} + m(2 + K_{\text{grp}})\} \\
& - \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}}^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(\frac{\nu_{\varepsilon}}{2}) \\
& - \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(\frac{\nu_{\text{gbl}}}{2}) - \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(\frac{\nu_{\text{grp}}}{2}) + \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}(\mathbf{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma})} \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}^{-1})}) \\
& + \sum_{j=1}^2 \log\Gamma(\frac{1}{2}(\xi_{\mathbf{q}(\mathbf{A}_{\Sigma})} + 2 - j)) - \sum_{j=1}^2 \log\Gamma(\frac{1}{2}(\nu_{\Sigma} + 4 - j)) - \frac{1}{2}(\xi_{\mathbf{q}(\boldsymbol{\Sigma})} - 1) \log |\mathbf{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma})}| \\
& + \sum_{j=1}^2 \log\Gamma(\frac{1}{2}(\xi_{\mathbf{q}(\boldsymbol{\Sigma})} + 2 - j)) - \frac{1}{2} \sum_{j=1}^2 1/(\nu_{\Sigma} s_{\Sigma,j}^2) (\mathbf{M}_{\mathbf{q}(\mathbf{A}_{\Sigma}^{-1})})_{jj} - \sum_{j=1}^2 \log\Gamma(\frac{1}{2}(3 - j)) \\
& - \frac{1}{2}(\xi_{\mathbf{q}(\mathbf{A}_{\Sigma})} - 1) \log |\mathbf{\Lambda}_{\mathbf{q}(\mathbf{A}_{\Sigma})}| + \frac{1}{2} \text{tr}(\mathbf{\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 \left. + \text{tr}(\mathbf{C}_{\text{gbl},i}^T \mathbf{C}_{\text{gbl},i} \boldsymbol{\Sigma}_{\mathbf{q}(\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_{\mathbf{q}} \left\{ \left(\begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\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}_{\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:

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

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

First we note that

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

where

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

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,

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

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

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

$$\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 |\mathbf{A}_{\mathbf{q}(\boldsymbol{\Sigma})}| - \frac{1}{2}(\xi_{\mathbf{q}(\boldsymbol{\Sigma})} + 2)E_{\mathbf{q}}\{\log |\boldsymbol{\Sigma}|\} - \frac{1}{2}\text{tr}(\mathbf{A}_{\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 |\mathbf{A}_{\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}(\mathbf{A}_{\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 $\log \underline{\mathbf{p}}(\mathbf{y}; \mathbf{q})$ 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 $E_{\mathbf{q}}\{\log(\sigma_{\text{gbl}}^2)\}$ 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 $E_{\mathbf{q}}\{\log(\sigma_{\text{grp}}^2)\}$ is

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

The coefficient of $E_{\mathbf{q}}\{\log|\boldsymbol{\Sigma}|\}$ is

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

The coefficient of $E_{\mathbf{q}}\{\log(a_{\varepsilon})\}$ is

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

The coefficient of $E_{\mathbf{q}}\{\log(a_{\text{gbl}})\}$ is

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

The coefficient of $E_{\mathbf{q}}\{\log(a_{\text{grp}})\}$ is

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

The coefficient of $E_{\mathbf{q}}\{\log|\boldsymbol{A}_{\boldsymbol{\Sigma}}|\}$ is

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

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

S.7 Derivation of Result 3

If \mathbf{B} and \mathbf{b} have the same forms given by equation (7) in Nolan & Wand (2020) with

$$\begin{aligned} \mathbf{b}_{ij} &\equiv \begin{bmatrix} \sigma_{\varepsilon}^{-1} \mathbf{y}_{ij} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{B}_{ij} \equiv \begin{bmatrix} \sigma_{\varepsilon}^{-1} \mathbf{X}_{ij} & \sigma_{\varepsilon}^{-1} \mathbf{Z}_{\text{gbl},ij} \\ \mathbf{O} & (\sum_{i=1}^m n_i)^{-1/2} \sigma_{\text{gbl}}^{-1} \mathbf{I}_{K_{\text{gbl}}} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix}, \\ \dot{\mathbf{B}}_{ij} &\equiv \begin{bmatrix} \sigma_{\varepsilon}^{-1} \mathbf{X}_{ij} & \sigma_{\varepsilon}^{-1} \mathbf{Z}_{\text{grp},ij}^g \\ \mathbf{O} & \mathbf{O} \\ n_i^{-1/2} \boldsymbol{\Sigma}_g^{-1/2} & \mathbf{O} \\ \mathbf{O} & n_i^{-1/2} \sigma_{\text{grp},g}^{-1} \mathbf{I}_{K_{\text{grp}}^g} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \end{bmatrix} \quad \text{and} \quad \ddot{\mathbf{B}}_{ij} \equiv \begin{bmatrix} \sigma_{\varepsilon}^{-1} \mathbf{X}_{ij} & \sigma_{\varepsilon}^{-1} \mathbf{Z}_{\text{grp},ij}^h \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} \\ \Sigma_h^{-1/2} & \mathbf{O} \\ \mathbf{O} & \sigma_{\text{grp},h}^{-1} \mathbf{I}_{K_{\text{grp}}^h} \end{bmatrix}, \end{aligned}$$

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

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

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 $\boldsymbol{\mu}_{q(\beta, u)}$ and $\boldsymbol{\Sigma}_{q(\beta, u)}$ updates, given at (2.12) but with \mathbf{D}_{MFVB} as given in (3.6), may be written as

$$\boldsymbol{\mu}_{q(\beta, u)} \longleftarrow (\mathbf{B}^T \mathbf{B})^{-1} \mathbf{B}^T \mathbf{b} \quad \text{and} \quad \boldsymbol{\Sigma}_{q(\beta, u)} \longleftarrow (\mathbf{B}^T \mathbf{B})^{-1}$$

where \mathbf{B} and \mathbf{b} have the forms given by equation (7) in Nolan & Wand (2020) with

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

$$\dot{\mathbf{B}}_{ij} \equiv \begin{bmatrix} \mu_{q(1/\sigma_{\varepsilon}^2)}^{1/2} \mathbf{X}_{ij} & \mu_{q(1/\sigma_{\varepsilon}^2)}^{1/2} \mathbf{Z}_{\text{grp},ij}^g \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ n_i^{-1/2} \mathbf{M}_{q(\Sigma_g^{-1})}^{1/2} & \mathbf{0} \\ \mathbf{0} & n_i^{-1/2} \mu_{q(1/\sigma_{\text{grp},g}^2)}^{1/2} \mathbf{I}_{K_{\text{grp}}^g} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \quad \text{and} \quad \ddot{\mathbf{B}}_{ij} \equiv \begin{bmatrix} \mu_{q(1/\sigma_{\varepsilon}^2)}^{1/2} \mathbf{X}_{ij} & \mu_{q(1/\sigma_{\varepsilon}^2)}^{1/2} \mathbf{Z}_{\text{grp},ij}^h \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \\ \mathbf{M}_{q(\Sigma_h^{-1})}^{1/2} & \mathbf{0} \\ \mathbf{0} & \mu_{q(1/\sigma_{\text{grp},h}^2)}^{1/2} \mathbf{I}_{K_{\text{grp}}^h} \end{bmatrix}.$$

Result 4 immediately follows from Theorem 3.3 of Nolan & Wand (2020).

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

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

where

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

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 \mathbf{D}_{MFVB} as given in (3.3),

$\mathbf{q}(\sigma_\varepsilon^2)$ is an Inverse- χ^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

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

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

$$= \mu_{\mathbf{q}(1/a_\varepsilon)} + \sum_{i=1}^m \sum_{j=1}^{n_i} \left\{ \left\| E_{\mathbf{q}} \left(\mathbf{y}_{ij} - \mathbf{C}_{\text{gbl},ij} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}} \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^g \begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g \end{bmatrix} - \mathbf{C}_{\text{grp},ij}^h \begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp},ij}^h \end{bmatrix} \right) \right\|^2 \right\}$$

$$\begin{aligned} &+ \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)}) \\ &+ 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] \\ &+ 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] \\ &+ 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] \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- χ^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- χ^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 $\mu_{\mathbf{q}(1/\sigma_{\text{grp},g}^2)} = \xi_{\mathbf{q}(\sigma_{\text{grp},g}^2)}/\lambda_{\mathbf{q}(\sigma_{\text{grp},g}^2)}$,

$\mathbf{q}(\boldsymbol{\Sigma}_g)$ is an Inverse-G-Wishart $(G_{\text{full}}, \xi_{\mathbf{q}(\boldsymbol{\Sigma}_g)}, \boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_g)})$ density function

where $\xi_{\mathbf{q}(\boldsymbol{\Sigma}_g)} = \nu_{\boldsymbol{\Sigma}_g} + 2 + m$ and

$$\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_g)} = \mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_g}^{-1})} + \sum_{i=1}^m \left(\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}^g)} \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}^g)}^T + \boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{lin},i}^g)} \right),$$

with inverse moment $\mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}_g^{-1})} = (\xi_{\mathbf{q}(\boldsymbol{\Sigma}_g)} - 1) \boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_g)}^{-1}$

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

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

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

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

$\mathbf{q}(\boldsymbol{\Sigma}_h)$ is an Inverse-G-Wishart $(G_{\text{full}}, \xi_{\mathbf{q}(\boldsymbol{\Sigma}_h)}, \boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_h)})$ density function

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

$$\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_h)} = \mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_h}^{-1})} + \sum_{i=1}^m \sum_{j=1}^{n_i} \left(\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h)} \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h)}^T + \boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h)} \right),$$

with inverse moment $\mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}_h^{-1})} = (\xi_{\mathbf{q}(\boldsymbol{\Sigma}_h)} - 1) \boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_h)}^{-1}$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\boldsymbol{\Lambda}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_g})} = \text{diag}\{\text{diagonal}(\mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}_g^{-1})})\} + \boldsymbol{\Lambda}_{\mathbf{A}_{\boldsymbol{\Sigma}_g}}$$

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

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

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

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

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 $(G_{\text{diag}}, \xi_{\mathbf{q}(\mathbf{A}_{\Sigma_h})}, \boldsymbol{\Lambda}_{\mathbf{q}(\mathbf{A}_{\Sigma_h})})$ density function

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

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

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

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

$$\begin{aligned}
& \log \underline{\mathbf{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}}^g) + \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(\boldsymbol{\Sigma}_{\boldsymbol{\beta}}^{-1} \left\{ (\boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta})} - \boldsymbol{\mu}_{\boldsymbol{\beta}}) (\boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta})} - \boldsymbol{\mu}_{\boldsymbol{\beta}})^T + \boldsymbol{\Sigma}_{\mathbf{q}(\boldsymbol{\beta})} \right\} \right) - \frac{1}{2} \log |\boldsymbol{\Sigma}_{\boldsymbol{\beta}}| + \frac{1}{2} \log |\boldsymbol{\Sigma}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u})}| \\
& -\frac{1}{2} \text{tr} \left(\mathbf{M}_{\mathbf{q}(\boldsymbol{\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 + \boldsymbol{\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}(\boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{grp}, ij}^h)}) \right\} \\
& -\frac{1}{2} \text{tr} \left(\mathbf{M}_{\mathbf{q}(\boldsymbol{\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 + \boldsymbol{\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}(\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\} - \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}_{\boldsymbol{\Sigma}_g}^{-1})} \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}_g^{-1})}) + \frac{1}{2} \text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_g)} \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}_g^{-1})}) - \frac{1}{2} \text{tr}(\mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_h}^{-1})} \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}_h^{-1})}) + \frac{1}{2} \text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_h)} \mathbf{M}_{\mathbf{q}(\boldsymbol{\Sigma}_h^{-1})}) \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2} (\xi_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_g})} + 2 - j)\right) - \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2} (\nu_{\boldsymbol{\Sigma}_g} + 4 - j)\right) - \frac{1}{2} (\xi_{\mathbf{q}(\boldsymbol{\Sigma}_g)} - 1) \log |\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_g)}| \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2} (\xi_{\mathbf{q}(\boldsymbol{\Sigma}_g)} + 2 - j)\right) - \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} - \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2} (3 - j)\right) \\
& - \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} \text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_g})} \mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_g}^{-1})}) \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2} (\xi_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\Sigma}_h})} + 2 - j)\right) - \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2} (\nu_{\boldsymbol{\Sigma}_h} + 4 - j)\right) - \frac{1}{2} (\xi_{\mathbf{q}(\boldsymbol{\Sigma}_h)} - 1) \log |\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_h)}| \\
& + \sum_{j=1}^2 \log \Gamma\left(\frac{1}{2} (\xi_{\mathbf{q}(\boldsymbol{\Sigma}_h)} + 2 - j)\right) - \frac{1}{2} \sum_{j=1}^2 1/(\nu_{\boldsymbol{\Sigma}_h} s_{\boldsymbol{\Sigma}_h, j}^2) \left(\mathbf{M}_{\mathbf{q}(\mathbf{A}_{\boldsymbol{\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_{q(A_{\Sigma_h})}-1)\log|A_{q(A_{\Sigma_h})}| + \frac{1}{2}\text{tr}(A_{q(A_{\Sigma_h})}M_{q(A_{\Sigma_h}^{-1})}) \\
& -\frac{1}{2}\mu_{q(1/\sigma_\varepsilon^2)}\sum_{i=1}^m\sum_{j=1}^{n_i}\left\{\left\|E_q\left(\mathbf{y}_{ij}-C_{\text{gbl},ij}\begin{bmatrix}\boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl},i}\end{bmatrix}-C_{\text{grp},ij}^g\begin{bmatrix}\mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp},i}^g\end{bmatrix}-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. \\
& +\text{tr}\left(C_{\text{gbl},ij}^T C_{\text{gbl},ij} \Sigma_{q(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})}\right) + \text{tr}\left(C_{\text{grp},ij}^g{}^T C_{\text{grp},ij}^g \Sigma_{q(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g)}\right) \\
& +\text{tr}\left(C_{\text{grp},ij}^h{}^T C_{\text{grp},ij}^h \Sigma_{q(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h)}\right) \\
& +2\text{tr}\left[C_{\text{grp},ij}^g{}^T C_{\text{gbl},ij} E_q\left\{\left(\begin{bmatrix}\boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}}\end{bmatrix}-\boldsymbol{\mu}_{q(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})}\right)\left(\begin{bmatrix}\mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp}}^g\end{bmatrix}-\boldsymbol{\mu}_{q(\mathbf{u}_{\text{lin},i}^g, \mathbf{u}_{\text{grp},i}^g)}\right)^T\right\}\right] \\
& +2\text{tr}\left[C_{\text{grp},ij}^h{}^T C_{\text{gbl},ij} E_q\left\{\left(\begin{bmatrix}\boldsymbol{\beta} \\ \mathbf{u}_{\text{gbl}}\end{bmatrix}-\boldsymbol{\mu}_{q(\boldsymbol{\beta}, \mathbf{u}_{\text{gbl}})}\right)\left(\begin{bmatrix}\mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp}}^h\end{bmatrix}-\boldsymbol{\mu}_{q(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h)}\right)^T\right\}\right] \\
& \left.+2\text{tr}\left[C_{\text{grp},ij}^g{}^T C_{\text{grp},ij}^h E_q\left\{\left(\begin{bmatrix}\mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp}}^g\end{bmatrix}-\boldsymbol{\mu}_{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}}^h\end{bmatrix}-\boldsymbol{\mu}_{q(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h)}\right)^T\right\}\right]\right].
\end{aligned}$$

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

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

First we note that

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

where

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

and

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

Therefore,

$$\begin{aligned}
E_{\mathbf{q}}\{\log \mathbf{p}(\mathbf{y} | \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{glob},ij} \begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{glob},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 + \text{tr} \left(\mathbf{C}_{\text{glob},ij}^T \mathbf{C}_{\text{glob},ij} \boldsymbol{\Sigma}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{glob}})} \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) \\
&\quad + \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) \\
&\quad + 2 \text{tr} \left[\mathbf{C}_{\text{grp},ij}^g {}^T \mathbf{C}_{\text{glob},ij} E_{\mathbf{q}} \left\{ \left(\begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{glob}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{glob}})} \right) \left(\begin{bmatrix} \mathbf{u}_{\text{lin},i}^g \\ \mathbf{u}_{\text{grp}}^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{glob},ij} E_{\mathbf{q}} \left\{ \left(\begin{bmatrix} \boldsymbol{\beta} \\ \mathbf{u}_{\text{glob}} \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta}, \mathbf{u}_{\text{glob}})} \right) \left(\begin{bmatrix} \mathbf{u}_{\text{lin},ij}^h \\ \mathbf{u}_{\text{grp}}^h \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h)} \right)^T \right\} \right] \\
&\quad + 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}}^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}}^h \end{bmatrix} - \boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{lin},ij}^h, \mathbf{u}_{\text{grp},ij}^h)} \right)^T \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} | \sigma_{\text{glob}}^2, \sigma_{\text{grp},g}^2, \boldsymbol{\Sigma}_g, \sigma_{\text{grp},h}^2, \boldsymbol{\Sigma}_h)\} &= -\frac{1}{2} \{2 + K_{\text{glob}} + 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{glob}} E_{\mathbf{q}}\{\log(\sigma_{\text{glob}}^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{glob}}^2)} \left\{ \|\boldsymbol{\mu}_{\mathbf{q}(\mathbf{u}_{\text{glob}})}\|^2 + \text{tr}(\boldsymbol{\Sigma}_{\mathbf{q}(\mathbf{u}_{\text{glob}})}) \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\{ (\boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta})} - \boldsymbol{\mu}_{\boldsymbol{\beta}}) (\boldsymbol{\mu}_{\mathbf{q}(\boldsymbol{\beta})} - \boldsymbol{\mu}_{\boldsymbol{\beta}})^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}(\mathbf{u}_{\text{lin},i}^g)}^T + \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}(\mathbf{u}_{\text{lin},ij}^h)}^T + \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{glob}} + 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 $E_{\mathbf{q}}\{\log \mathbf{p}(\sigma_{\varepsilon}^2 | a_{\varepsilon})\}$, $E_{\mathbf{q}}\{\log \mathbf{q}^*(\sigma_{\varepsilon}^2)\}$, $E_{\mathbf{q}}\{\log \mathbf{p}(a_{\varepsilon})\}$, $E_{\mathbf{q}}\{\log \mathbf{q}^*(a_{\varepsilon})\}$, $E_{\mathbf{q}}\{\log \mathbf{p}(\sigma_{\text{glob}}^2 | a_{\text{glob}})\}$, $E_{\mathbf{q}}\{\log \mathbf{q}^*(\sigma_{\text{glob}}^2)\}$, $E_{\mathbf{q}}\{\log \mathbf{p}(a_{\text{glob}})\}$ and $E_{\mathbf{q}}\{\log \mathbf{q}^*(a_{\text{glob}})\}$ follow the same form as shown from the derivations in the two-level case.

Following on, we have

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

$$\begin{aligned}
E_{\mathbf{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_{\mathbf{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_{\mathbf{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_{\mathbf{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_{\mathbf{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_{\mathbf{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_{\mathbf{q}}[\log\{\mathbf{p}(\boldsymbol{\Sigma}_g|\boldsymbol{A}_{\boldsymbol{\Sigma}_g})\}] &= -\frac{1}{2}(\nu_{\boldsymbol{\Sigma}_g} + 1)E_{\mathbf{q}}\{\log|\boldsymbol{A}_{\boldsymbol{\Sigma}_g}|\} - \frac{1}{2}(\nu_{\boldsymbol{\Sigma}_g} + 4)E_{\mathbf{q}}\{\log|\boldsymbol{\Sigma}_g|\} - \frac{1}{2}\log(\pi) \\
&\quad - \frac{1}{2}\text{tr}(\boldsymbol{M}_{\mathbf{q}(\boldsymbol{A}_{\boldsymbol{\Sigma}_g}^{-1})}\boldsymbol{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_{\mathbf{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_{\mathbf{q}}\{\log|\boldsymbol{\Sigma}_g|\} - \frac{1}{2}\text{tr}(\boldsymbol{\Lambda}_{\mathbf{q}(\boldsymbol{\Sigma}_g)}\boldsymbol{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_{\mathbf{q}}[\log\{\mathbf{p}(\boldsymbol{A}_{\boldsymbol{\Sigma}_g})\}] &= -\frac{3}{2}E_{\mathbf{q}}\{\log|\boldsymbol{A}_{\boldsymbol{\Sigma}_g}|\} - \frac{1}{2}\sum_{j=1}^2 1/(\nu_{\boldsymbol{\Sigma}_g}s_{\boldsymbol{\Sigma}_g,j}^2) \left(\boldsymbol{M}_{\mathbf{q}(\boldsymbol{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

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

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

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

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

The coefficient of $E_{\mathbf{q}}\{\log(\sigma_{\text{gbl}}^2)\}$ 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 $E_{\mathbf{q}}\{\log(\sigma_{\text{grp},g}^2)\}$ 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 $E_{\mathbf{q}}\{\log(\sigma_{\text{grp},h}^2)\}$ 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 $E_{\mathbf{q}}\{\log|\boldsymbol{\Sigma}_g|\}$ 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 $E_{\mathbf{q}}\{\log|\boldsymbol{\Sigma}_h|\}$ 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 $E_{\mathbf{q}}\{\log(a_{\varepsilon})\}$ is

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

The coefficient of $E_{\mathbf{q}}\{\log(a_{\text{gbl}})\}$ is

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

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

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

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

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

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

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

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

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

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 as Algorithm A.2 in Nolan *et al.* (2020) and based on Theorem 2.3 of Nolan & Wand (2020). 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:

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

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:

$$\mathbf{B} \equiv \left[\begin{array}{c|c|c|c|c} \mathbf{B}_1 & \dot{\mathbf{B}}_1 & \mathbf{O} & \cdots & \mathbf{O} \\ \hline \mathbf{B}_2 & \mathbf{O} & \dot{\mathbf{B}}_2 & \cdots & \mathbf{O} \\ \hline \vdots & \vdots & \vdots & \ddots & \vdots \\ \hline \mathbf{B}_m & \mathbf{O} & \mathbf{O} & \cdots & \dot{\mathbf{B}}_m \end{array} \right] \quad \text{and} \quad \mathbf{b} = \left[\begin{array}{c} \mathbf{b}_1 \\ \hline \mathbf{b}_2 \\ \vdots \\ \hline \mathbf{b}_m \end{array} \right]. \quad (\text{S.5})$$

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

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

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

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

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

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.

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

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

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

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.

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

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

S.13 The SOLVETHREELEVELSPARSELEASTSQUARES Algorithm

The SOLVETHREELEVELSPARSELEASTSQUARES, listed as Algorithm A.4 in Nolan *et al.* (2020) is a proceduralization of Theorem 3.3 of Nolan & Wand (2020). 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

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

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:

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

and

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

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

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

$$\text{and } \mathbf{A}^{-1} = \left[\begin{array}{|c|c|c|c|c|c|c|c|} \hline \mathbf{A}^{11} & \mathbf{A}^{12,1} & \mathbf{A}^{12,11} & \mathbf{A}^{12,12} & \mathbf{A}^{12,2} & \mathbf{A}^{12,21} & \mathbf{A}^{12,22} & \mathbf{A}^{12,23} \\ \hline \mathbf{A}^{12,1T} & \mathbf{A}^{22,1} & \mathbf{A}^{12,1,1} & \mathbf{A}^{12,1,2} & \times & \times & \times & \times \\ \hline \mathbf{A}^{12,11T} & \mathbf{A}^{12,1,1T} & \mathbf{A}^{22,11} & \times & \times & \times & \times & \times \\ \hline \mathbf{A}^{12,12T} & \mathbf{A}^{12,1,2T} & \times & \mathbf{A}^{22,12} & \times & \times & \times & \times \\ \hline \mathbf{A}^{12,2T} & \times & \times & \times & \mathbf{A}^{22,2} & \mathbf{A}^{12,2,1} & \mathbf{A}^{12,2,2} & \mathbf{A}^{12,2,3} \\ \hline \mathbf{A}^{12,21T} & \times & \times & \times & \mathbf{A}^{12,2,1T} & \mathbf{A}^{22,21} & \times & \times \\ \hline \mathbf{A}^{12,22T} & \times & \times & \times & \mathbf{A}^{12,2,2T} & \times & \mathbf{A}^{22,22} & \times \\ \hline \mathbf{A}^{12,23T} & \times & \times & \times & \mathbf{A}^{12,2,3T} & \times & \times & \mathbf{A}^{22,23} \\ \hline \end{array} \right]$$

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.

Algorithm S.2 SOLVETHREELEVELSPARSELEASTSQUARES 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.

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

$\mathbf{d}_{1ij} \leftarrow \text{1st } q_2 \text{ rows of } \mathbf{d}_{0ij} ; \mathbf{d}_{2ij} \leftarrow \text{remaining rows of } \mathbf{d}_{0ij} ; \omega_9 \leftarrow \begin{bmatrix} \omega_9 \\ \mathbf{d}_{2ij} \end{bmatrix}$

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

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

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.

$\mathbf{c}_{0i} \leftarrow \mathbf{Q}_i^T \omega_9 ; \mathbf{C}_{0i} \leftarrow \mathbf{Q}_i^T \Omega_{10}$

$\mathbf{c}_{1i} \leftarrow \text{1st } q_1 \text{ rows of } \mathbf{c}_{0i} ; \mathbf{c}_{2i} \leftarrow \text{remaining rows of } \mathbf{c}_{0i} ; \omega_7 \leftarrow \begin{bmatrix} \omega_7 \\ \mathbf{c}_{2i} \end{bmatrix}$

$\mathbf{C}_{1i} \leftarrow \text{1st } q_1 \text{ rows of } \mathbf{C}_{0i} ; \mathbf{C}_{2i} \leftarrow \text{remaining rows of } \mathbf{C}_{0i} ; \Omega_8 \leftarrow \begin{bmatrix} \Omega_8 \\ \mathbf{C}_{2i} \end{bmatrix}$

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.

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

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 $j = 1, \dots, n_i$:

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

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

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

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

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

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