SUPPLEMENT TO SECOND-ORDER ACCURATE INFERENCE ON EIGENVALUES OF COVARIANCE AND CORRELATION MATRICES

Robert J. Boik
Department of Mathematical Sciences
Montana State University — Bozeman
Bozeman, MT 59717-2400
Email: rjboik@math.montana.edu

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Contents

1 Introduction

This supplement gives derivatives and other details concerning the parameterization covariance and correlation matrices in terms of eigenvalues and eigenvectors.

2 Errata

The published article

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contains several typographical errors. The errors did not affect the computations or theoretical results. The known errors are listed below.

1. Equation (11) should be

$$\mathrm{E}\begin{pmatrix} \widetilde{\gamma}_{22} \\ \mathbf{ss}' \\ 2\,\mathbf{N}_p[\mathbf{S}\otimes\mathbf{S})] \end{pmatrix} = \left\{ \frac{1}{n}\begin{pmatrix} c_2 & [c_1 - c_2] & [c_1 - c_2] \\ \dfrac{c_1}{n} & \left[n - \dfrac{c_1}{n}\right] & \left[1 - \dfrac{c_1}{n}\right] \\ \dfrac{2c_1}{n} & 2\left[1 - \dfrac{c_1}{n}\right] & \left[n + 1 - \dfrac{2c_1}{n}\right] \end{pmatrix} \otimes \mathbf{I}_{p^2} \right\} \begin{pmatrix} \gamma_{22} \\ \boldsymbol{\sigma}\boldsymbol{\sigma}' \\ 2\,\mathbf{N}_p[\boldsymbol{\Sigma}\otimes\boldsymbol{\Sigma}] \end{pmatrix}.$$

2. The note below Table 4 should be

$$\kappa_{3j} = \mathrm{E}\left[(Y_j - \mu_j)^3\right]/\sigma_j^3, \quad \kappa_{4j} = \mathrm{E}\left[(Y_j - \mu_j)^4\right]/\sigma_j^4 - 3,$$

   rather than

$$\kappa_{3j} = (Y_j - \mu_j)^3/\sigma_j^3, \quad \kappa_{4j} = (Y_j - \mu_j)^4/\sigma_j^4 - 3,$$

3. Line 2 in Appendix A should be

$$\mathbf{W} = \mathbf{D}^{-1}\mathbf{W}^*, \text{ where } \mathbf{D} = n \oplus n^3\mathbf{I}_4 \oplus n^2\mathbf{I}_7, \quad \mathbf{W}^* = \begin{pmatrix} \mathbf{w}_1^* & \mathbf{w}_2^* & \cdots & \mathbf{w}_{12}^* \end{pmatrix}.$$

   Note that there are two corrections: $\mathbf{I}_3$ should be $\mathbf{I}_4$ and $\mathbf{I}_8$ should be $\mathbf{I}_7$.

3 Expressions For Derivatives

3.1 Arrangement of Derivatives

Let $\mathbf{A} = \mathbf{A}(\mathbf{B})$ be an $a \times q$ matrix whose elements are functions of the $b \times s$ matrix $\mathbf{B}$. The derivative of $\mathbf{A}$ with respect to $\mathbf{B}$ is defined to be $ab \times qs$ matrix of derivatives $\{\partial\, a_{ij}/\partial\, b_{st}\}$ whose elements are arranged as follows:

$$\frac{\partial\,\mathbf{A}}{\partial\,\mathbf{B}} \overset{\text{def}}{=} \frac{\partial}{\partial\,\mathbf{B}} \otimes \partial\,\mathbf{A}.$$

To simplify the expressions of certain structured matrices, an elementary matrix will be used. Let $\mathbf{u}$ be a $t \times 1$ vector of positive integers and denote the i^{th} entry of $\mathbf{u}$ by u_i. The elementary matrix $\mathbf{E}_{i,\mathbf{u}}$ with dimension $b \times u_i$ for $1 \le i \le t$ is defined as

$$\mathbf{E}_{i,\mathbf{u}} = \sum_{j=1}^{u_i} \mathbf{e}_{a_i+j}^{b}\mathbf{e}_j^{u_i}{}' = \begin{pmatrix} \mathbf{0}_{a_i \times u_i} \\ \mathbf{I}_{u_i} \\ \mathbf{0}_{(b-a_i-u_i)\times u_i} \end{pmatrix}, \tag{20}$$

where $\mathbf{e}_i^b$ is the i^{th} column of $\mathbf{I}_b$, $a_i = -u_i + \sum_{j=1}^{i} u_j$, and $b = \sum_{j=1}^{t} u_j$. If $\mathbf{u} = \mathbf{1}_t$, then the elementary matrix $\mathbf{E}_{i,\mathbf{u}}$ simplifies to the elementary vector $\mathbf{e}_i^t$. To maintain consistency between the notation for elementary matrices and elementary vectors, $\mathbf{E}_{i,\mathbf{u}}$ in (20) has been defined as the transpose of $\mathbf{E}_{i,\mathbf{u}}$ in equation (12) of Boik (2002).

Partition $\boldsymbol{\theta}$ as $\boldsymbol{\theta} = \begin{pmatrix} \boldsymbol{\theta}_1' & \cdots & \boldsymbol{\theta}_k' \end{pmatrix}'$. For example, to parameterize a correlation matrix, set $k = 3$ and set $\boldsymbol{\theta} = \begin{pmatrix} \boldsymbol{\tau}' & \boldsymbol{\mu}' & \boldsymbol{\varphi}' \end{pmatrix}'$. Derivatives of $\operatorname{vec} \boldsymbol{\Sigma}$ with respect to $\boldsymbol{\theta}$ are arranged as follows:

$$
\begin{aligned}
\mathbf{F}^{(1)} &\overset{\text{def}}{=} \left.\frac{\partial \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = \left.\sum_{s=1}^{k} \frac{\partial \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}_s'} \mathbf{E}_{s,\boldsymbol{\nu}}'\right|_{\boldsymbol{\mu}=\mathbf{0}}; \\
\mathbf{F}^{(2)} &\overset{\text{def}}{=} \left.\frac{\partial^2 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}' \otimes \partial \boldsymbol{\theta}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = \left.\sum_{s=1}^{k}\sum_{t=1}^{k} \frac{\partial^2 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}_s' \otimes \partial \boldsymbol{\theta}_t'} \left(\mathbf{E}_{s,\boldsymbol{\nu}} \otimes \mathbf{E}_{t,\boldsymbol{\nu}}\right)'\right|_{\boldsymbol{\mu}=\mathbf{0}}; \\
\mathbf{F}^{(11)} &\overset{\text{def}}{=} \left.\frac{\partial^2 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta} \otimes \partial \boldsymbol{\theta}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = \operatorname{dvec}\left(\mathbf{F}^{(2)}, p^2\dot{\nu}, \dot{\nu}\right); \\
\mathbf{F}^{(3)} &\overset{\text{def}}{=} \left.\frac{\partial^3 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}' \otimes \partial \boldsymbol{\theta}' \otimes \partial \boldsymbol{\theta}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} \\
&= \left.\sum_{s=1}^{k}\sum_{t=1}^{k}\sum_{u=1}^{k} \frac{\partial^3 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}_s' \otimes \partial \boldsymbol{\theta}_t' \otimes \partial \boldsymbol{\theta}_u'} \left(\mathbf{E}_{s,\boldsymbol{\nu}} \otimes \mathbf{E}_{t,\boldsymbol{\nu}} \otimes \mathbf{E}_{u,\boldsymbol{\nu}}\right)'\right|_{\boldsymbol{\mu}=\mathbf{0}}; \text{ and} \\
\mathbf{F}^{(111)} &\overset{\text{def}}{=} \left.\frac{\partial^3 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta} \otimes \partial \boldsymbol{\theta} \otimes \partial \boldsymbol{\theta}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = \operatorname{dvec}\left(\mathbf{F}^{(3)}, p^2\dot{\nu}^2, \dot{\nu}\right);
\end{aligned}
$$

where $\mathbf{E}_{s,\boldsymbol{\nu}}$ is defined in (20);

$$
\boldsymbol{\nu} = \begin{pmatrix} \nu_1 \\ \vdots \\ \nu_k \end{pmatrix} = \begin{pmatrix} \dim(\boldsymbol{\theta}_1) \\ \vdots \\ \dim(\boldsymbol{\theta}_k) \end{pmatrix}; \quad \dot{\nu} = \sum_{j=1}^{k} \nu_j;
$$

and $\operatorname{dvec}(\mathbf{A}, a, b)$ is the $a \times b$ matrix that satisfies $\operatorname{vec}(\mathbf{A}) = \operatorname{vec}\{\operatorname{dvec}(\mathbf{A}, a, b)\}$. The matrix $\mathbf{A}$ must have exactly ab elements. Higher-order derivatives can be rearranged by post-multiplying by commutation matrices. For example,

$$
\begin{aligned}
\frac{\partial^2 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}_t' \otimes \partial \boldsymbol{\theta}_s'} &= \frac{\partial^2 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}_s' \otimes \partial \boldsymbol{\theta}_t'} \mathbf{I}_{(\nu_t,\nu_s)} \text{ and} \\
\frac{\partial^3 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}_t' \otimes \partial \boldsymbol{\theta}_s' \otimes \partial \boldsymbol{\theta}_u'} &= \frac{\partial^3 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}_s' \otimes \partial \boldsymbol{\theta}_t' \otimes \partial \boldsymbol{\theta}_u'} \left(\mathbf{I}_{(\nu_t,\nu_s)} \otimes \mathbf{I}_{\nu_u}\right) \\
&= \frac{\partial^3 \operatorname{vec}(\boldsymbol{\Sigma})}{\partial \boldsymbol{\theta}_t' \otimes \partial \boldsymbol{\theta}_u' \otimes \partial \boldsymbol{\theta}_s'} \left(\mathbf{I}_{\nu_t} \otimes \mathbf{I}_{(\nu_s,\nu_u)}\right),
\end{aligned}
$$

where $\mathbf{I}_{(\,\cdot\,,\,\cdot\,)}$ is the commutation matrix (MacRae, 1974). The commutation matrix $\mathbf{I}_{(a,b)}$ is denoted by some writers as $\mathbf{K}_{b,a}$ (Magnus & Neudecker 1979, 1999 §3.7). The derivatives of $\operatorname{vec} \boldsymbol{\Sigma}$ with respect to $\boldsymbol{\theta}$ satisfy the following multiplicative invariance properties:

$$
\mathbf{F}^{(1)} = \mathbf{I}_{(p,p)} \mathbf{F}^{(1)};
$$

$$
\begin{aligned}
\mathbf{F}^{(2)} &= \mathbf{I}_{(p,p)}\,\mathbf{F}^{(2)} = \mathbf{F}^{(2)}\,\mathbf{I}_{(\dot\nu,\dot\nu)};\\
\mathbf{F}^{(11)} &= (\mathbf{I}_{\dot\nu}\otimes\mathbf{I}_{(p,p)})\,\mathbf{F}^{(11)};\\
\mathbf{F}^{(3)} &= \mathbf{I}_{(p,p)}\,\mathbf{F}^{(3)} = \mathbf{F}^{(3)}\,\mathbf{I}_{(\dot\nu,\dot\nu^2)} = \mathbf{F}^{(3)}\,\mathbf{I}_{(\dot\nu^2,\dot\nu)};\\
&= \mathbf{F}^{(3)}(\mathbf{I}_{\dot\nu}\otimes\mathbf{I}_{(\dot\nu,\dot\nu)}) = \mathbf{F}^{(3)}(\mathbf{I}_{(\dot\nu,\dot\nu)}\otimes\mathbf{I}_{\dot\nu});\ \text{and}\\
\mathbf{F}^{(111)} &= (\mathbf{I}_{(p,p)}\otimes\mathbf{I}_{\dot\nu^2})\,\mathbf{F}^{(111)} = (\mathbf{I}_{p^2}\otimes\mathbf{I}_{(\dot\nu,\dot\nu)})\,\mathbf{F}^{(111)}\,.
\end{aligned}
$$

These properties are useful when simplifying expressions.

The derivatives of $\boldsymbol{\lambda}$, $\operatorname{vec}\mathbf{G}$, and $\operatorname{vec}\boldsymbol{\Sigma}$ involve several structured matrices. For ease of reference, these structured matrices are defined below:

$$
\begin{array}{ll}
\mathbf{N}_a = \frac{1}{2}\left(\mathbf{I}_{a^2}+\mathbf{I}_{(a,a)}\right); & \mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}} = \left(\boldsymbol{\Lambda}^{-1}\otimes\mathbf{I}_p\right);\\
\mathbf{N}^*_a = \frac{1}{2}\left(\mathbf{I}_{a^2}-\mathbf{I}_{(a,a)}\right); & \mathbf{I}^{(3)}_{p} = (\mathbf{I}_p\otimes\operatorname{vec}\mathbf{I}_p\otimes\mathbf{I}_p)';\\
\mathbf{J}_a = \mathbf{I}_{a^3}+\mathbf{I}_{(a,a^2)}+(\mathbf{I}_a\otimes\mathbf{I}_{(a,a)}); & \mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}} = (\mathbf{I}_p\otimes\operatorname{vec}\boldsymbol{\Lambda}\otimes\mathbf{I}_p)';\\
\mathbf{J}^*_a = \mathbf{I}_{a^3}+\mathbf{I}_{(a,a^2)}+(\mathbf{I}_{(a,a)}\otimes\mathbf{I}_a); & \mathbf{I}^{(4)}_{p} = (\mathbf{I}_p\otimes\operatorname{vec}\mathbf{I}_p\otimes\operatorname{vec}\mathbf{I}_p\otimes\mathbf{I}_p)';\\
\mathbf{J}_{a,b} = \mathbf{I}_{(b,ab)}+(\mathbf{I}_b\otimes\mathbf{I}_{(b,a)}); & \mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}} = (\mathbf{I}_p\otimes\operatorname{vec}\boldsymbol{\Lambda}\otimes\mathbf{I}_p)';\\
\mathbf{J}^*_{a,b} = \mathbf{I}_{ab^2}+(\mathbf{I}_{(b,b)}\otimes\mathbf{I}_a); &
\end{array}
\tag{21}
$$

where a and b are positive integers. The matrix $\mathbf{N}_a$ is the perpendicular projection operator that projects onto the vector space generated by symmetric matrices. That is, $\mathbf{N}'_a=\mathbf{N}_a$, $\mathbf{N}^2_a=\mathbf{N}_a$, and if $\mathbf{A}$ is an $a\times a$ matrix, then $\operatorname{vec}\mathbf{A}=\mathbf{N}_a\operatorname{vec}\mathbf{A}$ if and only if $\mathbf{A}$ is symmetric. The matrix $\mathbf{N}^{\perp}_a$ is the perpendicular projection operator that projects onto the vector space generated by skew-symmetric matrices. That is, $(\mathbf{N}^{\perp}_a)'=\mathbf{N}^{\perp}_a$, $(\mathbf{N}^{\perp}_a)^2=\mathbf{N}^{\perp}_a$ and if $\mathbf{A}$ is an $a\times a$ matrix, then $\operatorname{vec}\mathbf{A}=\mathbf{N}^{\perp}_a\operatorname{vec}\mathbf{A}$ if and only if $\mathbf{A}$ is skew-symmetric.

3.2 Correlation Matrices

Denote the correlation matrix by $\boldsymbol{\Psi}$. Then, the covariance matrix can be written as

$$
\boldsymbol{\Sigma}=\boldsymbol{\Sigma}(\boldsymbol{\theta})=\boldsymbol{\sigma}_D\boldsymbol{\Psi}\boldsymbol{\sigma}_D,\ \text{where } \boldsymbol{\theta}=\begin{pmatrix}\boldsymbol{\tau}\\ \boldsymbol{\mu}\\ \boldsymbol{\varphi}\end{pmatrix},\quad \boldsymbol{\Psi}=\boldsymbol{\Gamma}\boldsymbol{\Lambda}\boldsymbol{\Gamma}',
$$

$$
\boldsymbol{\sigma}_D=\operatorname{Diag}(\boldsymbol{\sigma}_d),\quad \boldsymbol{\sigma}_d=\boldsymbol{\sigma}_d(\boldsymbol{\tau}),\quad \boldsymbol{\Gamma}=\boldsymbol{\Gamma}\mathbf{G}(\boldsymbol{\mu},\boldsymbol{\varphi})\big|_{\boldsymbol{\mu}=\mathbf{0}},\quad \boldsymbol{\Lambda}=\operatorname{Diag}(\boldsymbol{\lambda}),\quad \boldsymbol{\lambda}=\boldsymbol{\lambda}(\boldsymbol{\varphi}),
$$

and $\boldsymbol{\Gamma}\in\mathcal{O}(p)$, the space of $p\times p$ orthogonal matrices.

3.2.1 Derivatives of Scale Parameters

The vector of scale parameters, $\boldsymbol{\sigma}_d$, is parameterized as

$$
\boldsymbol{\sigma}_d=\mathbf{T}_1\exp\{\odot\mathbf{T}_2\boldsymbol{\tau}\},
$$

where $\mathbf{T}_1$ and $\mathbf{T}_2$ are full column-rank design matrices with dimensions $p \times q_1$ and $q_1 \times \nu_1$, respectively.

Theorem 3. *The first three derivatives of* $\boldsymbol{\sigma}_d$ *with respect to* $\boldsymbol{\tau}'$ *are*

$$\begin{aligned}
\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}} &= \frac{\partial\,\boldsymbol{\sigma}_d}{\partial\,\boldsymbol{\tau}'} = \mathbf{T}_1\,\text{Diag}\left(\exp\{\odot\mathbf{T}_2\boldsymbol{\tau}\}\right)\mathbf{T}_2, \\
\mathbf{D}^{(2)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau},\boldsymbol{\tau}} &= \frac{\partial^2\boldsymbol{\sigma}_d}{\partial\,\boldsymbol{\tau}'\otimes\partial\,\boldsymbol{\tau}'} = \mathbf{T}_1\sum_{i=1}^{q_1}\mathbf{e}_i^{q_1}\exp\{\mathbf{e}_i^{q_1\prime}\mathbf{T}_2\boldsymbol{\tau}\}(\mathbf{e}_i^{q_1\prime}\mathbf{T}_2\otimes\mathbf{e}_i^{q_1\prime}\mathbf{T}_2),\ \textit{and} \\
\mathbf{D}^{(3)}_{\boldsymbol{\sigma}:\boldsymbol{\tau},\boldsymbol{\tau},\boldsymbol{\tau}} &= \frac{\partial^3\boldsymbol{\sigma}_d}{\partial\,\boldsymbol{\tau}'\otimes\partial\,\boldsymbol{\tau}'\otimes\partial\,\boldsymbol{\tau}'} = \mathbf{T}_1\sum_{i=1}^{q_1}\mathbf{e}_i^{q_1}\exp\{\mathbf{e}_i^{q_1\prime}\mathbf{T}_2\boldsymbol{\tau}\}(\mathbf{e}_i^{q_1\prime}\mathbf{T}_2\otimes\mathbf{e}_i^{q_1\prime}\mathbf{T}_2\otimes\mathbf{e}_i^{q_1\prime}\mathbf{T}_2),
\end{aligned}$$

where $\mathbf{e}_i^{q_1}$ *is the* i^{th} *column of* $\mathbf{I}_{q_1}$.

□

3.2.2 Derivatives of Eigenvalues of $\boldsymbol{\Psi}$

The vector of eigenvalues of $\boldsymbol{\Psi}$ is parameterized as

$$\boldsymbol{\lambda} = wp\mathbf{T}_3\exp\{\odot\mathbf{T}_4\boldsymbol{\xi}\} \text{ subject to } \mathbf{C}_1'\boldsymbol{\lambda} = \mathbf{c}_0, \text{ where } w = \left(\mathbf{1}_p'\mathbf{T}_3\exp\{\odot\mathbf{T}_4\boldsymbol{\xi}\}\right)^{-1} \tag{22}$$

and $\mathbf{T}_3$ and $\mathbf{T}_4$ are full column-rank design matrices with dimensions $p \times q_3$ and $q_3 \times q_4$ respectively. The design matrix $\mathbf{T}_4$ satisfies rank $\begin{pmatrix}\mathbf{T}_4 & \mathbf{1}_{q_3}\end{pmatrix} = q_4 + 1$. The q_4-vector $\boldsymbol{\xi}$ is parameterized as $\boldsymbol{\xi} = \boldsymbol{\xi}(\boldsymbol{\varphi}) = \mathbf{V}_1\boldsymbol{\eta} + \mathbf{V}_2\boldsymbol{\varphi}$, where $\mathbf{V}_1$ and $\mathbf{V}_2$ are full column-rank matrices with dimensions $q_4 \times r_2$ and $q_4 \times (q_4 - r_2)$, respectively; $\mathbf{V}_1'\mathbf{V}_2 = \mathbf{0}$; $\boldsymbol{\eta}$ is an implicit function of $\boldsymbol{\varphi}$; $\boldsymbol{\xi}$ is subject to the constraints $\mathbf{C}_2'\exp\{\odot\mathbf{T}_4\boldsymbol{\xi}\} = \mathbf{0}$; $r_2 = \text{rank}(\mathbf{C_2})$; $\mathbf{C}_2$ is a full column-rank matrix whose columns form a basis for $\mathcal{R}\left[\mathbf{T}_3'(\mathbf{C}_1 - \mathbf{1}_p p^{-1}\mathbf{c}_0')\right]$, and $\mathcal{R}(\mathbf{M})$ is the vector space generated by the columns of $\mathbf{M}$.

Theorem 4. *Define* $\mathbf{W}_{\boldsymbol{\xi},1}$ *as* $\mathbf{W}_{\boldsymbol{\xi},1} = \text{Diag}\left(\exp\{\odot\mathbf{T}_4\boldsymbol{\xi}\}\right)\mathbf{T}_4$. *It is assumed that* $\mathbf{C}_2'\mathbf{W}_{\boldsymbol{\xi},1}$ *has full row rank in an open neighborhood of the solution. Accordingly,* $\mathbf{C}_2'\mathbf{W}_{\boldsymbol{\xi},1}$ *can be expressed in terms of its singular values and vectors as follows:*

$$\mathbf{C}_2'\mathbf{W}_{\boldsymbol{\xi},1} = \mathbf{U}_{\boldsymbol{\xi}}\begin{pmatrix}\mathbf{D}_{\boldsymbol{\xi}} & \mathbf{0}\end{pmatrix}\begin{pmatrix}\mathbf{A}_{\boldsymbol{\xi},1}' \\ \mathbf{A}_{\boldsymbol{\xi},2}'\end{pmatrix} = \mathbf{U}_{\boldsymbol{\xi}}\mathbf{D}_{\boldsymbol{\xi}}\mathbf{A}_{\boldsymbol{\xi},1}'; \tag{23}$$

where $\mathbf{D}_{\boldsymbol{\xi}}$ *is an* $r_2 \times r_2$ *diagonal matrix of nonzero singular values;* $r_2 = \text{rank}(\mathbf{C}_2)$*;* $\mathbf{U}_{\boldsymbol{\xi}} \in \mathcal{O}_{r_2}$*;* $\mathbf{A}_{\boldsymbol{\xi},1}$ *has dimension* $q_4 \times r_2$*;* $\mathbf{A}_{\boldsymbol{\xi},2}$ *has dimension* $q_4 \times \nu_3$*;* $\nu_3 = q_4 - r_2$*; and* $\begin{pmatrix}\mathbf{A}_{\boldsymbol{\xi},1} & \mathbf{A}_{\boldsymbol{\xi},2}\end{pmatrix} \in \mathcal{O}_{q_4}$. *Let* $\mathbf{V}_1$ *be any matrix whose columns form a basis for* $\mathcal{R}(\mathbf{A}_{\boldsymbol{\xi},1})$. *Similarly, let* $\mathbf{V}_2$ *be any matrix whose columns form a basis for* $\mathcal{R}(\mathbf{A}_{\boldsymbol{\xi},2})$. *This choice of* $\mathbf{V} = \begin{pmatrix}\mathbf{V}_1 & \mathbf{V}_2\end{pmatrix}$ *is delicate because* $\mathbf{V}$ *is defined as a function of* $\boldsymbol{\xi}$*, yet it will be treated as a constant when taking derivatives. For fixed* $\mathbf{V}$*, the first three derivatives of* $\boldsymbol{\lambda}$ *with respect to* $\boldsymbol{\varphi}'$ *are*

$$\begin{aligned}
\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}} &= \frac{\partial\,\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'} = wp\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_3\mathbf{W}_{\boldsymbol{\xi},1}\mathbf{V}_2, \quad w \textit{ is defined in (22)}; \\
\mathbf{H}_{\boldsymbol{\lambda}} &= \mathbf{I}_p - \frac{1}{p}\boldsymbol{\lambda}\mathbf{1}_p'; \\
\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}} &= \frac{\partial^2\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'}
\end{aligned}$$

$$
\begin{aligned}
&= -2w\left(\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}} \otimes \mathbf{1}_p'\mathbf{T}_3\mathbf{W}_{\boldsymbol{\xi},1}\mathbf{V}_2\right)\mathbf{N}_{\nu_3} + wp\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_3\mathbf{H}_{\boldsymbol{\xi}}\mathbf{W}_{\boldsymbol{\xi},2}\left(\mathbf{V}_2 \otimes \mathbf{V}_2\right);\\
\mathbf{H}_{\boldsymbol{\xi}} &= \mathbf{I}_{q_3} - \mathbf{W}_{\boldsymbol{\xi},1}(\mathbf{C}_2'\mathbf{W}_{\boldsymbol{\xi},1})^{+}\mathbf{C}_2';\\
(\mathbf{C}_2'\mathbf{W}_{\boldsymbol{\xi},1})^{+} &= \mathbf{A}_{\boldsymbol{\xi},1}\mathbf{D}_{\boldsymbol{\xi}}^{-1}\mathbf{U}_{\boldsymbol{\xi}}' \text{ \textit{is the Moore-Penrose inverse of} } \mathbf{C}_2'\mathbf{W}_{\boldsymbol{\xi},1};\\
\mathbf{W}_{\boldsymbol{\xi},2} &= \sum_{j=1}^{q_3}\mathbf{e}_j^{q_3}\exp\{\mathbf{e}_j^{q_3\prime}\mathbf{T}_4\boldsymbol{\xi}\}(\mathbf{e}_j^{q_3\prime}\mathbf{T}_4 \otimes \mathbf{e}_j^{q_3\prime}\mathbf{T}_4);\\
\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}} &= \frac{\partial^3\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}' \otimes \partial\,\boldsymbol{\varphi}' \otimes \partial\,\boldsymbol{\varphi}'}\\
&= -wp\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_3\mathbf{H}_{\boldsymbol{\xi}}\mathbf{W}_{\boldsymbol{\xi},2}\left[(\mathbf{C}_2'\mathbf{W}_{\boldsymbol{\xi},1})^{+}\mathbf{C}_2'\mathbf{W}_{\boldsymbol{\xi},2}\left(\mathbf{V}_2 \otimes \mathbf{V}_2\right) \otimes \mathbf{V}_2\right]\mathbf{J}_{\nu_3}\\
&\quad -w\left(\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}} \otimes \mathbf{1}_p'\mathbf{T}_3\mathbf{W}_{\boldsymbol{\xi},1}\mathbf{V}_2\right)\mathbf{J}_{\nu_3}\\
&\quad -w\left[\mathbf{1}_p'\mathbf{T}_3\mathbf{H}_{\boldsymbol{\xi}}\mathbf{W}_{\boldsymbol{\xi},2}\left(\mathbf{V}_2 \otimes \mathbf{V}_2\right) \otimes \mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\right]\mathbf{J}_{\nu_3}\\
&\quad +wp\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_3\mathbf{H}_{\boldsymbol{\xi}}\mathbf{W}_{\boldsymbol{\xi},3}\left(\mathbf{V}_2 \otimes \mathbf{V}_2 \otimes \mathbf{V}_2\right);\ \text{\textit{and}}\\
\mathbf{W}_{\boldsymbol{\xi},3} &= \sum_{j=1}^{q_3}\mathbf{e}_j^{q_3}\exp\{\mathbf{e}_j^{q_3\prime}\mathbf{T}_4\boldsymbol{\xi}\}(\mathbf{e}_j^{q_3\prime}\mathbf{T}_4 \otimes \mathbf{e}_j^{q_3\prime}\mathbf{T}_4 \otimes \mathbf{e}_j^{q_3\prime}\mathbf{T}_4).
\end{aligned}
$$

□

To reduce memory and computational requirements, matrix derivatives can be stored as sparse matrices. Also, to decrease the number of non-zero entries in the matrix derivatives, $\mathbf{V}_2$ can be equated to the transpose of the row reduced echelon form of $\mathbf{A}_{\boldsymbol{\xi},2}'$.

Corollary 1. If $\mathbf{C}_2$ in (5) has rank 0 (i.e., there are no additional constraints beyond $\mathbf{1}_p'\boldsymbol{\lambda} = p$), then $r_2 = 0$, $\mathbf{V}_2 = \mathbf{I}_{q_4}$, $\nu_3 = q_4$, $\boldsymbol{\varphi} = \boldsymbol{\xi}$ and the derivatives of $\boldsymbol{\lambda}$ simplify to

$$
\begin{aligned}
\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}} &= wp\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_3\mathbf{W}_{\boldsymbol{\xi},1},\\
\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}} &= -2w\left(\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}} \otimes \mathbf{1}_p'\mathbf{T}_3\mathbf{W}_{\boldsymbol{\xi},1}\right)\mathbf{N}_{\nu_3} + pw\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_3\mathbf{W}_{\boldsymbol{\xi},2};\\
\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}} &= -w\left(\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}} \otimes \mathbf{1}_p'\mathbf{T}_3\mathbf{W}_{\boldsymbol{\xi},1}\right)\mathbf{J}_{\nu_3} - w\left(\mathbf{1}_p'\mathbf{T}_3\mathbf{W}_{\boldsymbol{\xi},2} \otimes \mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\right)\mathbf{J}_{\nu_3} + wp\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_3\mathbf{W}_{\boldsymbol{\xi},3};
\end{aligned}
$$

where $\mathbf{N}_{\nu_3}$ and $\mathbf{J}_{\nu_3}$ are defined in (21). □

3.2.3 Derivatives of Eigenvectors of $\boldsymbol{\Psi}$

If Theorem 2 in Boik (2003) is satisfied with $k = 1$, then the correlation matrix $\boldsymbol{\Psi}$ can be written as

$$
\boldsymbol{\Psi} = \boldsymbol{\Gamma}\mathbf{G}\boldsymbol{\Lambda}\mathbf{G}'\boldsymbol{\Gamma}'\Big|_{\boldsymbol{\mu}=\mathbf{0}}, \text{ where } \mathbf{G} = \mathbf{G}(\boldsymbol{\mu}, \boldsymbol{\varphi}). \tag{24}
$$

Denote the vector of eigenvalue multiplicities that corresponds to $\mathbf{\Psi}$ by $\mathbf{m}$ and let $\mathbf{V}^*$ be a $(p^2-\mathbf{m}'\mathbf{m})/2 \times (p^2-\mathbf{m}'\mathbf{m})/2$ nonsingular matrix that can be partitioned as $\mathbf{V}^* = \begin{pmatrix}\mathbf{V}_3 & \mathbf{V}_4\end{pmatrix}$, where $\mathbf{V}_3$ has dimension $(p^2-\mathbf{m}'\mathbf{m})/2 \times (p-1)$, $\mathbf{V}_4$ has dimension $(p^2-\mathbf{m}'\mathbf{m})/2 \times \nu_2$, $\nu_2 = [(p-1)^2+1-\mathbf{m}'\mathbf{m}]/2$, and $\mathbf{V}_3'\mathbf{V}_4 = \mathbf{0}$. Then, $\operatorname{vec}\mathbf{G}$ can be written as

$$\mathbf{g} \overset{\text{def}}{=} \operatorname{vec}\mathbf{G} = \mathbf{A}_1\boldsymbol{\eta}^* + \mathbf{A}_2\boldsymbol{\mu}^* = \begin{pmatrix}\mathbf{A}_1 & \mathbf{A}_2\mathbf{V}_3\end{pmatrix}\begin{pmatrix}\boldsymbol{\eta}_1 \\ \boldsymbol{\eta}_2\end{pmatrix} + \mathbf{A}_2\mathbf{V}_4\boldsymbol{\mu}, \tag{25}$$

where $\boldsymbol{\eta}_1 = \boldsymbol{\eta}^*$; $\boldsymbol{\eta}_2 = (\mathbf{V}_3'\mathbf{V}_3)^{-1}\mathbf{V}_3'\boldsymbol{\mu}^*$; $\boldsymbol{\mu} = (\mathbf{V}_4'\mathbf{V}_4)^{-1}\mathbf{V}_4'\boldsymbol{\mu}^*$; and $\mathbf{A}_1$ and $\mathbf{A}_2$ are known semi-orthogonal indicator matrices of order $p^2 \times p(p+1)/2$ and $p^2 \times (p^2-\mathbf{m}'\mathbf{m})/2$, respectively. These matrices satisfy $\mathbf{A}_1'\operatorname{vec}\mathbf{G} = \boldsymbol{\eta}^*$, $\mathbf{A}_2'\operatorname{vec}\mathbf{G} = \boldsymbol{\mu}^*$, and $\mathbf{A}_1'\mathbf{A}_2 = \mathbf{0}$ (see §2.3 in Boik (2003)).

Expressions for the derivatives of $\mathbf{g} = \operatorname{vec}\mathbf{G}$ with respect to $\boldsymbol{\mu}'$ and $\boldsymbol{\varphi}'$ for a specific choice of $\mathbf{V}^*$ are given in Theorem 5. The following definitions are used in Theorem 5 and throughout the remainder of this supplement:

$$\mathbf{L}_p = \sum_{i=1}^{p}(\mathbf{e}_i^p \otimes \mathbf{e}_i^p)\mathbf{e}_i^{p\prime} \text{ and } \mathbf{C}_3 = \sum_{j=1}^{p-1}(\mathbf{e}_j^p \otimes \mathbf{e}_j^p)\mathbf{e}_j^{p\prime}. \tag{26}$$

Theorem 5. *Define* $\mathbf{W}_{\boldsymbol{\rho}}$ *as* $\mathbf{W}_{\boldsymbol{\rho}} = 2\mathbf{C}_3'(\mathbf{\Gamma\Lambda}\otimes\mathbf{\Gamma})\mathbf{N}_p^*\mathbf{A}_2$, *where* $\mathbf{N}_p^*$ *is given in (21). Express* $\mathbf{W}_{\boldsymbol{\rho}}$ *in terms of its singular values and vectors:*

$$\mathbf{W}_{\boldsymbol{\rho}} = \mathbf{U}_{\boldsymbol{\rho}}\begin{pmatrix}\mathbf{D}_{\boldsymbol{\rho}} & \mathbf{0}\end{pmatrix}\begin{pmatrix}\mathbf{A}_{\boldsymbol{\rho},1}' \\ \mathbf{A}_{\boldsymbol{\rho},2}'\end{pmatrix} = \mathbf{U}_{\boldsymbol{\rho}}\mathbf{D}_{\boldsymbol{\rho}}\mathbf{A}_{\boldsymbol{\rho},1}';$$

where $\mathbf{D}_{\boldsymbol{\rho}}$ *is a* $(p-1)\times(p-1)$ *diagonal matrix of singular values;* $\mathbf{U}_{\boldsymbol{\rho}} \in \mathcal{O}(p-1)$; $\mathbf{A}_{\boldsymbol{\rho},1}$ *has dimension* $(p^2-\mathbf{m}'\mathbf{m})/2\times(p-1)$; $\mathbf{A}_{\boldsymbol{\rho},2}$ *has dimension* $(p^2-\mathbf{m}'\mathbf{m})/2\times(p^2-\mathbf{m}'\mathbf{m})/2-p+1$; *and* $\mathbf{A}_{\boldsymbol{\rho}} = \begin{pmatrix}\mathbf{A}_{\boldsymbol{\rho},1} & \mathbf{A}_{\boldsymbol{\rho},2}\end{pmatrix} \in \mathcal{O}[(p^2-\mathbf{m}'\mathbf{m})/2]$. *Let* $\mathbf{V}_3$ *be any matrix whose columns form a basis for* $\mathcal{R}(\mathbf{A}_{\boldsymbol{\rho},1})$ *and let* $\mathbf{V}_4$ *be any matrix whose columns form a basis for* $\mathcal{R}(\mathbf{A}_{\boldsymbol{\rho},2})$. *This choice of* $\mathbf{V}^* = \begin{pmatrix}\mathbf{V}_3 & \mathbf{V}_4\end{pmatrix}$, *like the choice of* $\mathbf{V}$ *in Theorem 4, is delicate because* $\mathbf{V}^*$ *is a function of* $\boldsymbol{\rho} = \operatorname{vec}\mathbf{\Psi}$, *yet it will be treated as a constant when taking derivatives with respect to* $\boldsymbol{\varphi}$. *For fixed* $\mathbf{V}^*$, *the first three derivatives of* $\mathbf{g} = \operatorname{vec}\mathbf{G}$ *with respect to* $\boldsymbol{\mu}'$ *and* $\boldsymbol{\varphi}'$ *are*

$$\begin{aligned}
\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}} &= \left.\frac{\partial\operatorname{vec}\mathbf{G}}{\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\mathbf{N}_p^*\mathbf{A}_2\mathbf{V}_4;\\
\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}} &= \left.\frac{\partial^2\operatorname{vec}\mathbf{G}}{\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = \left[(\mathbf{I}-\mathbf{H}_{\boldsymbol{\rho}})\mathbf{A}_1\mathbf{D}_p'\mathbf{I}_p^{(3)} + \mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\right]\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right);\\
\mathbf{H}_{\boldsymbol{\rho}}, &= 2\mathbf{N}_p^*\mathbf{A}_2\mathbf{W}_{\boldsymbol{\rho}}^+\mathbf{C}_3'(\mathbf{\Gamma\Lambda}\otimes\mathbf{\Gamma});\\
\mathbf{W}_{\boldsymbol{\rho}}^+ &= \mathbf{A}_{\boldsymbol{\rho},3}\mathbf{D}_{\boldsymbol{\rho}}^{-1}\mathbf{U}_{\boldsymbol{\rho}}' \textit{ is the Moore-Penrose inverse of } \mathbf{W}_{\boldsymbol{\rho}};\\
\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu},\boldsymbol{\mu}} &= \left.\frac{\partial^3\operatorname{vec}\mathbf{G}}{\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}}\\
&= -\left[(\mathbf{I}-\mathbf{H}_{\boldsymbol{\rho}})\mathbf{A}_1\mathbf{D}_p'\mathbf{I}_p^{(3)} + \mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\right]\left(\mathbf{I}_{(p,p)}\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\mathbf{J}_{\nu_2};\\
\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}} &= \left.\frac{\partial\operatorname{vec}\mathbf{G}}{\partial\,\boldsymbol{\varphi}'}\right|_{\boldsymbol{\mu}=\mathbf{0}}
\end{aligned}$$

$$
\begin{aligned}
&= -\frac{1}{2}\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p_i,\boldsymbol{\lambda}_i}\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}};\\
\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi}} &= \left.\frac{\partial^2 \operatorname{vec}\mathbf{G}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'}\right|_{\boldsymbol{\mu}=\mathbf{0}}\\
&= \left[(\mathbf{I}-\mathbf{H}_{\boldsymbol{\rho}})\mathbf{A}_1\mathbf{D}'_p\mathbf{I}^{(3)}_p+\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\right]\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)\\
&\quad +2\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_p\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\right)\mathbf{N}_{\nu_3}-\frac{1}{2}\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}};\\
\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}} &= \left.\frac{\partial^3 \operatorname{vec}\mathbf{G}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'}\right|_{\boldsymbol{\mu}=\mathbf{0}}\\
&= -\left[(\mathbf{I}-\mathbf{H}_{\boldsymbol{\rho}})\mathbf{A}_1\mathbf{D}'_p\mathbf{I}^{(3)}_p+\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\right]\left(\mathbf{I}_{(p,p)}\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)\mathbf{J}_{\nu_3}\\
&\quad +\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(4)}_p\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)\mathbf{J}^*_{\nu_3}-\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_p\\
&\quad \times\Big[\left(\mathbf{I}_{(p,p)}\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\right)+\left(\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)\Big]\mathbf{J}_{\nu_3}\\
&\quad -\frac{1}{2}\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{L}_p\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}};\\
\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu}} &= \left.\frac{\partial^2 \operatorname{vec}\mathbf{G}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}}\\
&= \left[(\mathbf{I}-\mathbf{H}_{\boldsymbol{\rho}})\mathbf{A}_1\mathbf{D}'_p\mathbf{I}^{(3)}_p+\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\right]\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\\
&\quad -\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_p\left(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right);\\
\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\mu}} &= \left.\frac{\partial^3 \operatorname{vec}\mathbf{G}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}}\\
&= -\left[(\mathbf{I}-\mathbf{H}_{\boldsymbol{\rho}})\mathbf{A}_1\mathbf{D}'_p\mathbf{I}^{(3)}_p+\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\right]\Big[\left(\mathbf{I}_{(p,p)}\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\\
&\quad +\left(\mathbf{I}_{(p,p)}\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)\mathbf{J}_{\nu_2,\nu_3}\Big]-\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_p\\
&\quad \times\Big[\left(\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)+\left(\mathbf{I}_{(p,p)}\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\right)\mathbf{J}_{\nu_2,\nu_3}\Big]\\
&\quad +\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(4)}_p\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\mathbf{J}^*_{\nu_2,\nu_3};
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu},\boldsymbol{\mu}} &= \left.\frac{\partial^3 \operatorname{vec}\mathbf{G}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} \\
&= -\Big[(\mathbf{I}-\mathbf{H}_{\boldsymbol{\rho}})\mathbf{A}_1\mathbf{D}'_p\mathbf{I}^{(3)}_p + \mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\Big]\left(\mathbf{I}_{(p,p)}\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\mathbf{J}^{**}_{\nu_2,\nu_3} \\
&\quad +\Big[(\mathbf{I}-\mathbf{H}_{\boldsymbol{\rho}})\mathbf{A}_1\mathbf{D}'_p\mathbf{I}^{(3)}_p + \mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_{p_i,\boldsymbol{\lambda}_i}\Big]\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}\right) \\
&\quad +\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(4)}_p\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\left(\mathbf{I}_{(\nu_3,\nu_2)}\otimes\mathbf{I}_{\nu_2}\right) \\
&\quad -\mathbf{H}_{\boldsymbol{\rho}}\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}\mathbf{I}^{(3)}_p\left(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}\right);
\end{aligned}
$$

where $\mathbf{D}_p$ *is the duplication matrix of order* $p^2 \times p(p+1)/2$ *(Magnus and Neudecker, 1999, §3.8),* $\mathbf{N}^*_a$, $\mathbf{J}_a$, $\mathbf{J}^*_a$, $\mathbf{J}_{a,b}$, $\mathbf{J}^*_{a,b}$, $\mathbf{J}^{**}_{a,b}$, $\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}$, $\mathbf{I}^{(3)}_p$, $\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}$, *and* $\mathbf{I}^{(4)}_p$ *are defined in (21), and* $\mathbf{L}_p$ *is defined in* (26).

□

3.2.4 Derivatives of $\boldsymbol{\Sigma}$

Theorem 6 (First-Order Derivatives of $\operatorname{vec}\boldsymbol{\Sigma}$**).** *Assume that* $\boldsymbol{\theta}$ *is partitioned as in equation (3) in Boik (2003). First-order derivatives of* $\operatorname{vec}\boldsymbol{\Sigma}$ *with respect to the components of* $\boldsymbol{\theta}$*, evaluated at* $\boldsymbol{\mu}=\mathbf{0}$ *are*

$$
\begin{aligned}
\left.\frac{\partial\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\tau}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} &= 2\,\mathbf{N}_p(\boldsymbol{\sigma}_D\boldsymbol{\Psi}\otimes\mathbf{I}_p)\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}; \\
\left.\frac{\partial\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} &= (\boldsymbol{\sigma}_D\otimes\boldsymbol{\sigma}_D)\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\mu}}; \\
\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\mu}} &= \left.\frac{\partial\operatorname{vec}\boldsymbol{\Psi}}{\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\Gamma}\boldsymbol{\Lambda}\otimes\boldsymbol{\Gamma})\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}};\ \textit{and} \\
\left.\frac{\partial\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\varphi}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} &= (\boldsymbol{\sigma}_D\otimes\boldsymbol{\sigma}_D)\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\varphi}}; \\
\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\varphi}} &= \left.\frac{\partial\operatorname{vec}\boldsymbol{\Psi}}{\partial\,\boldsymbol{\varphi}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\Gamma}\otimes\boldsymbol{\Gamma})\left[(\boldsymbol{\Lambda}\otimes\mathbf{I}_p)\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}+\frac{1}{2}\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\right];
\end{aligned}
$$

where the derivatives of $\boldsymbol{\sigma}_d$, $\boldsymbol{\lambda}$, *and* $\mathbf{g}$ *are given in Theorems 3, 4, and 5, respectively;* $\mathbf{N}_p$ *is defined in (21); and* $\mathbf{L}_p$ *is defined in* (26).

To obtain expressions for second- and third-order derivatives, the identities

$$
\begin{aligned}
(\mathbf{ABC}\otimes\mathbf{D})\mathbf{E} &= \Big\{\mathbf{A}\otimes[\operatorname{vec}(\mathbf{C}')]'\otimes\mathbf{D}\Big\}[\operatorname{vec}(\mathbf{B}')\otimes\mathbf{E}]\ \text{ and} \\
(\mathbf{A}\otimes\mathbf{BCD})\mathbf{E} &= [\mathbf{A}\otimes(\operatorname{vec}\mathbf{D})'\otimes\mathbf{B}]\,(\mathbf{E}\otimes\operatorname{vec}\mathbf{C}),
\end{aligned}
$$

are repeatedly used, where **A**, **B**, **C**, **D**, and **E** are any matrices that are conformable for multiplication.

Theorem 7 (Second-Order Derivatives of $\operatorname{vec}\boldsymbol{\Sigma}$**).** *Second-order derivatives of* $\operatorname{vec}\boldsymbol{\Sigma}$ *with respect to the components of* $\boldsymbol{\theta}$*, evaluated at* $\boldsymbol{\mu}=\mathbf{0}$ *are*

$$\begin{aligned}
\left.\frac{\partial^2 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\tau}'\otimes\partial\boldsymbol{\tau}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} &= 2\,\mathbf{N}_p\Big[(\boldsymbol{\sigma}_D\boldsymbol{\Psi}\otimes\mathbf{I}_p)\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau},\boldsymbol{\tau}} \\
&\quad +(\mathbf{I}_p\otimes\operatorname{vec}\boldsymbol{\Psi}\otimes\mathbf{I}_p)'(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}})\Big];
\end{aligned}$$

$$\left.\frac{\partial^2 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\tau}'\otimes\partial\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\mathbf{I}_p\otimes\boldsymbol{\sigma}_D)\mathbf{I}^{(3)}_p\left(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\otimes\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\mu}}\right)$$

$$\left.\frac{\partial^2 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\mu}'\otimes\partial\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\sigma}_D\otimes\boldsymbol{\sigma}_D)\mathbf{D}^{(2)}_{\boldsymbol{\rho}:\boldsymbol{\mu},\boldsymbol{\mu}};$$

$$\mathbf{D}^{(2)}_{\boldsymbol{\rho}:\boldsymbol{\mu},\boldsymbol{\mu}} = \left.\frac{\partial^2 \operatorname{vec}\boldsymbol{\Psi}}{\partial\boldsymbol{\mu}'\otimes\partial\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\Gamma}\otimes\boldsymbol{\Gamma})\left[(\boldsymbol{\Lambda}\otimes\mathbf{I}_p)\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}-\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}})\right];$$

$$\left.\frac{\partial^2 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\varphi}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = (\boldsymbol{\sigma}_D\otimes\boldsymbol{\sigma}_D)\mathbf{D}^{(2)}_{\boldsymbol{\rho}:\boldsymbol{\varphi},\boldsymbol{\varphi}};$$

$$\begin{aligned}
\mathbf{D}^{(2)}_{\boldsymbol{\rho}:\boldsymbol{\varphi},\boldsymbol{\varphi}} &= \left.\frac{\partial^2 \operatorname{vec}\boldsymbol{\Psi}}{\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\varphi}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\Gamma}\otimes\boldsymbol{\Gamma})\Big[2\mathbf{I}^{(3)}_p\left(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)\mathbf{N}_{\nu_3} \\
&\quad -\mathbf{I}^{(3)}_p\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)+(\boldsymbol{\Lambda}\otimes\mathbf{I}_p)\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi}}+\frac{1}{2}\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\Big];
\end{aligned}$$

$$\left.\frac{\partial^2 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = (\boldsymbol{\sigma}_D\otimes\boldsymbol{\sigma}_D)\mathbf{D}^{(2)}_{\boldsymbol{\rho}:\boldsymbol{\varphi},\boldsymbol{\mu}};$$

$$\begin{aligned}
\mathbf{D}^{(2)}_{\boldsymbol{\rho}:\boldsymbol{\varphi},\boldsymbol{\mu}} &= \left.\frac{\partial^2 \operatorname{vec}\boldsymbol{\Psi}}{\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\Gamma}\otimes\boldsymbol{\Gamma})\Big[(\boldsymbol{\Lambda}\otimes\mathbf{I}_p)\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu}}-\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right) \\
&\quad +\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\left(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\Big];\ \textit{and}
\end{aligned}$$

$$\left.\frac{\partial^2 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\tau}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\sigma}_D\otimes\mathbf{I}_p)\mathbf{I}^{(3)}_p\left(\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\right);$$

where the derivatives of $\boldsymbol{\sigma}_d$*,* $\boldsymbol{\lambda}$*, and* $\mathbf{g}$ *are given in Theorems 3, 4, and 5, respectively;* $\mathbf{N}_p$*,* $\mathbf{I}^{(3)}_p$*, and* $\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}$ *are defined in (21); and* $\mathbf{L}_p$ *is defined in* (26)*.*

Theorem 8 (Third-Order Derivatives of $\operatorname{vec}\boldsymbol{\Sigma}$**).** *Third-order derivatives of* $\operatorname{vec}\boldsymbol{\Sigma}$ *with respect to the components of* $\boldsymbol{\theta}$*, evaluated at* $\boldsymbol{\mu}=\mathbf{0}$ *are*

$$\left.\frac{\partial^3 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\tau}'\otimes\partial\boldsymbol{\tau}'\otimes\partial\boldsymbol{\tau}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p\Big[(\mathbf{I}_p\otimes\operatorname{vec}\boldsymbol{\Psi}\otimes\mathbf{I}_p)'\left(\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau},\boldsymbol{\tau}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\right)\mathbf{J}_{\nu_1}$$

$$+(\boldsymbol{\sigma}_{D}\boldsymbol{\Psi}\otimes\mathbf{I}_p)\mathbf{L}_p\mathbf{D}^{(3)}_{\boldsymbol{\sigma}:\boldsymbol{\tau},\boldsymbol{\tau},\boldsymbol{\tau}}\Bigg];$$

$$\left.\frac{\partial^3 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\mu}'\otimes\partial\boldsymbol{\mu}'\otimes\partial\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\sigma}_{D}\boldsymbol{\Gamma}\otimes\boldsymbol{\sigma}_{D}\boldsymbol{\Gamma})\Bigg\{\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\left(\mathbf{I}_{(p,p)}\,\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\mathbf{J}_{\nu_2}+(\boldsymbol{\Lambda}\otimes\mathbf{I}_p)\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu},\boldsymbol{\mu}}\Bigg\};$$

$$\begin{aligned}\left.\frac{\partial^3 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\varphi}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} &= 2\,\mathbf{N}_p(\boldsymbol{\sigma}_{D}\boldsymbol{\Gamma}\otimes\boldsymbol{\sigma}_{D}\boldsymbol{\Gamma})\Bigg\{\Bigg[\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\left(\mathbf{I}_{(p,p)}\,\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)\\ &\quad +\mathbf{I}^{(3)}_{p}\Big[\left(\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)+\left(\mathbf{I}_{(p,p)}\,\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\right)\Big]\Bigg]\mathbf{J}_{\nu_3}\\ &\quad -\mathbf{I}^{(4)}_{p}\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)\mathbf{J}^{*}_{\nu_3}+(\boldsymbol{\Lambda}\otimes\mathbf{I}_p)\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}}+\frac{1}{2}\mathbf{L}_p\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}}\Bigg\}\end{aligned}$$

$$\begin{aligned}\left.\frac{\partial^3 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\mu}'\otimes\partial\boldsymbol{\tau}'\otimes\partial\boldsymbol{\tau}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} &= 2\,\mathbf{N}_p\Bigg\{\mathbf{I}^{(4)}_{p}\left(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\otimes\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\mu}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\right)\left(\mathbf{I}_{(\nu_2,\nu_1)}\otimes\mathbf{I}_{\nu_1}\right)\\ &\quad +(\boldsymbol{\sigma}_{D}\otimes\mathbf{I}_p)\mathbf{I}^{(3)}_{p}\left(\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\mu}}\otimes\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau},\boldsymbol{\tau}}\right)\Bigg\};\end{aligned}$$

$$\begin{aligned}\left.\frac{\partial^3 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\tau}'\otimes\partial\boldsymbol{\tau}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} &= 2\,\mathbf{N}_p\Bigg\{\mathbf{I}^{(4)}_{p}\left(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\otimes\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\right)\left(\mathbf{I}_{(\nu_3,\nu_1)}\otimes\mathbf{I}_{\nu_1}\right)\\ &\quad +(\boldsymbol{\sigma}_{D}\otimes\mathbf{I}_p)\mathbf{I}^{(3)}_{p}\left(\mathbf{D}^{(1)}_{\boldsymbol{\rho}:\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau},\boldsymbol{\tau}}\right)\Bigg\};\end{aligned}$$

$$\left.\frac{\partial^3 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\mu}'\otimes\partial\boldsymbol{\mu}'\otimes\partial\boldsymbol{\tau}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\sigma}_{D}\otimes\mathbf{I}_p)\mathbf{I}^{(3)}_{p}\left(\mathbf{D}^{(2)}_{\boldsymbol{\rho}:\boldsymbol{\mu},\boldsymbol{\mu}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\right);$$

$$\left.\frac{\partial^3 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\tau}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\,\mathbf{N}_p(\boldsymbol{\sigma}_{D}\otimes\mathbf{I}_p)\mathbf{I}^{(3)}_{p}\left(\mathbf{D}^{(2)}_{\boldsymbol{\rho}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\right);$$

$$\begin{aligned}\left.\frac{\partial^3 \operatorname{vec}\boldsymbol{\Sigma}}{\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\varphi}'\otimes\partial\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} &= 2\,\mathbf{N}_p(\boldsymbol{\sigma}_{D}\boldsymbol{\Gamma}\otimes\boldsymbol{\sigma}_{D}\boldsymbol{\Gamma})\Bigg\{\mathbf{I}^{(3)}_{p}\Big[\left(\mathbf{I}_{(p,p)}\,\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\\ &\quad +\left(\mathbf{I}_{(p,p)}\,\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\right)\mathbf{J}_{\nu_2,\nu_3}\Big]\\ &\quad +\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}\Big[\left(\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)+\left(\mathbf{I}_{(p,p)}\,\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\right)\mathbf{J}_{\nu_2,\nu_3}\Big]\\ &\quad -\mathbf{I}^{(4)}_{p}\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\mathbf{J}^{*}_{\nu_2,\nu_3}+(\boldsymbol{\Lambda}\otimes\mathbf{I}_p)\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\mu}}\Bigg\};\end{aligned}$$

$$\left.\frac{\partial^3 \operatorname{vec} \mathbf{\Sigma}}{\partial\, \boldsymbol{\varphi}' \otimes \partial\, \boldsymbol{\mu}' \otimes \partial\, \boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\, \mathbf{N}_p(\boldsymbol{\sigma}_{\scriptscriptstyle D}\mathbf{\Gamma} \otimes \boldsymbol{\sigma}_{\scriptscriptstyle D}\mathbf{\Gamma})\Big\{\mathbf{I}_p^{(3)} \left(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}} \otimes \mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}\right)$$

$$-\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}} \left[\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\varphi}} \otimes \mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}\right) - \left(\mathbf{I}_{(p,p)}\, \mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu}} \otimes \mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right) \mathbf{J}^{**}_{\nu_2,\nu_3}\right]$$

$$-\mathbf{I}_p^{(4)} \left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}} \otimes \mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}} \otimes \mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right) \left(\mathbf{I}_{(\nu_3,\nu_2)} \otimes \mathbf{I}_{\nu_2}\right) + (\mathbf{\Lambda} \otimes \mathbf{I}_p)\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\varphi},\boldsymbol{\mu},\boldsymbol{\mu}}\Big\};$$

$$\left.\frac{\partial^3 \operatorname{vec} \mathbf{\Sigma}}{\partial\, \boldsymbol{\varphi}' \otimes \partial\, \boldsymbol{\mu}' \otimes \partial\, \boldsymbol{\tau}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = 2\, \mathbf{N}_p(\boldsymbol{\sigma}_{\scriptscriptstyle D} \otimes \mathbf{I}_p)\mathbf{I}_p^{(3)} \left(\mathbf{D}^{(2)}_{\boldsymbol{\rho}:\boldsymbol{\varphi},\boldsymbol{\varphi}} \otimes \mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\sigma}_d:\boldsymbol{\tau}}\right);$$

where the derivatives of $\boldsymbol{\sigma}_d$, $\boldsymbol{\lambda}$, *and* $\mathbf{g}$ *are given in Theorems 3, 4, and 5, respectively;* $\mathbf{N}_p$, $\mathbf{J}_a$, $\mathbf{J}_{a,b}$, $\mathbf{J}^*_{a,b}$, $\mathbf{J}^{**}_{a,b}$, $\mathbf{I}^{(2)}_{p,\boldsymbol{\lambda}}$, $\mathbf{I}^{(3)}_p$, $\mathbf{I}^{(3)}_{p,\boldsymbol{\lambda}}$, *and* $\mathbf{I}^{(4)}_p$ *are defined in (21); and* $\mathbf{L}_p$ *is defined in* (26).

3.3 Covariance Matrices

If interest is in the eigenvalues of the covariance matrix, then it is useful to write the covariance matrix as

$$\mathbf{\Sigma} = \mathbf{\Sigma}(\boldsymbol{\theta}) = \mathbf{\Gamma\Lambda\Gamma}', \text{ where } \boldsymbol{\theta} = \begin{pmatrix}\boldsymbol{\mu}\\ \boldsymbol{\varphi}\end{pmatrix},$$

$$\mathbf{\Gamma} = \mathbf{\Gamma G}(\boldsymbol{\mu})\big|_{\boldsymbol{\mu}=\mathbf{0}}, \quad \mathbf{\Lambda} = \operatorname{Diag}(\boldsymbol{\lambda}), \quad \boldsymbol{\lambda} = \boldsymbol{\lambda}(\boldsymbol{\varphi}),$$

and $\mathbf{\Gamma} \in \mathcal{O}(p)$.

3.3.1 Derivatives of Eigenvalues of $\mathbf{\Sigma}$

The vector of eigenvalues of $\mathbf{\Sigma}$ is parameterized either as

$$\boldsymbol{\lambda} = \mathbf{T}_1 \exp\{\odot \mathbf{T}_2\boldsymbol{\xi}\} \text{ subject to } \mathbf{C}_1'\boldsymbol{\lambda} = \mathbf{c}_0 \text{ or as} \tag{27}$$

$$\boldsymbol{\lambda} = \varphi_1 w \mathbf{T}_1 \exp\{\odot \mathbf{T}_2\boldsymbol{\xi}\} \text{ subject to } \mathbf{C}_1'\boldsymbol{\lambda} = \mathbf{c}_0\varphi_1, \tag{28}$$

$$\text{where } w = \left(\mathbf{1}_p'\mathbf{T}_1 \exp\{\odot \mathbf{T}_2\boldsymbol{\xi}\}\right)^{-1};$$

$\mathbf{T}_1$ and $\mathbf{T}_2$ are full column-rank model matrices with dimensions $p \times q_1$ and $q_1 \times q_2$, respectively; and $\mathbf{C}_1$ and $\mathbf{c}_0$ are matrices (vectors) of known constants that satisfy $\mathbf{c}_0 \in \mathcal{R}(\mathbf{C}_1')$. The model matrix $\mathbf{T}_2$ in (28) satisfies $\operatorname{rank}\begin{pmatrix}\mathbf{T}_2 & \mathbf{1}_{q_1}\end{pmatrix} = q_2 + 1$.

The q_2-vector $\boldsymbol{\xi}$ is subject to the restriction

$$\mathbf{C}_1'\boldsymbol{\lambda} = \mathbf{c}_0 \iff \mathbf{C}_2' \exp\{\odot \mathbf{T}_2\boldsymbol{\xi}\} - \mathbf{c}_1 = \mathbf{0} \text{ in (27) and}$$

$$\mathbf{C}_1'\boldsymbol{\lambda} = \mathbf{c}_0\varphi_1 \iff \mathbf{C}_2' \exp\{\odot \mathbf{T}_2\boldsymbol{\xi}\} = \mathbf{0} \text{ in (28)},$$

where $\mathbf{C}_2$ and $\mathbf{c}_1$ are constructed as follows. For the parameterization in (27), $\mathbf{c}_1 = \left(\mathbf{A}'\mathbf{A}\right)^{-1}\mathbf{A}'\mathbf{c}_0$ and $\mathbf{AC}_2'$ is any full column-rank factorization of $\mathbf{C}_1'\mathbf{T}_1$. For the parameterization in (28), $\mathbf{C}_2$ is any full column-rank matrix whose columns form a basis set for $\mathcal{R}\left[\mathbf{T}_1'(\mathbf{C}_1 - \mathbf{1}_p\mathbf{c}_0')\right]$. The q_2-vector $\boldsymbol{\xi}$ is parameterized as

$$\boldsymbol{\xi} = \boldsymbol{\xi}(\boldsymbol{\varphi}) = \mathbf{V}_1\boldsymbol{\eta} + \mathbf{V}_2\boldsymbol{\varphi} \text{ in (27) and}$$

$$\boldsymbol{\xi} = \boldsymbol{\xi}(\boldsymbol{\varphi}_2) = \mathbf{V}_1\boldsymbol{\eta} + \mathbf{V}_2\boldsymbol{\varphi}_2 \text{ in } (28)$$

where $\mathbf{V}_1$ and $\mathbf{V}_2$ are full column-rank matrices with dimensions $q_2 \times r_2$ and $q_2 \times (q_2 - r_2)$, respectively; $\mathbf{V}_1'\mathbf{V}_2 = \mathbf{0}$; $\boldsymbol{\eta}$ is an implicit function of $\boldsymbol{\varphi}_2$; and $r_2 = \operatorname{rank}(\mathbf{C}_2)$. See Boik (2003) for details. Derivatives of $\boldsymbol{\lambda}$ in (27) with respect to $\boldsymbol{\varphi}'$ are given in Theorem 9 and derivatives of $\boldsymbol{\lambda}$ in (28) with respect to $\boldsymbol{\varphi}'$ are given in Theorem 10

Theorem 9. *Suppose that $\boldsymbol{\lambda}$ is parameterized as in* (27). *Define $\mathbf{W}_{1;\boldsymbol{\xi}}$ as*

$$\mathbf{W}_{1;\boldsymbol{\xi}} = \operatorname{Diag}\left(\exp\{\odot\mathbf{T}_2\boldsymbol{\xi}\}\right)\mathbf{T}_2.$$

It is assumed that $\mathbf{C}_2'\mathbf{W}_{1;\boldsymbol{\xi}}$ has full row-rank in an open neighborhood of the solution. Accordingly, $\mathbf{C}_2'\mathbf{W}_{1;\boldsymbol{\xi}}$ can be expressed in terms of its singular values and vectors as follows:

$$\mathbf{C}_2'\mathbf{W}_{1;\boldsymbol{\xi}} = \mathbf{U}_{\boldsymbol{\xi}}\begin{pmatrix}\mathbf{D}_{\boldsymbol{\xi}} & \mathbf{0}\end{pmatrix}\begin{pmatrix}\mathbf{A}_{\boldsymbol{\xi},1}' \\ \mathbf{A}_{\boldsymbol{\xi},2}'\end{pmatrix} = \mathbf{U}_{\boldsymbol{\xi}}\mathbf{D}_{\boldsymbol{\xi}}\mathbf{A}_{\boldsymbol{\xi},1}'; \tag{29}$$

where $\mathbf{D}_{\boldsymbol{\xi}}$ is an $r_2 \times r_2$ diagonal matrix of nonzero singular values; $r_2 = \operatorname{rank}(\mathbf{C}_2)$; $\mathbf{U}_{\boldsymbol{\xi}} \in \mathcal{O}_{r_2}$; $\mathbf{A}_{\boldsymbol{\xi},1}$ has dimension $q_2 \times r_2$; $\mathbf{A}_{\boldsymbol{\xi},2}$ has dimension $q_2 \times \nu_2$; $\nu_2 = q_2 - r_2$; and $\begin{pmatrix}\mathbf{A}_{\boldsymbol{\xi},1} & \mathbf{A}_{\boldsymbol{\xi},2}\end{pmatrix} \in \mathcal{O}_{q_2}$. Let $\mathbf{V}_1$ be any matrix whose columns form a basis for $\mathcal{R}(\mathbf{A}_{\boldsymbol{\xi},1})$. Similarly, let $\mathbf{V}_2$ be any matrix whose columns form a basis for $\mathcal{R}(\mathbf{A}_{\boldsymbol{\xi},2})$. This choice of $\mathbf{V} = \begin{pmatrix}\mathbf{V}_1 & \mathbf{V}_2\end{pmatrix}$ is delicate because $\mathbf{V}$ is defined as a function of $\boldsymbol{\xi}$, yet it will be treated as a constant when taking derivatives.

For fixed $\mathbf{V}$, the first three derivatives of $\boldsymbol{\lambda}$ with respect to $\boldsymbol{\varphi}'$ are as follows:

$$\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}} = \frac{\partial\,\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'} = \mathbf{T}_1\mathbf{W}_{1;\boldsymbol{\xi}}\mathbf{V}_2;$$

$$\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}} = \frac{\partial^2\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'} = \mathbf{T}_1\mathbf{H}_{\boldsymbol{\xi}}\mathbf{W}_{2;\boldsymbol{\xi}}\left(\mathbf{V}_2\otimes\mathbf{V}_2\right);$$

$$\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}} = \frac{\partial^3\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'} = \mathbf{T}_1\mathbf{H}_{\boldsymbol{\xi}}\mathbf{W}_{3;\boldsymbol{\xi}}\left(\mathbf{V}_2\otimes\mathbf{V}_2\otimes\mathbf{V}_2\right)$$

$$-\mathbf{T}_1\mathbf{H}_{\boldsymbol{\xi}}\mathbf{W}_{2;\boldsymbol{\xi}}\left[\left(\mathbf{C}_2'\mathbf{W}_{1:\boldsymbol{\xi}}\right)^+\mathbf{C}_2'\mathbf{W}_{2;\boldsymbol{\xi}}\left(\mathbf{V}_2\otimes\mathbf{V}_2\right)\otimes\mathbf{V}_2\right]\mathbf{J}_{\nu_2} \text{ where}$$

$$\mathbf{H}_{\boldsymbol{\xi}} = \mathbf{I}_{q_1} - \mathbf{W}_{1;\boldsymbol{\xi}}\left(\mathbf{C}_2'\mathbf{W}_{1;\boldsymbol{\xi}}\right)^+\mathbf{C}_2';$$

$$\left(\mathbf{C}_2'\mathbf{W}_{1;\boldsymbol{\xi}}\right)^+ = \mathbf{A}_{\boldsymbol{\xi},1}\mathbf{D}_{\boldsymbol{\xi}}^{-1}\mathbf{U}_{\boldsymbol{\xi}}' \text{ is the Moore-Penrose inverse of } \mathbf{C}_2'\mathbf{W}_{1;\boldsymbol{\xi}};$$

$$\mathbf{W}_{2;\boldsymbol{\xi}} = \sum_{i=1}^{q_1}\left[\mathbf{e}_i^{q_1}\exp\{\mathbf{e}_i^{q_1\prime}\mathbf{T}_2\boldsymbol{\xi}\}\mathbf{e}_i^{q_1\prime}\otimes\mathbf{e}_i^{q_1\prime}\right]\left(\mathbf{T}_2\otimes\mathbf{T}_2\right); \text{ and}$$

$$\mathbf{W}_{3;\boldsymbol{\xi}} = \sum_{i=1}^{q_1}\left[\mathbf{e}_i^{q_1}\exp\{\mathbf{e}_i^{q_1\prime}\mathbf{T}_2\boldsymbol{\xi}\}\mathbf{e}_i^{q_1\prime}\otimes\mathbf{e}_i^{q_1\prime}\otimes\mathbf{e}_i^{q_1\prime}\right]\left(\mathbf{T}_2\otimes\mathbf{T}_2\otimes\mathbf{T}_2\right);$$

where $\mathbf{J}_{\nu_2}$ is defined in (21). □

Corollary 2. If $\mathbf{C}_2$ in (27) has rank 0 (i.e., there are no constraints on $\boldsymbol{\lambda}$), then $r_2 = 0$, $\nu_2 = q_2$, $\mathbf{V}_2 = \mathbf{I}_{q_2}$, $\boldsymbol{\varphi} = \boldsymbol{\xi}$ and the derivatives of $\boldsymbol{\lambda}$ simplify to

$$\frac{\partial\,\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'} = \mathbf{T}_1\mathbf{W}_{1;\boldsymbol{\xi}}; \quad \frac{\partial^2\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'} = \mathbf{T}_1\mathbf{W}_{2;\boldsymbol{\xi}} \text{ and;}$$

$$\frac{\partial^3 \boldsymbol{\lambda}}{\partial \boldsymbol{\varphi}' \otimes \partial \boldsymbol{\varphi}' \otimes \partial \boldsymbol{\varphi}'} = \mathbf{T}_1 \mathbf{W}_{3;\boldsymbol{\xi}}.$$

$\square$

Theorem 10. *Suppose that* $\boldsymbol{\lambda}$ *is parameterized as in* (28). *Partition* $\boldsymbol{\varphi}$ *as*

$$\boldsymbol{\varphi} = \begin{pmatrix} \varphi_1 \\ \boldsymbol{\varphi}_2 \end{pmatrix} \text{ and define } \boldsymbol{\nu}_2 \overset{\text{def}}{=} \begin{pmatrix} \nu_{21} \\ \nu_{22} \end{pmatrix} = \begin{pmatrix} 1 \\ q_2 - r_2 \end{pmatrix}$$

where $r_2 = \operatorname{rank}(\mathbf{C}_2)$ *and the entries in* $\boldsymbol{\nu}_2$ *represent the dimensions of* φ_1 *and* $\boldsymbol{\varphi}_2$. *Define* $\mathbf{V}_1$, $\mathbf{V}_2$, $\mathbf{W}_{1;\boldsymbol{\xi}}$, $\mathbf{W}_{2;\boldsymbol{\xi}}$, $\mathbf{W}_{3;\boldsymbol{\xi}}$, *and* $\mathbf{H}_{\boldsymbol{\xi}}$ *as in Theorem 9, except denote the dimension of* $\mathbf{V}_2$ *as* $q_2 \times (\nu_{22})$.

For fixed $\mathbf{V}$, *the first three derivatives of* $\boldsymbol{\lambda}$ *with respect to* $\boldsymbol{\varphi}'$ *are*

$$\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}} = \sum_{s=1}^{2} \mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_s} \mathbf{E}'_{s,\boldsymbol{\nu}_2},$$

$$\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}} = \sum_{s=1}^{2} \sum_{t=1}^{2} \mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_s,\boldsymbol{\varphi}_t} \left(\mathbf{E}'_{s,\boldsymbol{\nu}_2} \otimes \mathbf{E}'_{t,\boldsymbol{\nu}_2}\right),$$

$$\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}} = \sum_{s=1}^{2} \sum_{t=1}^{2} \sum_{u=1}^{2} \mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_s,\boldsymbol{\varphi}_t,\boldsymbol{\varphi}_u} \left(\mathbf{E}'_{s,\boldsymbol{\nu}_2} \otimes \mathbf{E}'_{t,\boldsymbol{\nu}_2} \otimes \mathbf{E}'_{u,\boldsymbol{\nu}_2}\right), \text{ where}$$

$$\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_s} = \frac{\partial \boldsymbol{\lambda}}{\partial \boldsymbol{\varphi}'_s}; \quad \mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_s,\boldsymbol{\varphi}_t} = \frac{\partial^2 \boldsymbol{\lambda}}{\partial \boldsymbol{\varphi}'_s \otimes \partial \boldsymbol{\varphi}'_t};$$

$$\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_s,\boldsymbol{\varphi}_t,\boldsymbol{\varphi}_u} = \frac{\partial^3 \boldsymbol{\lambda}}{\partial \boldsymbol{\varphi}'_s \otimes \partial \boldsymbol{\varphi}'_t \otimes \partial \boldsymbol{\varphi}'_u};$$

$$\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\varphi_1} = \boldsymbol{\lambda} \frac{1}{\varphi_1};$$

$$\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2} = w\varphi_1 \mathbf{H}_{\boldsymbol{\lambda}} \mathbf{T}_1 \mathbf{W}_{1;\boldsymbol{\xi}} \mathbf{V}_2, \quad w \text{ is defined in (28)};$$

$$\mathbf{H}_{\boldsymbol{\lambda}} = \mathbf{I}_p - \frac{1}{\varphi_1} \boldsymbol{\lambda} \mathbf{1}'_p;$$

$$\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\varphi_1,\varphi_1} = \mathbf{0}_{p\times 1}; \quad \mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2,\varphi_1} = w \mathbf{H}_{\boldsymbol{\lambda}} \mathbf{T}_1 \mathbf{W}_{1;\boldsymbol{\xi}} \mathbf{V}_2;$$

$$\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2,\boldsymbol{\varphi}_2} = -2w \left(\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2} \otimes \mathbf{1}'_p \mathbf{T}_1 \mathbf{W}_{1;\boldsymbol{\xi}} \mathbf{V}_2\right) \mathbf{N}_{\nu_{22}} + w\varphi_1 \mathbf{H}_{\boldsymbol{\lambda}} \mathbf{T}_1 \mathbf{H}_{\boldsymbol{\xi}} \mathbf{W}_{2;\boldsymbol{\xi}} \left(\mathbf{V}_2 \otimes \mathbf{V}_2\right);$$

$$\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2,\boldsymbol{\varphi}_2,\boldsymbol{\varphi}_2} = w\varphi_1 \mathbf{H}_{\boldsymbol{\lambda}} \mathbf{T}_1 \mathbf{H}_{\boldsymbol{\xi}} \mathbf{W}_{3;\boldsymbol{\xi}} \left(\mathbf{V}_2 \otimes \mathbf{V}_2 \otimes \mathbf{V}_2\right)$$

$$-w\varphi_1 \mathbf{H}_{\boldsymbol{\lambda}} \mathbf{T}_1 \mathbf{H}_{\boldsymbol{\xi}} \mathbf{W}_{2;\boldsymbol{\xi}} \left[(\mathbf{C}'_2 \mathbf{W}_{1;\boldsymbol{\xi}})^{+} \mathbf{C}'_2 \mathbf{W}_{2;\boldsymbol{\xi}} \left(\mathbf{V}_2 \otimes \mathbf{V}_2\right) \otimes \mathbf{V}_2\right] \mathbf{J}_{\nu_{22}}$$

$$-w \left(\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2,\boldsymbol{\varphi}_2} \otimes \mathbf{1}'_p \mathbf{T}_1 \mathbf{W}_{1;\boldsymbol{\xi}} \mathbf{V}_2\right) \mathbf{J}_{\nu_{22}} - w \left[\mathbf{1}'_p \mathbf{T}_1 \mathbf{H}_{\boldsymbol{\xi}} \mathbf{W}_{2;\boldsymbol{\xi}} \left(\mathbf{V}_2 \otimes \mathbf{V}_2\right) \otimes \mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2}\right] \mathbf{J}_{\nu_{22}};$$

$$\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\varphi_1,\varphi_1,\boldsymbol{\varphi}_2} = \mathbf{0}_{p\times\nu_{22}}; \quad \mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\varphi_1,\varphi_1,\varphi_1} = \mathbf{0}_{p\times 1}; \quad \mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\varphi_1,\boldsymbol{\varphi}_2,\boldsymbol{\varphi}_2} = \frac{1}{\varphi_1}\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2,\boldsymbol{\varphi}_2};$$

$\mathbf{E}_{s,\boldsymbol{\nu}_2}$ *is defined in* (20)*, and* $\mathbf{N}_{\nu_{22}}$ *and* $\mathbf{J}_{\nu_{22}}$ *are defined in* (21)*.*

□

To reduce memory and computational requirements, matrix derivatives can be stored as sparse matrices. Also, to decrease the number of non-zero entries in the matrix derivatives, $\mathbf{V}_2$ can be equated to the transpose of the row reduced echelon form of $\mathbf{A}'_{\boldsymbol{\xi},2}$.

Corollary 3. If $\mathbf{C}_2$ in (5) has rank 0 (i.e., there are no additional constraints beyond $\mathbf{1}'_p\boldsymbol{\lambda} = p$), then $r_2 = 0$, $\mathbf{V}_2 = \mathbf{I}_{q_2}$, $\nu_{22} = q_2$, $\boldsymbol{\varphi}_2 = \boldsymbol{\xi}$ and the derivatives of $\boldsymbol{\lambda}$ simplify to

$$\frac{\partial\,\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'_2} = w\varphi_1\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_1\mathbf{W}_{1;\boldsymbol{\xi}};$$

$$\frac{\partial^2\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'_2\otimes\partial\,\boldsymbol{\varphi}'_2} = -2w\left(\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2}\otimes\mathbf{1}'_p\mathbf{T}_1\mathbf{W}_{1;\boldsymbol{\xi}}\right)\mathbf{N}_{\nu_{22}} + w\varphi_1\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_1\mathbf{W}_{2;\boldsymbol{\xi}};$$

$$\frac{\partial^3\boldsymbol{\lambda}}{\partial\,\boldsymbol{\varphi}'_2\otimes\partial\,\boldsymbol{\varphi}'_2\otimes\partial\,\boldsymbol{\varphi}'_2} = -w\left(\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2,\boldsymbol{\varphi}_2}\otimes\mathbf{1}'_p\mathbf{T}_1\mathbf{W}_{1;\boldsymbol{\xi}}\right)\mathbf{J}_{\nu_{22}} - w\left(\mathbf{1}'_p\mathbf{T}_1\mathbf{W}_{2;\boldsymbol{\xi}}\otimes\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}_2}\right)\mathbf{J}_{\nu_{22}}$$

$$+w\varphi_1\mathbf{H}_{\boldsymbol{\lambda}}\mathbf{T}_1\mathbf{W}_{3;\boldsymbol{\xi}};$$

where $\mathbf{N}_{\nu_{22}}$ and $\mathbf{J}_{\nu_{22}}$ are defined in (21).

□

3.3.2 Derivatives of Eigenvectors of $\boldsymbol{\Sigma}$

The matrix of eigenvectors of $\boldsymbol{\Sigma}$ is parameterized as

$$\boldsymbol{\Gamma} = \boldsymbol{\Gamma}\mathbf{G}(\boldsymbol{\mu})\big|_{\boldsymbol{\mu}=\mathbf{0}}, \text{ where } \operatorname{vec}\mathbf{G} = \mathbf{g} = \mathbf{A}_1\boldsymbol{\mu} + \mathbf{A}_2\boldsymbol{\eta};$$

$\boldsymbol{\eta}$ is an implicit function of $\boldsymbol{\mu}$ and the indicator matrices $\mathbf{A}_1$ and $\mathbf{A}_2$ are defined in the appendix of Boik (2002). Theorem A1 in Boik (2002) gives the derivatives of $\mathbf{g}$ with respect to $\boldsymbol{\mu}'$. For completeness, the derivatives are reproduced in Theorem 11 below.

Theorem 11. *The first three derivatives of* $\operatorname{vec}\mathbf{G}$ *with respect to* $\boldsymbol{\mu}$*, evaluated at* $\boldsymbol{\mu} = \mathbf{0}$*, can be written as follows:*

$$\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}} = \left.\frac{\partial\,\operatorname{vec}(\mathbf{G})}{\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = (\mathbf{I}_{p^2} - \mathbf{A}_3)\mathbf{A}_1 = (\mathbf{I}_{p^2} - \mathbf{I}_{(p,p)})\mathbf{A}_1,$$

$$\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}} = \left.\frac{\partial^2\operatorname{vec}(\mathbf{G})}{\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = \mathbf{A}_3\left(\mathbf{I}_p\otimes\operatorname{vec}\mathbf{I}_p\otimes\mathbf{I}_p\right)'(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}), \text{ and}$$

$$\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu},\boldsymbol{\mu}} = \left.\frac{\partial^3\ \operatorname{vec}(\mathbf{G})}{\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'}\right|_{\boldsymbol{\mu}=\mathbf{0}} = -\mathbf{A}_3\left(\mathbf{I}_p\otimes\operatorname{vec}\mathbf{I}_p\otimes\mathbf{I}_p\right)'\Big[(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\otimes\mathbf{I}_{(p,p)}\mathbf{D}^{(2)}_{G})$$

$$-(\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}})\left\{\mathbf{I}_{\nu_1^3} + (\mathbf{I}_{\nu_1}\otimes\mathbf{I}_{(\nu_1,\nu_1)})\right\}\Big], \text{ where}$$

$$\mathbf{A}_3 = \sum_{i=1}^{p}\sum_{j=i}^{p}(2-\delta_{ij})(\mathbf{e}_i^p\mathbf{e}_i^{p\prime}\otimes\mathbf{e}_j^p\mathbf{e}_j^{p\prime})\,\mathbf{N}_p,$$

$\mathbf{N}_p$ *is defined in (21) and* δ_{ij} *is Kronecker's delta.* □

3.3.3 Derivatives of $\boldsymbol{\Sigma}$

It is assumed that $\boldsymbol{\Sigma}$ is parameterized as

$$\boldsymbol{\Sigma} = \boldsymbol{\Gamma}\mathbf{G}\boldsymbol{\Lambda}\mathbf{G}'\boldsymbol{\Gamma}'\big|_{\boldsymbol{\mu}=\mathbf{0}},$$

where $\mathbf{G}=\mathbf{G}(\boldsymbol{\mu})$, $\boldsymbol{\Lambda}=\boldsymbol{\Lambda}(\boldsymbol{\varphi})$ and $\boldsymbol{\theta}$ is partitioned as

$$\boldsymbol{\theta} = \begin{pmatrix}\boldsymbol{\mu}\\ \boldsymbol{\varphi}\end{pmatrix}.$$

Theorem 12 (First-Order Derivatives of $\operatorname{vec}\boldsymbol{\Sigma}$**).** *First-order derivatives of* $\operatorname{vec}\boldsymbol{\Sigma}$ *with respect to the components of* $\boldsymbol{\theta}$*, evaluated at* $\boldsymbol{\mu}=\mathbf{0}$ *are*

$$\frac{\partial\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\mu}'} = 2\,\mathbf{N}_p(\boldsymbol{\Gamma}\boldsymbol{\Lambda}\otimes\boldsymbol{\Gamma})\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}} \text{ and}$$

$$\frac{\partial\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\varphi}'} = (\boldsymbol{\Gamma}\otimes\boldsymbol{\Gamma})\mathbf{L}\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}};$$

where $\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}$ *is given in Theorem 11; and, depending on the parameterization,* $\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}$ *is given either in Theorem 9 or in Theorem 10.*

□

Theorem 13 (Second-Order Derivatives of $\operatorname{vec}\boldsymbol{\Sigma}$**).** *Second-order derivatives of* $\operatorname{vec}\boldsymbol{\Sigma}$ *with respect to the components of* $\boldsymbol{\theta}$*, evaluated at* $\boldsymbol{\mu}=\mathbf{0}$ *are*

$$\frac{\partial^2\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'} = 2\,\mathbf{N}_p\left[(\boldsymbol{\Gamma}\boldsymbol{\Lambda}\otimes\boldsymbol{\Gamma})\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}} - \{\boldsymbol{\Gamma}\otimes(\operatorname{vec}\boldsymbol{\Lambda})'\otimes\boldsymbol{\Gamma}\}\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\right];$$

$$\frac{\partial^2\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\mu}'} = 2\,\mathbf{N}_p\{\boldsymbol{\Gamma}\otimes(\operatorname{vec}\mathbf{I}_p)'\otimes\boldsymbol{\Gamma}\}\left\{\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right\};\ \text{and}$$

$$\frac{\partial^2\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'} = (\boldsymbol{\Gamma}\otimes\boldsymbol{\Gamma})\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}};$$

where $\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}$ *and* $\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}$ *are given in Theorem 11; and, depending on the parameterization,* $\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}$ *and* $\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}}$ *are given either in Theorem 9 or in Theorem 10.*

□

Theorem 14 (Third-Order Derivatives of $\operatorname{vec}\boldsymbol{\Sigma}$**).** *Third-order derivatives of* $\operatorname{vec}\boldsymbol{\Sigma}$ *with respect to the components of* $\boldsymbol{\theta}$*, evaluated at* $\boldsymbol{\mu}=\mathbf{0}$ *are*

$$\frac{\partial^3\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'} = 2\,\mathbf{N}_p\Big[(\boldsymbol{\Gamma}\boldsymbol{\Lambda}\otimes\boldsymbol{\Gamma})\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu},\boldsymbol{\mu}}$$

$$+\left\{\boldsymbol{\Gamma}\otimes(\operatorname{vec}\boldsymbol{\Lambda})'\otimes\boldsymbol{\Gamma}\right\}\left(\mathbf{I}_{(p,p)}\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\left\{\mathbf{I}_{(\nu_1,\nu_1^2)}+(\mathbf{I}_{\nu_1}\otimes 2\,\mathbf{N}_{\nu_1})\right\}\Bigg];$$

$$\frac{\partial^3\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\mu}'\otimes\partial\,\boldsymbol{\mu}'}=2\,\mathbf{N}_p\Bigg[\left\{\boldsymbol{\Gamma}\otimes(\operatorname{vec}\mathbf{I}_p)'\otimes\boldsymbol{\Gamma}\right\}\left(\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}\right)$$

$$-\left(\boldsymbol{\Gamma}\otimes(\operatorname{vec}\mathbf{I}_p)'\otimes(\operatorname{vec}\mathbf{I}_p)'\otimes\boldsymbol{\Gamma}\right)\left(\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\otimes\mathbf{L}_p\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right)\left(\mathbf{I}_{(\nu_2,\nu_1)}\otimes\mathbf{I}_{\nu_1}\right)\Bigg];$$

$$\frac{\partial^3\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\mu}'}=2\,\mathbf{N}_p\left\{\boldsymbol{\Gamma}\otimes(\operatorname{vec}\mathbf{I}_p)'\otimes\boldsymbol{\Gamma}\right\}\left(\mathbf{L}_p\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}}\otimes\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}\right);$$

$$\frac{\partial^3\operatorname{vec}\boldsymbol{\Sigma}}{\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'\otimes\partial\,\boldsymbol{\varphi}'}=(\boldsymbol{\Gamma}\otimes\boldsymbol{\Gamma})\mathbf{L}_p\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}};$$

where $\mathbf{D}^{(1)}_{\mathbf{g}:\boldsymbol{\mu}}$, $\mathbf{D}^{(2)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu}}$, *and* $\mathbf{D}^{(3)}_{\mathbf{g}:\boldsymbol{\mu},\boldsymbol{\mu},\boldsymbol{\mu}}$ *are given in Theorem 11; and, depending on the parameterization,* $\mathbf{D}^{(1)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi}}$, $\mathbf{D}^{(2)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi}}$, *and* $\mathbf{D}^{(3)}_{\boldsymbol{\lambda}:\boldsymbol{\varphi},\boldsymbol{\varphi},\boldsymbol{\varphi}}$ *are given either in Theorem 9 or in Theorem 10.*

□

4 Matrix Expressions for $\mathbf{Z}_j$ and $\mathbf{K}_j$

The terms $\mathbf{Z}_j$ for $j=1,\ldots$ in (27) are linear functions of $\mathbf{s}-\boldsymbol{\sigma}=\operatorname{vec}(\mathbf{S}-\boldsymbol{\Sigma})$ whose coefficients depend on the derivatives of $\boldsymbol{\Sigma}$ with respect to $\boldsymbol{\theta}$. For convenience, define $\ddot{\mathbf{F}}^{(1)}$, $\ddot{\mathbf{F}}^{(2)}$, $\dddot{\mathbf{F}}^{(1)}$, and $\dddot{\mathbf{F}}^{(2)}$ as

$$\begin{aligned}\ddot{\mathbf{F}}^{(1)} &= \left(\boldsymbol{\Sigma}^{-1}\otimes\boldsymbol{\Sigma}^{-1}\right)\mathbf{F}^{(1)};\quad \ddot{\mathbf{F}}^{(2)}=\left(\boldsymbol{\Sigma}^{-1}\otimes\boldsymbol{\Sigma}^{-1}\right)\mathbf{F}^{(2)};\\ \dddot{\mathbf{F}}^{(1)} &= \left(\boldsymbol{\Sigma}^{-1}\otimes\operatorname{vec}\boldsymbol{\Sigma}^{-1}\otimes\boldsymbol{\Sigma}^{-1}\right)\mathbf{F}^{(1)}\text{ and }\dddot{\mathbf{F}}^{(2)}=\left(\boldsymbol{\Sigma}^{-1}\otimes\operatorname{vec}\boldsymbol{\Sigma}^{-1}\otimes\boldsymbol{\Sigma}^{-1}\right)\mathbf{F}^{(2)}.\end{aligned}$$

Expressions for $\mathbf{Z}_j$ and $\mathbf{K}_j$ are as follows:

$$\begin{aligned}\mathbf{Z}_1 &= \frac{1}{2}\,\ddot{\mathbf{F}}^{(1)\prime}\sqrt{n}\,(\mathbf{s}-\boldsymbol{\sigma});\\
\mathbf{Z}_2 &= \frac{1}{2}\,\mathbf{F}^{(11)\prime}\left\{\mathbf{I}_{\dot{\nu}}\otimes\left(\boldsymbol{\Sigma}^{-1}\otimes\boldsymbol{\Sigma}^{-1}\right)\sqrt{n}\,(\mathbf{s}-\boldsymbol{\sigma})\right\}-\dddot{\mathbf{F}}^{(1)\prime}\left\{\mathbf{F}^{(1)}\otimes\sqrt{n}(\mathbf{s}-\boldsymbol{\sigma})\right\};\\
\mathbf{Z}_3 &= \left(\operatorname{vec}\ddot{\mathbf{F}}^{(1)}\otimes\ddot{\mathbf{F}}^{(1)}\right)'\left(\mathbf{I}_{p\dot{\nu}}\otimes\mathbf{I}_{(p,p)}\otimes\mathbf{I}_p\right)\left\{\mathbf{I}_{\dot{\nu}}\otimes\mathbf{F}^{(1)}\otimes\sqrt{n}(\mathbf{s}-\boldsymbol{\sigma})\right\}\\
&+ 2\,\dddot{\mathbf{F}}^{(1)\prime}\left[\mathbf{F}^{(1)}\otimes\mathbf{N}_p\left(\mathbf{I}_p\otimes\operatorname{vec}\boldsymbol{\Sigma}^{-1}\otimes\mathbf{I}_p\right)'\left\{\mathbf{F}^{(1)}\otimes\sqrt{n}(\mathbf{s}-\boldsymbol{\sigma})\right\}\right]\\
&+ \frac{1}{2}\,\mathbf{F}^{(111)\prime}\left\{\mathbf{I}_{\dot{\nu}^2}\otimes\left(\boldsymbol{\Sigma}^{-1}\otimes\boldsymbol{\Sigma}^{-1}\right)\sqrt{n}\,(\mathbf{s}-\boldsymbol{\sigma})\right\}\\
&- 2\,\mathbf{F}^{(11)\prime}\left(\mathbf{I}_{\dot{\nu}}\otimes\boldsymbol{\Sigma}^{-1}\otimes\operatorname{vec}\boldsymbol{\Sigma}^{-1}\otimes\boldsymbol{\Sigma}^{-1}\right)'\left\{\left(\mathbf{I}_{\dot{\nu}}\otimes\mathbf{F}^{(1)}\right)\mathbf{N}_{\dot{\nu}}\otimes\sqrt{n}(\mathbf{s}-\boldsymbol{\sigma})\right\}\\
&- \dddot{\mathbf{F}}^{(1)\prime}\left\{\mathbf{F}^{(2)}\otimes\sqrt{n}(\mathbf{s}-\boldsymbol{\sigma})\right\};\end{aligned}$$

$$
\begin{aligned}
\mathbf{K}_2 &= -\frac{1}{2}\,\ddot{\mathbf{F}}^{(1)\prime}\,\mathbf{F}^{(1)} = -\bar{\mathbf{I}}_{\boldsymbol{\theta}};\\
\mathbf{K}_3 &= 2\,\dddot{\mathbf{F}}^{(1)\prime}\left(\mathbf{F}^{(1)}\otimes\mathbf{F}^{(1)}\right)\mathbf{N}_{\dot\nu} - \mathbf{F}^{(11)\prime}\left(\mathbf{I}_{\dot\nu}\otimes\ddot{\mathbf{F}}^{(1)}\right)\mathbf{N}_{\dot\nu} - \frac{1}{2}\,\ddot{\mathbf{F}}^{(1)\prime}\,\mathbf{F}^{(2)};\ \text{and}\\
\mathbf{K}_4 &= \mathbf{F}^{(11)\prime}\left\{\mathbf{I}_{\dot\nu}\otimes\left(\boldsymbol{\Sigma}^{-1}\otimes\operatorname{vec}\boldsymbol{\Sigma}^{-1}\otimes\boldsymbol{\Sigma}^{-1}\right)'\left(\mathbf{F}^{(1)}\otimes\mathbf{F}^{(1)}\right)\right\}\left\{4\left(\mathbf{N}_{\dot\nu}\otimes\mathbf{I}_{\dot\nu}\right)+2\mathbf{I}_{(\dot\nu^2,\dot\nu)}\right\}\\
&+ 4\,\dddot{\mathbf{F}}^{(1)\prime}\left(\mathbf{F}^{(2)}\otimes\mathbf{F}^{(1)}\right)\left\{\left(\mathbf{I}_{\dot\nu}\otimes\mathbf{N}_{\dot\nu}\right)+\frac{1}{2}\mathbf{I}_{(\dot\nu,\dot\nu^2)}\right\}\\
&- \mathbf{F}^{(1)\prime}(\boldsymbol{\Sigma}^{-1}\otimes\operatorname{vec}\boldsymbol{\Sigma}^{-1}\otimes\operatorname{vec}\boldsymbol{\Sigma}^{-1}\otimes\boldsymbol{\Sigma}^{-1})'\left(\mathbf{F}^{(1)}\otimes\mathbf{F}^{(1)}\otimes\mathbf{F}^{(1)}\right)\\
&\times \left\{2\mathbf{I}_{(\dot\nu,\dot\nu^2)}+3\mathbf{I}_{(\dot\nu^2,\dot\nu)}+4\left(\mathbf{N}_{\dot\nu}\otimes\mathbf{I}_{\dot\nu}\right)\right\}\\
&- \mathbf{F}^{(111)\prime}\left(\mathbf{I}_{\dot\nu^2}\otimes\ddot{\mathbf{F}}^{(1)}\right)\left\{\left(\mathbf{I}_{\dot\nu}\otimes\mathbf{N}_{\dot\nu}\right)+\frac{1}{2}\mathbf{I}_{(\dot\nu,\dot\nu^2)}\right\}\\
&- \mathbf{F}^{(11)\prime}\left(\mathbf{I}_{\dot\nu}\otimes\ddot{\mathbf{F}}^{(2)}\right)\left\{\left(\mathbf{N}_{\dot\nu}\otimes\mathbf{I}_{\dot\nu}\right)+\frac{1}{2}\mathbf{I}_{(\dot\nu^2,\dot\nu)}\right\} - \frac{1}{2}\,\ddot{\mathbf{F}}^{(1)\prime}\,\mathbf{F}^{(3)};
\end{aligned}
$$

where $\mathbf{N}_{\dot\nu} = \frac{1}{2}\left(\mathbf{I}_{\dot\nu}+\mathbf{I}_{(\dot\nu,\dot\nu)}\right)$.

5 References

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