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APPENDIX A TO

ON THE PERFORMANCE OF EQUIANGULAR MASCON SOLUTION IN GRACE-LIKE MISSIONS

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The model of observation equations is of the form

$$y = Ax + e,\ \mathrm{D}(y) = Q_y \qquad \text{(A.1)}$$

Where y is a vector of m observations, A is the $m \times n$ design matrix, x is a vector of n unknowns. The $m \times m$ covariance matrix Q_y is written as

$$Q_y = Q_0 + \sum_{k=1}^{p} \sigma_k Q_k \qquad \text{(A.2)}$$

where Q_0 and $Q_k, k = 1, \ldots, p$ are some $m \times m$ known cofactor matrices. The unknown variance components $\sigma_k,\ k = 1, \ldots, p$ can be estimated as $\hat{\sigma}_0 = N_s^{-1} \ell_s$, where the entries of the vector N_s and the vector ℓ_s are [Teunissen and Amiri-Simkooei, 2008]

$$N_s^{(i,j)} = \frac{1}{2} \mathrm{tr}\left(Q_i Q_y^{-1} P_A^{\perp} Q_j Q_y^{-1} P_A^{\perp}\right) \qquad \text{(A.3)}$$

and

$$\ell_s^{(i)} = \frac{1}{2} \hat{e}^T Q_y^{-1} Q_i Q_y^{-1} \hat{e} - \frac{1}{2} \mathrm{tr}\left(Q_0 Q_y^{-1} P_A^{\perp} Q_i Q_y^{-1} P_A^{\perp}\right) \qquad \text{(A.4)}$$

where $P_A^{\perp} = I - A N_\alpha^{-1} A^T Q_y^{-1}$ is an orthogonal projector. The structure introduced in Eq. (16) is of the form

$$Q_y = \begin{bmatrix} 0 & 0 \\ 0 & C_2 \end{bmatrix} + \sigma_0^2 \begin{bmatrix} Q & 0 \\ 0 & 0 \end{bmatrix} \qquad \text{(A.5)}$$

where $C_2 = s^2 C$ is inverted to $C_2^{-1} = s^{-2} C^{-1} = \alpha P$. For this application, Q_0 is the known term and there is only one unknown variance component, $\sigma_1 = \sigma_0^2$ as we have $p = 1$. We therefore have

$$A \equiv \begin{bmatrix} A \\ I \end{bmatrix}, \; y \equiv \begin{bmatrix} y \\ y_0 \end{bmatrix}, Q_0 = \begin{bmatrix} 0 & 0 \\ 0 & C_2 \end{bmatrix}, Q_1 = \begin{bmatrix} Q & 0 \\ 0 & 0 \end{bmatrix} \tag{A.6}$$

The covariance matrix Q_y is inverted to

$$Q_y^{-1} = \begin{bmatrix} \sigma_0^{-2} Q^{-1} & 0 \\ 0 & C_2^{-1} \end{bmatrix} = \begin{bmatrix} W & 0 \\ 0 & C_2^{-1} \end{bmatrix} \tag{A.7}$$

The projector $P_A^{\perp}$ can be further developed as

$$P_A^{\perp} = \begin{bmatrix} I_m & 0 \\ 0 & I_n \end{bmatrix} - \begin{bmatrix} A \\ I \end{bmatrix} N_\alpha^{-1} [A^T \; I] \begin{bmatrix} W & 0 \\ 0 & C_2^{-1} \end{bmatrix} \tag{A.8}$$

or

$$P_A^{\perp} = \begin{bmatrix} I_m & 0 \\ 0 & I_n \end{bmatrix} - \begin{bmatrix} A \\ I \end{bmatrix} [N_\alpha^{-1} A^T W \quad N_\alpha^{-1} C_2^{-1}] \tag{A.9}$$

and finally

$$P_A^{\perp} = \begin{bmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{bmatrix} \tag{A.10}$$

where

$$P_{11} = I_m - A N_\alpha^{-1} A^T W \tag{A.11}$$

$$P_{12} = -A \, N_\alpha^{-1} C_2^{-1} \tag{A.12}$$

$$P_{21} = -N_\alpha^{-1} A^T W \tag{A.13}$$

$$P_{22} = I_n - \; N_\alpha^{-1} C_2^{-1} \tag{A.14}$$

Further, the $Q_1 Q_y^{-1}$ simplifies as

$$Q_1 Q_y^{-1} = \begin{bmatrix} Q & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} W & 0 \\ 0 & C_2^{-1} \end{bmatrix} = \begin{bmatrix} \sigma_0^{-2} I_m & 0 \\ 0 & 0 \end{bmatrix} \tag{A.15}$$

and

$$Q_1 Q_y^{-1} P_A^{\perp} = \begin{bmatrix} \sigma_0^{-2} P_{11} & \sigma_0^{-2} P_{12} \\ 0 & 0 \end{bmatrix} \tag{A.16}$$

This gives

$$Q_1 Q_y^{-1} P_A^{\perp} Q_1 Q_y^{-1} P_A^{\perp} = \begin{bmatrix} \sigma_0^{-4} P_{11} P_{11} & \sigma_0^{-4} P_{11} P_{12} \\ 0 & 0 \end{bmatrix} \tag{A.17}$$

and

$$Q_0 Q_y^{-1} P_A^{\perp} Q_1 Q_y^{-1} P_A^{\perp} = \begin{bmatrix} 0 & 0 \\ \sigma_0^{-4} P_{21} P_{11} & \sigma_0^{-4} P_{21} P_{12} \end{bmatrix} \tag{A.18}$$

The 1×1 normal matrix N_s simplifies to

$$N_s^{(1,1)} = n_{11} = \frac{1}{2\sigma_0^4} \mathrm{tr}(P_{11} P_{11}) \tag{A.19}$$

or, finally

$$N_s^{(1,1)} = n_{11} = \frac{1}{2\sigma_0^4} (m - 2\mathrm{tr}(\, N_\alpha^{-1} N) + \mathrm{tr}(\, N_\alpha^{-1} N N_\alpha^{-1} N)) \tag{A.20}$$

The first terms of ℓ_s in Eq. (A.4) can be worked out as

$$\frac{1}{2}\hat{e}^T Q_y^{-1} Q_1 Q_y^{-1}\hat{e} = \frac{1}{2}[\hat{e}^T\ \hat{e}_0^T]\begin{bmatrix} W & 0 \\ 0 & C_2^{-1}\end{bmatrix}\begin{bmatrix}\sigma_0^{-2} I_m & 0 \\ 0 & 0\end{bmatrix}\begin{bmatrix}\hat{e} \\ \hat{e}_0\end{bmatrix} \tag{A.21}$$

or

$$\frac{1}{2}\hat{e}^T Q_y^{-1} Q_1 Q_y^{-1}\hat{e} = \frac{1}{2}[\hat{e}^T\ \hat{e}_0^T]\begin{bmatrix}\sigma_0^{-2} W & 0 \\ 0 & 0\end{bmatrix}\begin{bmatrix}\hat{e} \\ \hat{e}_0\end{bmatrix} \tag{A.22}$$

which gives

$$\frac{1}{2}\hat{e}^T Q_y^{-1} Q_1 Q_y^{-1}\hat{e} = \frac{1}{2\sigma_0^2}\hat{e}^T W\hat{e} \tag{A.23}$$

The second term of ℓ_s is

$$\frac{1}{2}\mathrm{tr}(Q_0 Q_y^{-1} P_A^{\perp} Q_1 Q_y^{-1} P_A^{\perp}) = \frac{1}{2\sigma_0^2}\mathrm{tr}(P_{21}P_{12}) \tag{A.24}$$

or

$$\frac{1}{2}\mathrm{tr}(Q_0 Q_y^{-1} P_A^{\perp} Q_1 Q_y^{-1} P_A^{\perp}) = \frac{1}{2\sigma_0^2}\mathrm{tr}(N_\alpha^{-1} N N_\alpha^{-1} C_2^{-1}) \tag{A.25}$$

which gives the ℓ_s as

$$\ell_s = \frac{1}{2\sigma_0^4}\hat{e}^T W\hat{e} - \frac{1}{2\sigma_0^2}\mathrm{tr}(N_\alpha^{-1} N N_\alpha^{-1} C_2^{-1}) \tag{A.26}$$

$$\ell_s = \ell_1 = \frac{\hat{e}^T Q^{-1}\hat{e}}{2\sigma_0^4} - \frac{\mathrm{tr}(N_\alpha^{-1} N N_\alpha^{-1}(\alpha P))}{2\sigma_0^2} \tag{A.27}$$

This completes the proof.

The variance component can be estimated as $\hat{\sigma}_0^2 = N_s^{-1}\ell_s$. The equation $N_s\hat{\sigma}_0^2 = \ell_s$, with terms from Eqs. (A.20) and (A.27) and leaving out the term $2\sigma^2$ from the denominators of both sides, gives: $m - 2\mathrm{tr}(N_\alpha^{-1}N) + \mathrm{tr}(N_\alpha^{-1}NN_\alpha^{-1}N) = (\hat{e}^T Q^{-1}\hat{e})/\sigma^2 - \mathrm{tr}(N_\alpha^{-1}NN_\alpha^{-1}(\alpha P))$. This equation can further simplify to

$$m - 2\mathrm{tr}(N_\alpha^{-1}N) + \mathrm{tr}(N_\alpha^{-1}NN_\alpha^{-1}(\overbrace{N + \alpha P}^{N_\alpha})) = \frac{\hat{e}^T Q^{-1}\hat{e}}{\sigma_0^2} \tag{A.28}$$

or finally, the least squares estimate of the variance component σ_0^2 is

$$\hat{\sigma}_0^2 = \frac{\hat{e}^T Q^{-1}\hat{e}}{m - \mathrm{tr}(N_\alpha^{-1}N)} \tag{A.29}$$