

On BIQUE Procedures Applied to GPS Pseudorange Measurements

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Abstract. Best-Invariant-Quadratic-Unbiased-Estimation (BIQUE) of the variance factors is used in this work to evaluate the adequacy, or goodness, of different stochastic models affecting GPS pseudorange measurements (assumed uncorrelated), using the linear Gauss-Markov functional model. Four different stochastic models of the observations are tested, verifying that incorrect results of the BIQUE estimates (i.e. negative variance components) imply large inaccuracies of GPS-derived user positions. Results on real measurement campaigns show that the SNR (Signal to Noise Ratio) is effective in reducing the GPS position errors, by using models with SNR and SNR squared. BIQUE estimations with negative variance components allowed us to reject one of the four chosen stochastic models. No significant differences have been noted using slightly different (high) values of the redundancy r of the observations ($r = 20$ and $r = 28$). We use formulas in which the BIQUE methodology does not require the evaluation of least-squares (LS) residuals. Therefore, the BIQUE of the variance and covariance components could be performed in pre-adjustment, without the necessity of cumbersome LS adjustments during each iteration.

Keywords: BIQUE · VCE · Variance-covariance component estimation · Variance factors · Stochastic models · GPS pseudorange measurements · Functional models · Gauss-Markov

1 Introduction

Estimation of the variance and covariance components for GPS pseudorange measurements, i.e. adoption of a suitable stochastic model of the observations, is a crucial step to assess the accuracy of GPS-derived user coordinates. In the last two decades, many methodologies for VCE (Variance-Covariance Estimation) have been presented in the statistical and geodetic literatures (Moghtased-Azar et al. 2014; Junhuan et al. 2011). Among them, BIQUE (Best Invariant Quadratic Unbiased Estimation) techniques, in the framework of least-squares adjustment, can be basically categorized with respect to the adopted stochastic and functional models (with or without unknown

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parameters). Iterative formulas have already been developed and they have different expressions, depending on the selected models.

This work presents BIQUE methods to evaluate the effectiveness, or validity, of different stochastic models applied to some GPS observables (in particular, pseudorange measurements, assumed uncorrelated), verifying that incorrect results of the BIQUE estimates (i.e. negative variance components) imply bad choices of the stochastic models, and therefore large inaccuracies of GPS-derived user positions.

Let us suppose that the $(n, 1)$ random GPS pseudorange measurements vector $\boldsymbol{l}$ is normally distributed and that the observations are uncorrelated. Denoting the k unknown variance and covariance components σ_i^2 and σ_{ij}, respectively, we define the $(k, 1)$ vector $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_k)^{\mathrm{T}}$ (T denotes transposition).

Regarding the stochastic model, we model the definite positive (n, n) covariance matrix $\boldsymbol{\Sigma}_{\boldsymbol{l}}$ of the observables as a linear combination of the unknown vector $\boldsymbol{\sigma}$:

$$\boldsymbol{\Sigma}_l = \sum_1^k \sigma_i \mathbf{Q}_i \tag{1.1}$$

with assigned (n, n) symmetrical cofactor matrices $\mathbf{Q}_i$.

The observation weight matrix is:

$$\mathbf{P} = \boldsymbol{\Sigma}_l^{-1} \tag{1.2}$$

In Appendix A we will derive the relations for the BIQUE of $\boldsymbol{\sigma}$ in the functional model of condition only. This model will be the starting point for the general BIQUE of the variance-covariance components.

Generally, it must be noted that formulating the condition equations (see Appendix A, Eq. A.1) of the functional model of condition only can be very difficult. As far as GPS pseudorange measurements are concerned, the well-known GPS navigation equations and the Gauss-Markov functional model are used. In the case of GPS pseudorange observations, in next section we will apply the general formulations (derived in Appendix B) in the case of Gauss-Markov functional model.

The paper is structured as follows: after introducing the general linear stochastic model, we apply (Sect. 2) the BIQUE estimation to the Gauss-Markov functional model, which is the model adopted for GPS pseudorange measurements (Li et al. 2011). In Sect. 3 we will show numerical results of the least-squares adjustment of GPS observables (pseudorange) by considering different stochastic models and testing the effectiveness of the model via the BIQUE procedure. Section 4 contains concluding remarks. In Sect. 5 (Appendix A) we derive formally the BIQUE estimation equations under the hypothesis of a condition adjustment functional model, whereas in Sect. 6 (Appendix B) we show a generalized methodology for BIQUE.

2 BIQUE of the GPS Pseudorange Variance Factors (Gauss-Markov Model)

As it will be shown in Appendix B, the methodology for the BIQUE VCE of the observed GPS pseudoranges (for which we adopt the Gauss-Markov functional model) implies the iterative resolution of the system:

$$\mathbf{H}\hat{\sigma} = \mathbf{f} \tag{2.1}$$

where:

$$\mathbf{H} = \left\{h_{ij} = tr(\mathbf{M}\mathbf{Q}_i\mathbf{M}\mathbf{Q}_j)\right\} \tag{2.2}$$

$$\mathbf{f} = \left\{\mathrm{f}_i = l^{\mathrm{T}}\mathbf{M}\mathbf{Q}_i\mathbf{M}l\right\} \tag{2.3}$$

$$\mathbf{M} = \mathbf{P}\mathbf{Q}_{\hat{\mathbf{v}}}\mathbf{P} = \mathbf{P}\mathbf{R} \tag{2.4}$$

and $\mathbf{M}$ is a symmetric matrix defined in Appendix B (Eq. B.1).

We will show in Appendix B (Eq. (B.12)) that it is not necessary to perform a least-squares adjustment, which could imply great computational cost. Therefore, it is possible to avoid the evaluation of the least-squares (LS) residuals $\hat{\mathbf{v}}$, and (B.12) reduces to (2.3). Moreover, in our case of Gauss-Markov functional model, the expression of the cofactor matrix $\mathbf{Q}_{\hat{\mathbf{v}}}$ of the least-squares residuals, used in (2.4), turns out to be:

$$\mathbf{Q}_{\hat{\mathbf{v}}} = \mathbf{P}^{-1} - \mathbf{A}\left(\mathbf{A}^{\mathrm{T}}\mathbf{P}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathrm{T}} \tag{2.5}$$

where $\mathbf{A}$ is the known (n, u) design matrix of the linearized pseudorange equations (Rahemi et al. 2014), with $\mathrm{rank}(\mathbf{A}) = u \leq n$. Therefore, (2.4) becomes:

$$\mathbf{M} = \mathbf{P}\mathbf{Q}_{\hat{\mathbf{v}}}\mathbf{P} = \mathbf{P}\mathbf{R} = \mathbf{P} - \mathbf{P}\mathbf{A}\left(\mathbf{A}^{\mathrm{T}}\mathbf{P}\mathbf{A}\right)^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{P} \tag{2.6}$$

Since the matrix $\mathbf{M}$, defined in Eq. (2.6) and required in (2.2) and (2.3), contains the weight matrix $\mathbf{P}$ of the pseudorange observations and hence the covariance matrix $\boldsymbol{\Sigma}_l$ (that is, the vector $\boldsymbol{\sigma}$ of variance-covariance components) it is necessary to implement an iterative numerical procedure. Starting with a reasonable vector $\hat{\boldsymbol{\sigma}}^{(0)}$ of a priori variance-covariance components, a first estimation $\hat{\boldsymbol{\sigma}}^{(1)}$ is carried out. The resulting values of the components are then multiplied by the corresponding cofactor matrices, obtaining improved matrices $\mathbf{Q}_i^{(1)} = \hat{\boldsymbol{\sigma}}^{(1)}\hat{\boldsymbol{\sigma}}^{(0)}\mathbf{Q}_i$, from which the updated covariance matrix $\boldsymbol{\Sigma}_l^{(1)} = \sum_1^k \mathbf{Q}_i^{(1)}$ is computed. This new covariance matrix represents the input of the subsequent iteration. The procedure is repeated until the estimates will reproduce themselves (in the case of process convergence), namely until $\hat{\boldsymbol{\sigma}}^{(v)}$ converges to the

vector $(1,\ldots,1)^{\mathrm{T}}$. Supposing convergence after v iterations, the final values of the variance-covariance components are expressed as:

$$\hat{\sigma}_i = \prod_{\alpha=0}^{v} \hat{\sigma}_i^{(\alpha)}, i = 1,\ldots,k \tag{2.7}$$

The sum of the elements h_{ij} of the matrix $\mathbf{H}$, defined in (2.2), equals the total redundancy r (Crocetto et al. 2000):

$$\sum_{i,j=1}^{k} h_{ij} = r \tag{2.8}$$

Furthermore (Crocetto et al. 2000), the k elements of the vector $\mathbf{f}$ (see (2.3)) add up to the total quadratic form of the weighted least-squares residuals of the observations:

$$\sum_{1}^{k} \mathrm{f}_i = \boldsymbol{l}^{\mathrm{T}}\mathbf{M}\boldsymbol{l} \tag{2.9}$$

From (2.8) and (2.9), we can observe that the total quadratic form $\boldsymbol{l}^{\mathrm{T}}\mathbf{M}\boldsymbol{l}$ is somewhat spread among the f_i, as well as the total redundancy over the elements of $\mathbf{H}$.

3 Case Study: GPS Pseudorange Measurements

The BIQUE technique will be applied to the estimation of the phase center coordinates of a GPS receiver antenna and of the receiver clock offset by means of redundant pseudorange measurements. The test antenna was placed in a point of the regional GNSS network (located in southern Italy).

We have assumed four stochastic models for the measured pseudoranges (assumed uncorrelated), to carry out a correct LS adjustment, as follows:

(SA): constant variance (σ_ρ^2) of all pseudorange measurements;

(SB): constant term with additive term depending on the measured pseudorange value;

(SC): constant term with additive term inversely proportional to the measurement Signal-to-Noise Ratio (SNR), derived from the receiver;

(SD): constant term with additive term inversely proportional to the SNR squared.

In formulas:

$$\text{(SA)} \qquad \sigma_\rho^2 = cost = \sigma_{01}^2 \quad \Leftrightarrow \quad \boldsymbol{\Sigma}_{\boldsymbol{ll}} = \sigma_{01}^2 \mathbf{Q}_1 \tag{3.1}$$

$$\text{with} \qquad \mathbf{Q}_1 = \mathbf{I} \tag{3.2}$$

$$\text{(SB)} \qquad \sigma_\rho^2 = \sigma_{01}^2 + (\sigma_{02}\rho)^2 \quad \Leftrightarrow \quad \boldsymbol{\Sigma}_l = \sigma_{01}^2\mathbf{Q}_1 + \sigma_{02}^2\mathbf{Q}_2 \tag{3.3}$$

$$\text{with} \qquad \mathbf{Q}_1 = \mathbf{I} \text{ and } \mathbf{Q}_2 = diag\left[\rho_i^2\right] \tag{3.4}$$

$$\text{(SC)} \qquad \sigma_\rho^2 = \sigma_{01}^2 + \left(\frac{\sigma_{02}}{\text{SNR}}\right)^2 \quad \Leftrightarrow \quad \boldsymbol{\Sigma}_l = \sigma_{01}^2\mathbf{Q}_1 + \sigma_{02}^2\mathbf{Q}_2 \tag{3.5}$$

$$\text{with} \qquad \mathbf{Q}_1 = \mathbf{I} \text{ and } \mathbf{Q}_2 = diag\left[\left(\frac{1}{\text{SNR}_i}\right)^2\right] \tag{3.6}$$

$$\text{(SD)} \qquad \sigma_\rho^2 = \sigma_{01}^2 + \left(\frac{\sigma_{02}}{\text{SNR}^2}\right)^2 \quad \Leftrightarrow \quad \boldsymbol{\Sigma}_l = \sigma_{01}^2\mathbf{Q}_1 + \sigma_{02}^2\mathbf{Q}_2 \tag{3.7}$$

$$\text{with} \qquad \mathbf{Q}_1 = \mathbf{I} \text{ and } \mathbf{Q}_2 = diag\left[\left(\frac{1}{\text{SNR}_i^2}\right)^2\right] \tag{3.8}$$

where σ_ρ^2 is the variance of the pseudorange ρ, σ_{01}^2 is the first constant part of σ_ρ^2, and σ_{02}^2 is the second variance factor.

The satellite's clock offset and coordinates are derived from a precise ephemerides file in the SP3 format (Standard Product 3, Hilla 2007). The pseudorange measurements are derived from the C/A (Coarse/Acquisition) code embedded in the transmitted signal and are input in the format RINEX 3.01 (Receiver Independent Exchange) (IGS 2013). As for the SNR, the values retrieved from the RINEX files have range from 0 to 80.

Two measurement campaigns have been performed. In the first session, data obtained by dual-frequency receivers were gathered. Ephemeris data of eight satellites were considered, with four 15-min measurement epochs, between 16:00 h and 16:45 h on Oct. 10, 2018. The total number of observations is n = 32, and the global redundancy r is equal to 28. In a second measurement session, 24 observations were collected (in three measurement epochs), with r = 20.

Table 1. BIQUE values with the selected stochastic models and $r = 20$.

Stochastic model	$\hat{\sigma}_{01}$ (m)	$\hat{\sigma}_{02}$ (m)
(SA)	8.9	
(SB)	Negative	Negative
(SC)	2.7	445
(SD)	1.8	25096

Tables 1 and 2 report the results of the BIQUE estimates with the chosen stochastic models SA, SB, SC, SD, for two values of r (20 and 28).

Since the BIQUE values for model (SB) are found to be negative, the stochastic model (SB) is not correct. This is because the pseudorange values lay in a small interval, therefore the elements of the matrix $\mathbf{Q_2}$ = diag$\left[\rho_i^2\right]$ (see Eq. (3.4)) are not

Table 2. BIQUE values with the selected stochastic models and $r = 28$.

Stochastic model	$\hat{\sigma}_{01}$ (m)	$\hat{\sigma}_{02}$ (m)
(SA)	8.4	
(SB)	Negative	Negative
(SC)	2.3	428
(SD)	2.1	23661

significantly different. Consequently, a stochastic model with two unknown variance components turns out to be not significant. Caspary (1985) suggests, in case of negative VCE, the reduction of the number of unknown variance-covariance components. In this work we explore, as an alternative, the possibilities of different stochastic models.

The variance component estimates in models (SC) and (SD) are positive, being the SNR values significantly different.

The receiver coordinates evaluated with the models (SA), (SC), (SD) were compared to very accurate values derived from phase measurements and by linking the GPS position to the IGS (International-GPS-Service-Geodynamics) network. Results of the estimated GPS coordinates are reported in Table 3.

Table 3. Estimated coordinate differences with the selected stochastic models, $r = 20$. Δs is the root sum squared (RSS) of the errors ΔX, ΔY, ΔZ.

Stochastic model	ΔX (m)	ΔY (m)	ΔZ (m)	Δs (m)
(SA)	6.9	−4.8	6.3	10.5
(SC)	−4.2	2.1	3.0	5.6
(SD)	2.8	3.4	−2.1	4.9

Models (SC) and (SD) improve the accuracy of the estimated coordinates with respect to model (SA). As can be deduced from Table 3, model (SD) best describes the pseudorange stochastic errors.

Results show that a suitable stochastic improves significantly the estimation accuracy, and the BIQUE methodology allows us to evaluate the adequacy of a selected model.

A fundamental hypothesis for effective application of VCE with BIQUE techniques is the absence of blunders in the observations. Gross measurement errors could cause the estimation of too great values of the variances, impairing the efficacy of the procedure and of the subsequent LS adjustment. A preliminary detection test of outliers with reasonable values of the variance factors (based on the experience of the experimenters) should therefore be performed in advance.

4 Conclusions

In this work we have performed VCE within the framework of the condition functional model, showing the BIQUE estimation equations (Appendix A) and generalizing the obtained results to all the functional models (Appendix B). As an example of the BIQUE methodology, we applied our theoretical results to GPS pseudorange measurements, using the linear Gauss-Markov functional model and testing four different stochastic models of the observations. The SNR flag retrieved from the RINEX files of GPS pseudorange measurement turned out to be effective in reducing the GPS position errors, by using models (SC) and (SD), with SNR and SNR squared respectively. Comparing the results obtained with two different redundancy values (r respectively equal to 20 and 28), we point out that large redundancies are necessary for good estimates, but no significant differences in the results have been noted when using slightly different (high) values of r. In both measurement campaigns, however, stochastic model (SB) turned out to be inadequate, providing negative values of the variance and covariance components, even with high redundancy values. This allowed us to reject model (SB).

It is worth stressing that Eq. (2.3) of our BIQUE technique does not require the evaluation of the least-squares residuals. Consequently, no cumbersome LS adjustments are necessary during each iteration, and the BIQUE methodology can be performed in pre-adjustment. This significantly reduces the computational effort, implying that the iterative BIQUE methodologies could easily be implemented in real-time data processing.

Furthermore, the BIQUE technique does not impose any constraint on the variance components, not forcing them to be positive. This could lead, in case of inadequate or erroneous stochastic modeling and/or observation groups with low redundancy, to negative values of the estimated variance components. The anomalous behavior of the BIQUE estimation turns out to be an advantage, rather than a weakness, because a VCE procedure with negative variances implies a bad choice of the stochastic model. BIQUE methodologies play therefore a significant role, allowing us to gain insight into the assessment of the goodness of the selected stochastic models.

5 Appendix A – BIQUE Estimation in Condition Functional Model

The condition (functional) adjustment model is the system of $r < n$ condition equations:

$$\mathbf{A}\mathbf{v} = \mathbf{w} = \mathbf{d} - \mathbf{A}\boldsymbol{l} \tag{A.1}$$

where $\mathbf{A}$ is a known (r, n) design matrix with $\text{rank}(\mathbf{A}) = r < n$, $\mathbf{v}$ is the $(n, 1)$ vector of the n observation errors, $\mathbf{w}$ is the $(r, 1)$ random normal misclosure vector which is determined by the observations, $\boldsymbol{l}$ is the $(n, 1)$ random vector of the observations which we will assume normally distributed, $\mathbf{d}$ is the $(r, 1)$ deterministic vector.

As stochastic model, we consider the general linear model (1.1).

As it is well known, for the LS solution of the (A.1) the following relations hold:

$$\begin{aligned}\hat{\mathbf{v}} &= \boldsymbol{\Sigma}_l \mathbf{A}^{\mathrm{T}} \left(\mathbf{A}\boldsymbol{\Sigma}_l \mathbf{A}^{\mathrm{T}}\right)^{-1} \mathbf{w} = \mathbf{P}^{-1}\mathbf{A}^{\mathrm{T}} \left(\mathbf{A}\mathbf{P}^{-1}\mathbf{A}^{\mathrm{T}}\right)^{-1} \mathbf{w} \\ \mathbf{Q}_{\hat{\mathbf{v}}} &= \boldsymbol{\Sigma}_l \mathbf{A}^{\mathrm{T}} \left(\mathbf{A}\boldsymbol{\Sigma}_l \mathbf{A}^{\mathrm{T}}\right)^{-1} \mathbf{A}\boldsymbol{\Sigma}_l = \mathbf{P}^{-1}\mathbf{A}^{\mathrm{T}} \left(\mathbf{A}\mathbf{P}^{-1}\mathbf{A}^{\mathrm{T}}\right)^{-1} \mathbf{A}\mathbf{P}^{-1}\end{aligned} \tag{A.2}$$

where $\boldsymbol{\Sigma}_l$ and $\mathbf{P}$ are given by Eqs. (1.1) and (1.2) respectively, $\hat{\mathbf{v}}$ is the vector of least-squares residuals and $\mathbf{Q}_{\hat{\mathbf{v}}}$ is the corresponding cofactor (variance-covariance) matrix.

$$\mathbf{p}^{\mathrm{T}}\boldsymbol{\sigma} = \sum_{1}^{k} p_i \, \sigma_i \tag{A.3}$$

where p_i are known coefficients.

The estimation is performed through a quadratic form of the misclosure vector $\mathbf{w}$:

$$q_w = \mathbf{w}^{\mathrm{T}}\mathbf{B}\mathbf{w} = \mathbf{p}^{\mathrm{T}}\hat{\boldsymbol{\sigma}} \tag{A.4}$$

where $\mathbf{B}$ is an arbitrary symmetric (r, r) matrix.

The criterion of unbiasedness implies:

$$E(q_w) = E\left(\mathbf{w}^{\mathrm{T}}\mathbf{B}\mathbf{w}\right) = \mathbf{p}^{\mathrm{T}}\boldsymbol{\sigma} \tag{A.5}$$

In addition, the minimum-variance criterion implies:

$$var(q_w) = \sigma_{q_w}^2 = var\left(\mathbf{w}^{\mathrm{T}}\mathbf{B}\mathbf{w}\right) = min \tag{A.6}$$

We recall that if $\mathbf{x}$ is a $(n, 1)$ random vector with expectation $E(\mathbf{x}) = \mathbf{0}$ and covariance matrix $\boldsymbol{\Sigma} = E(\mathbf{x}\mathbf{x}^{\mathrm{T}})$, then for the expectation of the quadratic form $q = \mathbf{x}^{\mathrm{T}}\mathbf{B}\mathbf{x}$ we have (Caspary 1987; Sjöberg 1984):

$$E(q) = tr(\mathbf{B}\boldsymbol{\Sigma}). \tag{A.7}$$

where $tr(\,)$ denotes the trace of a square matrix; furthermore, if $\mathbf{x}$ is normally distributed, the variance of q is given by (Caspary 1987; Sjöberg 1984):

$$\sigma_q^2 = 2tr(\mathbf{B}\boldsymbol{\Sigma}\mathbf{B}\boldsymbol{\Sigma}) \tag{A.8}$$

The misclosure vector $\mathbf{w}$ has expectation zero (in absence of bias on the observations), hence the unbiasedness and minimum variance criteria imply:

$$\begin{aligned} tr(\mathbf{B}\boldsymbol{\Sigma}_{\mathbf{w}}) &= \mathbf{p}^{\mathrm{T}}\boldsymbol{\sigma} \\ tr(\mathbf{B}\boldsymbol{\Sigma}_{\mathbf{w}}\mathbf{B}\boldsymbol{\Sigma}_{\mathbf{w}}) &= min \end{aligned} \tag{A.9}$$

For $\boldsymbol{\Sigma}_{\mathbf{w}}$, the (r, r) covariance matrix of $\mathbf{w}$, using the error propagation law to (A.1) and inserting (1.1), we have:

$$\mathbf{\Sigma_w} = \mathbf{A}\sum\nolimits_{\mathbf{v}}\mathbf{A}^{\mathrm{T}} = \mathbf{A}\sum\nolimits_{l}\mathbf{A}^{\mathrm{T}} = \mathbf{A}\left(\sum\nolimits_{1}^{k}\sigma_i\mathbf{Q}_i\right)\mathbf{A}^{\mathrm{T}} = \sum\nolimits_{1}^{k}\sigma_i\mathbf{A}\mathbf{Q}_i\mathbf{A}^{\mathrm{T}} = \sum\nolimits_{1}^{k}\sigma_i\tilde{\mathbf{Q}}_i \tag{A.10}$$

where:

$$\tilde{\mathbf{Q}}_i = \mathbf{A}\mathbf{Q}_i\mathbf{A}^{\mathrm{T}} \tag{A.11}$$

From the first of (A.9) and (A.10), we have:

$$tr(\mathbf{B}\Sigma_{\mathbf{w}}) = tr\left(\mathbf{B}\sum_{1}^{k}\sigma_i\widetilde{\mathbf{Q}}_i\right) = \sum_{1}^{\mathrm{k}}p_i\sigma_i \Leftrightarrow tr\left(\mathbf{B}\widetilde{\mathbf{Q}}_i\right) = p_i(i = 1, \ldots..k)$$

Consequently, for the unbiasedness and minimum variance criteria we obtain:

$$\begin{gathered} tr\left(\mathbf{B}\widetilde{\mathbf{Q}}_j\right) = p_j(j = 1, \ldots..k) \\ tr(\mathbf{B}\Sigma_{\mathbf{w}}\mathbf{B}\Sigma_{\mathbf{w}}) = min \end{gathered} \tag{A.12}$$

Hence the Lagrange function of the problem is expressed as:

$$L = tr(\mathbf{B}\Sigma_{\mathbf{w}}\mathbf{B}\Sigma_{\mathbf{w}}) - 2\sum_{1}^{k}\lambda_{\mathrm{j}}\left[tr\left(\mathbf{B}\widetilde{\mathbf{Q}}_j\right) - p_j\right] \tag{A.13}$$

where $\boldsymbol{\lambda} = (\lambda_1, \ldots..., \lambda_k)^{\mathrm{T}}$ is a k-vector of Lagrange multipliers. The solution is found by equating the partial derivatives of L with respect to $\mathbf{B}$ and $\boldsymbol{\lambda}$ to zero.

In order to do that, we recall that if $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are (n, n) matrices, the matrices of partial derivatives of the scalar functions $tr(\mathbf{AB})$ and $tr(\mathbf{ABAC})$ with respect to the elements of $\mathbf{A}$ are respectively (Caspary 1987):

$$\begin{gathered} \frac{\partial}{\partial\mathbf{A}}tr(\mathbf{AB}) = \mathbf{B}^{\mathrm{T}} \\ \frac{\partial}{\partial\mathbf{A}}tr(\mathbf{ABAC}) = (\mathbf{BAC} + \mathbf{CAB})^{\mathrm{T}} \end{gathered} \tag{A.14}$$

Because the matrices $\tilde{\mathbf{Q}}_i$ are symmetrical, the use of (A.14) yields:

$$\frac{\partial L}{\partial\mathbf{B}} = 2\mathbf{\Sigma_w}\mathbf{B}\mathbf{\Sigma_w} - 2\sum_{1}^{k}\lambda_{\mathrm{j}}\tilde{\mathbf{Q}}_j$$

and leads to the set of equations:

$$\begin{gathered} tr\left(\mathbf{B}\widetilde{\mathbf{Q}}_j\right) = p_j(j = 1, \ldots..k) \\ \mathbf{\Sigma_w}\mathbf{B}\mathbf{\Sigma_w} - \sum_{1}^{k}\lambda_{\mathrm{j}}\tilde{\mathbf{Q}}_j = 0 \end{gathered} \tag{A.15}$$

An auxiliary matrix $\mathbf{M}$ is introduced to solve Eqs. (A.15) for $\mathbf{B}$:

$$\mathbf{M} = \mathbf{N}^{-1} \tag{A.16}$$

with:

$$\mathbf{N} = \mathbf{\Sigma}_{\mathbf{w}} = \mathbf{A}\mathbf{\Sigma}_{i}\mathbf{A}^{\mathrm{T}} \tag{A.17}$$

and is selected to meet the conditions:

$$\mathbf{M}\mathbf{\Sigma}_{\mathbf{w}}\mathbf{B}\mathbf{\Sigma}_{\mathbf{w}}\mathbf{M} = \mathbf{N}^{-1}\mathbf{N}\mathbf{B}\mathbf{N}^{-1}\mathbf{N} = \mathbf{B}$$

Pre- and post-multiplication of the second equation of (A.15) with $\mathbf{M} = \mathbf{N}^{-1}$ yields:

$$\mathbf{B} = \sum\nolimits_{1}^{k} \lambda_{\mathrm{j}}\mathbf{N}^{-1}\tilde{\mathbf{Q}}_{j}\mathbf{N}^{-1} \tag{A.18}$$

Inserting (A.18) in the first of (A.15) we have:

$$tr\left(\mathbf{B}\tilde{\mathbf{Q}}_{i}\right) = \sum\nolimits_{i=1}^{k} \lambda_{\mathrm{j}} tr\left(\mathbf{N}^{-1}\tilde{\mathbf{Q}}_{i}\mathbf{N}^{-1}\tilde{\mathbf{Q}}_{j}\right) = p_{j}(j = 1, \ldots .k) \tag{A.19}$$

Let $\mathbf{H}$ be the (k, k) matrix composed of the elements:

$$h_{ij} = tr\left(\mathbf{N}^{-1}\tilde{\mathbf{Q}}_{i}\mathbf{N}^{-1}\tilde{\mathbf{Q}}_{j}\right)(i, j = 1, \ldots .k) \tag{A.20}$$

then Eq. (A.19) can be written in the concise form:

$$\mathbf{H}\lambda = \mathbf{p} \tag{A.21}$$

with the k-vectors $\boldsymbol{\lambda}$ and $\mathbf{p}$ defined as above.

Noting that the matrix $\mathbf{H}$ could turn out to be singular (i.e. non-full rank), a generalized solution of the (A.21) for $\boldsymbol{\lambda}$ requires the (Moore-Penrose) pseudoinverse $\mathbf{H}^{+}$ defined by:

$$\mathbf{H}\mathbf{H}^{+}\mathbf{H} = \mathbf{H}, \quad \mathbf{H}^{+}\mathbf{H}\mathbf{H}^{+} = \mathbf{H}^{+}, \quad (\mathbf{H}\mathbf{H}^{+})^{\mathrm{T}} = \mathbf{H}\mathbf{H}^{+}, \quad (\mathbf{H}^{+}\mathbf{H})^{\mathrm{T}} = \mathbf{H}^{+}\mathbf{H} \tag{A.22}$$

Therefore:

$$\boldsymbol{\lambda} = \mathbf{H}^{+}\mathbf{p} \Leftrightarrow \lambda_{i} = \mathbf{g}_{i}^{\mathrm{T}}\mathbf{p} = \mathbf{p}^{\mathrm{T}}\mathbf{g}_{i} \tag{A.23}$$

where $\mathbf{g}_{i}$ is the i–th column of the matrix $\mathbf{H}^{+}$. Substitution into Eq. (A.18) yields:

$$\mathbf{B} = \sum\nolimits_{1}^{k} \mathbf{p}^{\mathrm{T}}\mathbf{g}_{i}\mathbf{N}^{-1}\tilde{\mathbf{Q}}_{i}\mathbf{N}^{-1} \tag{A.24}$$

and results in the estimation for $\mathbf{p}^{\mathrm{T}}\boldsymbol{\sigma}$:

$$q_w = \mathbf{p}^{\mathrm{T}}\hat{\sigma} = \mathbf{w}^{\mathrm{T}}\mathbf{B}\mathbf{w} = \mathbf{w}^{\mathrm{T}}\sum\nolimits_1^k \mathbf{p}^{\mathrm{T}}\mathbf{g}_i\mathbf{N}^{-1}\tilde{\mathbf{Q}}_i\mathbf{N}^{-1}\mathbf{w} \tag{A.25}$$

Defining the k–vector $\mathbf{f}$ as:

$$\mathbf{f} = \left\{\mathrm{f}_i = \mathbf{w}^{\mathrm{T}}\mathbf{N}^{-1}\tilde{\mathbf{Q}}_i\mathbf{N}^{-1}\mathbf{w}\right\} \tag{A.26}$$

the Eq. (A.25) can be put in a more suitable form:

$$q_w = \mathbf{w}^{\mathrm{T}}\mathbf{B}\mathbf{w} = \sum\nolimits_1^k \mathbf{p}^{\mathrm{T}}\mathbf{g}_i\mathrm{f}_i = \mathbf{p}^{\mathrm{T}}\mathbf{H}^{+}\mathbf{f} = \mathbf{p}^{\mathrm{T}}\hat{\boldsymbol{\sigma}} \tag{A.27}$$

from which the final result is obtained as:

$$\hat{\sigma} = \mathbf{H}^{+}\mathbf{f} \tag{A.28}$$

Thus, the **locally** best invariant quadratic unbiased estimates $\hat{\sigma}_i^2$ and $\hat{\sigma}_{ij}$ of the variances and covariances are solutions of the system

$$\mathbf{H}\hat{\sigma} = \mathbf{f} \tag{A.29}$$

with:

$$\mathbf{N} = \mathbf{A}\boldsymbol{\Sigma}_l\mathbf{A}^{\mathrm{T}} \tag{A.30}$$

$$\tilde{\mathbf{Q}}_i = \mathbf{A}\mathbf{Q}_i\mathbf{A}^{\mathrm{T}} \tag{A.31}$$

$$\mathbf{H} = \left\{h_{ij} = tr\left(\mathbf{N}^{-1}\tilde{\mathbf{Q}}_i\mathbf{N}^{-1}\tilde{\mathbf{Q}}_j\right)\right\} \tag{A.32}$$

$$\mathbf{f} = \left\{\mathrm{f}_i = \mathbf{w}^{\mathrm{T}}\mathbf{N}^{-1}\tilde{\mathbf{Q}}_i\mathbf{N}^{-1}\mathbf{w}\right\} \tag{A.33}$$

We note that with the previous relations (A.29)–(A.33) the evaluation of the LS residuals is not required. Hence, with the functional model of condition only, the BIQUE VCE can be performed in pre-adjustment; furthermore, in this functional model there are no unknown parameters and a possible datum defect has no influence on the overall procedure.

It is worth noting that $\mathbf{N}$, defined in Eq. (A.30) and used in (A.32) and (A.33), contains the covariance matrix $\boldsymbol{\Sigma}_l$, i.e. the vector $\boldsymbol{\sigma}$. Therefore, it is mandatory to implement an iterative numerical approach, like the one depicted in Sect. 2.

A further observation concerns the Eqs. (A.1) of the functional model of condition only, which in some cases can be very difficult to write. Other functional models (with unknown parameters) turn out to be generally easier to formulate, and therefore are more frequently used. As a result, it is useful to elaborate a BIQUE VCE procedure which could be used in any functional model, given the stochastic model (1.1). This will be shown in Appendix B.

6 Appendix B – A Generalized Procedure for BIQUE VCE

In this section we show a generalization of the BIQUE procedure for all functional models. For this purpose, we introduce an (n, n) symmetric matrix $\mathbf{M}$:

$$\mathbf{M} = \mathbf{A}^{\mathrm{T}}\mathbf{N}^{-1}\mathbf{A} \tag{B.1}$$

As for the elements h_{ij}, inserting (A.30) into (A.31) and from (B.1), we have:

$$\begin{aligned} h_{ij} &= tr\left(\mathbf{N}^{-1}\tilde{\mathbf{Q}}_i\mathbf{N}^{-1}\tilde{\mathbf{Q}}_j\right) = tr\left(\mathbf{N}^{-1}\mathbf{A}\mathbf{Q}_i\mathbf{A}^{\mathrm{T}}\mathbf{N}^{-1}\mathbf{A}\mathbf{Q}_j\mathbf{A}^{\mathrm{T}}\right) \\ &= tr\left[\left(\mathbf{A}^{\mathrm{T}}\mathbf{N}^{-1}\mathbf{A}\right)\mathbf{Q}_i\left(\mathbf{A}^{\mathrm{T}}\mathbf{N}^{-1}\mathbf{A}\right)\mathbf{Q}_j\right] = tr\left(\mathbf{M}\mathbf{Q}_i\mathbf{M}\mathbf{Q}_j\right) \end{aligned} \tag{B.2}$$

and the elements f_i are expressed by using $\mathbf{w} = \mathbf{A}\hat{\mathbf{v}}$, inserting (A.30) into (A.32), and recalling (B.1):

$$\mathrm{f}_i = \mathbf{w}^{\mathrm{T}}\mathbf{N}^{-1}\tilde{\mathbf{Q}}_i\mathbf{N}^{-1}\mathbf{w} = \hat{\mathbf{v}}^{\mathrm{T}}(\mathbf{A}^{\mathrm{T}}\mathbf{N}^{-1}\mathbf{A})\mathbf{Q}_i\left(\mathbf{A}^{\mathrm{T}}\mathbf{N}^{-1}\mathbf{A}\right)\hat{\mathbf{v}} \tag{B.3}$$

Between the observation vector $\boldsymbol{l}$ and the least-squares residuals vector $\hat{\mathbf{v}}$ the following relation holds:

$$\hat{\mathbf{v}} = -\mathbf{R}\boldsymbol{l} \tag{B.4}$$

where the redundancy matrix $\mathbf{R}$ is equal to:

$$\mathbf{R} = \mathbf{Q}_{\hat{\mathbf{v}}}\mathbf{P} = \boldsymbol{\Sigma}_{\boldsymbol{l}}\mathbf{A}^{\mathrm{T}}\mathbf{N}^{-1}\mathbf{A} \tag{B.5}$$

and is idempotent, with:

$$rank(\mathbf{R}) = tr(\mathbf{R}) = r \tag{B.6}$$

From (B.1), (B.4), (B.5) and (A.29) we easily deduce the relations:

$$\mathbf{M}\hat{\mathbf{v}} = \mathbf{P}\hat{\mathbf{v}} = -\mathbf{M}\boldsymbol{l} \tag{B.7}$$

which, introduced into (B.3), yield

$$\mathrm{f}_i = \boldsymbol{l}^{\mathrm{T}}\mathbf{M}\mathbf{Q}_i\mathbf{M}\boldsymbol{l} = \hat{\mathbf{v}}^{\mathrm{T}}\mathbf{M}\mathbf{Q}_i\mathbf{M}\hat{\mathbf{v}} = \hat{\mathbf{v}}^{\mathrm{T}}\mathbf{P}\mathbf{Q}_i\mathbf{P}\hat{\mathbf{v}} \tag{B.8}$$

From (A.29) and the second of (A.2) we note that the matrix $\mathbf{M}$ (B.1) can be arranged in the compact general form:

$$\mathbf{M} = \mathbf{P}\mathbf{Q}_{\hat{\mathbf{v}}}\mathbf{P} \tag{B.9}$$

and it can be fully characterized by inserting the expression of $\mathbf{Q}_{\hat{\mathbf{v}}}$ related to the chosen functional model.

Therefore, assuming the linear stochastic model (1.1), the generalized BIQUE VCE consists in solving iteratively the system:

$$\mathbf{H}\hat{\boldsymbol{\sigma}} = \mathbf{f} \tag{B.10}$$

where:

$$\mathbf{H} = \left\{h_{ij} = tr\left(\mathbf{M}\mathbf{Q}_i\mathbf{M}\mathbf{Q}_j\right)\right\} \tag{B.11}$$

$$\mathbf{f} = \left\{\mathrm{f}_i = \boldsymbol{l}^{\mathrm{T}}\mathbf{M}\mathbf{Q}_i\mathbf{M}\boldsymbol{l} = \hat{\mathbf{v}}^{\mathrm{T}}\mathbf{M}\mathbf{Q}_i\mathbf{M}\hat{\mathbf{v}} = \hat{\mathbf{v}}^{\mathrm{T}}\mathbf{P}\mathbf{Q}_i\mathbf{P}\hat{\mathbf{v}}\right\} \tag{B.12}$$

$$\mathbf{M} = \mathbf{P}\mathbf{Q}_{\hat{\mathbf{v}}}\mathbf{P} \tag{B.13}$$

It is easy to verify that the formulas of the h_{ij} and f_i provided by other authors (Koch 1986; Ou 1989; Rao 1973; Sjöberg 1983; Yu 1992) are particular cases of the generalized expressions (B.10)–(B.13).

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