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ON THE RELIABILITY OF MIXED LS ADJUSTMENT MODELS

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Abstract. This paper examines the internal and external reliability criteria of the mixed LS adjustment model. We use the reliability concept to quantify the potential for detecting gross errors and to estimate their impact on the adjusted parameters. After a short introduction to the mixed adjustment model, the hat matrix and Baarda's data snooping we describe the theoretical tools developed to define the internal and external reliability in the mixed adjustment model. The paper presents the results of an example of LS adjustment of transformation parameters between two coordinate systems, indicating that the reliability can be used effectively for this model.

Keywords: least squares, reliability criteria, hat matrix, outlier detection.

Introduction

There are three main standard models of least squares (LS) adjustment: observation equation, condition equation, and mixed model. When the observations are explicitly related to the parameters, we can create observation equations in a way that $L^a = F(x^a)$, while L^a is a vector of n adjusted observations and x^a is a vector of u adjusted parameters. When there are no parameters at all–only conditions between the observations–we can create condition equations in such a way that $F(L^a) = 0$. In a mixed adjustment model, both parameters x^a and observations L^a are involved implicitly in a mixed adjustment model equation, as $F(x^a, L^a) = 0$. The observation equation model is also known as the Gauss-Markov Model (GMM) and the mixed adjustment model is known as the Gauss-Helmert Model (GHM). The GHM may be regarded as a general model, and the other two models can be derived from it as special cases (Leick, 2004). It is not forgotten that there are other LS models. For example, the observation equation model and the mixed model can be extended by adding constrains. Total least squares (TLS) model is also an alternative, although this kind of adjustment model can be described as an ordinary least squares solution (e.g., Neitzel, 2010). More than that, it is known that the observation equation model and the mixed model can be solved as a condition equation model (e.g., Mikhail & Ackermann, 1976). Nevertheless, the above three models are widely used in geodetic and surveying applications, and they will be at the focus of this study.

Measurements are the basis for the LS adjustment process. When measurements are made, for any reason, one or more measurements may contain a gross error. In the process of LS adjustment, a measurement with a gross error must be detected and eliminated from the data to prevent it from distorting the estimation of the adjustment parameters (Koch, 1999). There are two main approaches to detecting gross errors: statistical hypothesis testing and robust methods. Baarda (1968), in his pioneer work, created the basis for outlier detection by statistical tests and by introducing the data snooping method. Pope (1976), Heck (1981), Koch (1985), and others based their outlier detection methodologies on statistical tests as well. Krarup et al. (1980), Huber (1981), and others developed robust methods for gross error detection based on iterative reweighting of observations. In both, the LS adjustment plays an important role.

Reliability refers to the ability of an adjustment system to detect gross errors (blunders) and to estimate the effects that undetected errors may have on the adjusted solution. The reliability of a system is considered high when the system can identify even small blunders. Following Baarda's (1968) research, reliability theory has been extensively studied in geodesy and adjustment computations (e.g., Teunissen, 1985, 1998; Even-Tzur, 1999; Leick, 2004). The theory of Baarda's reliability assumes the presence of a

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single gross error in the data and is based on a hypothesis test theory, which decides between the null and a unique alternative hypothesis. Knight et al. (2010) extended the reliability theory in GMM for the case of multiple blunders. Hypothesis tests with multiple alternative hypotheses have been intensively studied recently (e.g., Yang et al., 2013, 2017; Teunissen, 2018). An overview of the latest advances in the reliability theory for geodesy is presented in Rofatto et al. (2020).

The studies have mainly focused on LS adjustment based on the observation equation model (GMM) and its extensively reviewed in the geodetic literature. Recently there are efforts to expand the reliability concept also to GHM. Koch (2014) uses the expectation maximization (EM) algorithm to detect outliers in GHM. Wang et al. (2020) applied Baarda's data snooping algorithm for the equality constrained, nonlinear GHM while using sensitivity analysis. Some aspects of minimum detectable bias (MDB) and statistical tests to identify outliers for the GHM are presented in Ettlinger and Neuner (2020).

In the current study, we restrict ourselves to the original Baarda concept of reliability and make a modest contribution to the study of reliability. This study examines the reliability criteria in the mixed LS adjustment model, deriving from it the criteria for the condition equation and observation equation models.

1. Mixed adjustment model

The mathematical model of the mixed adjustment model (e.g., Mikhail & Ackermann, 1976) is given by

$$F(\mathrm{x}^a, \mathrm{L}^a) = 0. \tag{1}$$

We denote the number of equations in Eq. (1) by r.

Let us define x^0 as a vector of approximate values of the parameters. Therefore, the vector of parameter corrections x is $\mathrm{x} = \mathrm{x}^a - \mathrm{x}^0$. Let us define L^b as a vector of measurements, then the vector of residuals v is defined as $\mathrm{v} = \mathrm{L}^a - \mathrm{L}^b$. The mathematical model of mixed adjustment can be written as

$$F(\mathrm{x}^0 + \mathrm{x}, \mathrm{L}^b + \mathrm{v}) = 0. \tag{2}$$

When the mathematical model is nonlinear, we define as a vector of approximate values of the measurements and the linearization of Eq. (1) is done around x^0 and L^0, while the ultimate solution is achieved by performing iterations (Pope, 1972). The linearization gives the fundamental form of condition equations for the adjustment of observations and parameters as

$$\mathrm{Bv} + \mathrm{Ax} + \mathrm{w} = 0, \tag{3}$$

where the design matrix A is $(r \times u)$, the observation matrix B is $(r \times n)$, and the misclosure vector w is $(r \times 1)$, which is equal to $\mathrm{w} = F(\mathrm{x}^0, \mathrm{L}^0) + \mathrm{B}(\mathrm{L}^b - \mathrm{L}^0)$ (e.g., Koch, 2014). The LS estimate of parameters is based on the minimization of the function $\mathrm{v}^T\mathrm{Pv}$ where P is the weight matrix of the measurements. When we perform iterations in the solution process, we set for the first iteration that L^0 is equal to L^b and therefore the well-known solution of x and v (e.g., Mikhail & Ackermann, 1976; Leick, 2004) is

$$\mathrm{x} = -(\mathrm{A}^T\mathrm{M}^{-1}\mathrm{A})^{-1}\mathrm{A}^T\mathrm{M}^{-1}\mathrm{w} = -\mathrm{N}^{-1}\mathrm{A}^T\mathrm{M}^{-1}\mathrm{w}; \tag{4}$$

$$\mathrm{v} = -\mathrm{P}^{-1}\mathrm{B}^T\mathrm{M}^{-1}(\mathrm{Ax} + \mathrm{w}), \tag{5}$$

with the covariance matrices

$$\Sigma_x = \sigma_0^2\mathrm{N}^{-1}; \tag{6}$$

$$\Sigma_v = \sigma_0^2\mathrm{P}^{-1}\mathrm{B}^T\mathrm{M}^{-1}(\mathrm{M} - \mathrm{AN}^{-1}\mathrm{A}^T)\mathrm{M}^{-1}\mathrm{BP}^{-1}, \tag{7}$$

while σ_0^2 is the variance of unit weight, $\mathrm{M} = \mathrm{BP}^{-1}\mathrm{B}^T$, and $\mathrm{N} = \mathrm{A}^T\mathrm{M}^{-1}\mathrm{A}$.

2. Hat matrix

The "hat matrix", H, is the matrix that converts values from the observed variable into estimations obtained with the LS method. The square matrix H is called the hat matrix as it puts a hat on L.

In a mixed adjustment model, the hat matrix defined by H_{AB} is

$$\begin{aligned}\hat{\mathrm{L}} &\equiv \mathrm{L}^a = \mathrm{L}^b + \mathrm{v} = \\ &\left[\mathrm{I} + \mathrm{P}^{-1}\mathrm{B}^T\mathrm{M}^{-1}\mathrm{A}(\mathrm{A}^T\mathrm{M}^{-1}\mathrm{A})^{-1}\mathrm{A}^T\mathrm{M}^{-1}\mathrm{B} - \mathrm{P}^{-1}\mathrm{B}^T\mathrm{M}^{-1}B\right]\mathrm{L}^b = \\ &\mathrm{H}_{AB}\mathrm{L}^b.\end{aligned} \tag{8}$$

The square matrix H_{AB} is $(n \times n)$, and H_{AB} is idempotent. The eigenvalues of an idempotent matrix are either 0 or 1 and the number of nonzero eigenvalues is equal to the rank of the matrix. The trace of an idempotent matrix equals the rank of the matrix. It is easy to notice that the trace of H_{AB} equals to $n + u - r$, therefore it has $n + u - r$ eigenvalues equal to 1 and the remaining ones are 0. Matrix H_{AB} is not symmetrical except when the weight matrix P equals the unit matrix; P = I.

LS adjustment with weight matrix P, which in general does not have to be diagonal, can be presented as an adjustment without weights by normalization of matrices A, B and L. The additional significance of the normalization process is that it allows us to take into account correlations between the measurements. Thus, Eq. (8) can be normalized by pre-multiplying matrix B by $\sqrt{\mathrm{P}^{-1}}$ as $\overline{\mathrm{B}} = \mathrm{B}\sqrt{\mathrm{P}^{-1}}$, and the vector L by $\sqrt{\mathrm{P}}$ as $\overline{\mathrm{L}}^b = \sqrt{\mathrm{P}}\,\mathrm{L}^b$. Since $\mathrm{M} = \overline{\mathrm{B}}\,\overline{\mathrm{B}}^T$ and matrix A remains unchanged, we get the normalized form of Eq. (8):

$$\begin{aligned}\hat{\overline{\mathrm{L}}} &= \left[\mathrm{I} - \overline{\mathrm{B}}^T\mathrm{M}^{-1}\overline{\mathrm{B}} + \overline{\mathrm{B}}^T\mathrm{M}^{-1}\mathrm{A}(\mathrm{A}^T\mathrm{M}^{-1}\mathrm{A})^{-1}\mathrm{A}^T\mathrm{M}^{-1}\overline{\mathrm{B}}\right]\overline{\mathrm{L}}^b = \\ &\overline{\mathrm{H}}_{AB}\overline{\mathrm{L}}^b.\end{aligned} \tag{9}$$

The normalized hat matrix $\overline{H}_{AB}$ is idempotent and symmetric and is called a projector. Let $\overline{h}_i$ be the *i*-th diagonal element of $\overline{H}_{AB}$. For a projector, the sum of the squares of the entries of each row is equal to the row diagonal entry: $\sum_k \overline{h}_{ik}^2 = \overline{h}_i$ (it is obtained only when the hat matrix is symmetric). The diagonal elements of matrix $\overline{H}_{AB}$ fulfill the inequality $0 \le \overline{h}_i \le 1$ (Hoaglin & Welsch, 1978).

The special cases of the hat matrix for the condition model and observation models can be obtained from Eq. (8). Putting A = 0 in Eq. (8), we get the hat matrix, H_B, which relates to the condition equation model

$$H_B = I - P^{-1}B^T M^{-1} B. \tag{10}$$

When B = –I and therefore M = P^{-1}, we get the well-known hat matrix H_A, which relates to the observation equation model

$$H_A = A(A^T PA)^{-1} A^T P. \tag{11}$$

Both H_A and H_B are not symmetrical matrices. Using the normalized form ensures their symmetricity. The normalized form can be obtained as above by using Eq. (9). For the condition equation model, we get

$$\overline{H}_B = I - \overline{B}^T M^{-1} \overline{B} \tag{12}$$

and for the observation equation model we get

$$\overline{H}_A = \sqrt{P} A(A^T PA)^{-1} A^T \sqrt{P} = \overline{A}(\overline{A}^T \overline{A})^{-1} \overline{A}^T. \tag{13}$$

Sometimes, a specific adjustment problem can be performed by observation model or a condition equation model. It is obvious in such a case that H_A must be equal to H_B. Let us multiply H_A and H_B by B on the left and we get

$$BA(A^T PA)^{-1} A^T P = B(I - P^{-1} B^T M^{-1} B). \tag{14}$$

Since BA = 0 (e.g., Mikhail & Ackermann, 1976) and $M = BP^{-1}B^T$, we can easily see that both sides of Eq. (14) are equal to zero; therefore $H_A = H_B$.

3. Baarda's data snooping for outlier identification in a mixed adjustment model

Data snooping is a method based on hypothesis testing for identification of a single outlier in LS adjustment, and it serves as a basis for understanding and developing tools in determining reliability. Data snooping is a very useful method for gross error identification and is routinely used in adjustment computations. Although data snooping was introduced as a testing procedure for use in geodetic networks, it is a generally applicable method (Lehmann, 2012). The *w* test introduced by Baarda (1968) plays a major role in the data snooping algorithm.

Let us define $\hat{d}_i$ as the difference between observed (ℓ_i) and calculated ($\hat{\ell}_i^c$) values, such that $\hat{d}_i = \hat{\ell}_i^c - \ell_i$ with standard error $\sigma_{\hat{d}_i}$. The *i*-th observed quantity is denoted as $\hat{\ell}_i^c$ of *n* observations ℓ that are computed from the parameters following from the adjustment of all observations except ℓ_i. We defined the test statistic k_i for uncorrelated measurements as

$$k_i = \frac{\hat{d}_i}{\sigma_{\hat{d}_i}}. \tag{15}$$

If $k_i \ge \sqrt{F(\alpha,1,\infty)}$, we reject the null hypothesis (H_0), which says that the measurement does not contain a gross error, and accept the alternative hypothesis (H_1) that says the measurement contains a gross error with α level of significance.

Since we are dealing with gross errors, it can be assumed that their size is relatively large in relation to the linearization errors. Thus, we can concentrate on the solution of the first iteration only. Therefore, if outliers are not present in the measurements, the misclosure vector w is equal to

$$w = F(L^b, x^0) = BL^b + Ax^0. \tag{16}$$

If the measurements contain gross errors, the physical relationship between the parameters and the observations is

$$w' + Bv + Ax = 0. \tag{17}$$

Whereas if the *i*-th observation included a gross error Δ_{ℓ_i} then the misclosure vector w' is equal to

$$w' = F(L^b + e_i \Delta_{\ell_i}, x^0) = B(L^b + e_i \Delta_{\ell_i}) + Ax^0 = w + Be_i \Delta_{\ell_i}, \tag{18}$$

where e_i is a unit vector with 1 at the *i*-th entry specifying which measurement is disturbed by Δ_{ℓ_i}. Since the LS estimates are unbiased, taking the expectation of $\hat{d}_i$ gives $E(\hat{d}_i) = \tilde{d}_i = \Delta_{\ell_i}$ (Cross, 1983) where $\tilde{d}_i$ is the true value of d_i; therefore, $w' = w + Be_i\tilde{d}_i$.

The linearization of Eq. (1) is now

$$Bv + Ax + w + Be_i\tilde{d}_i = 0. \tag{19}$$

The LS estimates of x, v, and $\tilde{d}_i$ which are defined as $\hat{x}$, $\hat{v}$, and $\hat{d}_i$ are obtained by applying Lagrange's method (e.g., Cross, 1983). By minimizing the function

$$\Phi = v^T Pv + 2\lambda^T (Bv + Ax + w + Be_i\tilde{d}_i) \Rightarrow \min \tag{20}$$

we can get the LS estimates in addition to the Lagrangian multipliers, $\hat{\lambda}$. Thus, we have

$$\frac{\partial \Phi}{\partial \hat{v}} = 2\hat{v}^T P + 2\hat{\lambda}^T B = 0 \;\Rightarrow\; P\hat{v} + B^T \hat{\lambda} = 0; \tag{21}$$

$$\frac{\partial \Phi}{\partial x} = 2\hat{\lambda}^T A = 0 \;\Rightarrow\; A^T \hat{\lambda} = 0; \tag{22}$$

$$\frac{\partial\Phi}{\partial\lambda} = 2(\hat{v}^T B^T \hat{x}^T A^T + w^T + \hat{d}_i^T e_i^T B^T) = 0 \Rightarrow$$

$$B\hat{v} + A\hat{x} + w + Be_i\hat{d}_i = 0, \tag{23}$$

$$\frac{\partial\Phi}{\partial\tilde{d}_i} = 2\hat{\lambda}^T Be_i = 0 \Rightarrow e_i^T B^T \hat{\lambda} = 0. \tag{24}$$

From Eq. (21) we can get

$$\hat{v} = -P^{-1} B^T \hat{\lambda}. \tag{25}$$

Substituting Eq. (25) in Eq. (23) gives

$$\hat{\lambda} = M^{-1}(A\hat{x} + w + Be_i\hat{d}_i). \tag{26}$$

Substituting Eq. (26) in Eq. (22) gives

$$\hat{x} = -N^{-1} A^T M^{-1}(w + Be_i\hat{d}_i). \tag{27}$$

Substituting Eq. (26) and Eq. (27) in Eq. (24) gives (after some manipulations)

$$(e_i^T B^T M^{-1} Be_i - e_i^T B^T M^{-1} AN^{-1} A^T M^{-1} Be_i)\hat{d}_i =$$
$$(e_i^T B^T M^{-1} AN^{-1} A^T M^{-1} - e_i^T B^T M^{-1})w. \tag{28}$$

Since

$$P(I - H_{AB}) = B^T M^{-1} B - B^T M^{-1} AN^{-1} A^T M^{-1} B, \tag{29}$$

using Eq. (4) and Eq. (5) we can rewrite Eq. (28) as

$$e_i^T P(I - H_{AB})e_i\hat{d}_i = e_i^T P\hat{v}. \tag{30}$$

Therefore

$$\hat{d}_i = (e_i^T P(I - H_{AB})e_i)^{-1} e_i^T Pv =$$
$$\frac{e_i^T Pv}{e_i^T P(I - H_{AB})e_i}. \tag{31}$$

The covariance matrix of v, Σ_v, can be presented by H_{AB} as

$$\Sigma_v = \sigma_0^2(I - H_{AB})P^{-1}. \tag{32}$$

Therefore, applying the propagation of error law gives

$$\sigma_{\hat{d}_i}^2 = (e_i^T P(I - H_{AB})e_i)^{-1} e_i^T P\Sigma_v Pe_i (e_i^T P(I - H_{AB})e_i)^{-1} =$$
$$\sigma_0^2(e_i^T P(I - H_{AB})e_i)^{-1} e_i^T P(I - H_{AB})\cancel{P}^{-1}\cancel{P}e_i (e_i^T P(I - H_{AB})e_i)^{-1} =$$
$$\sigma_0^2(e_i^T P(I - H_{AB})e_i)^{-1} = \sigma_0^2 / (e_i^T P(I - H_{AB})e_i). \tag{33}$$

In the normalized form we get

$$\hat{\bar{d}}_i = \frac{e_i^T\hat{\bar{v}}}{e_i^T(I - \bar{H}_{AB})e_i} = \frac{\hat{\bar{v}}_i}{1 - \bar{h}_i}. \tag{34}$$

and

$$\sigma_{\hat{\bar{d}}_i}^2 = \sigma_0^2 / (e_i^T(I - \bar{H}_{AB})e_i) = \frac{\sigma_0^2}{1 - \bar{h}_i}. \tag{35}$$

Since $\sigma_{\bar{v}_i} = \sigma_0\sqrt{(1 - \bar{h}_i)}$ we get $\sigma_0 = \sigma_{\bar{v}_i} / \sqrt{1 - \bar{h}_i}$; therefore,

$$\sigma_{\hat{\bar{d}}_i} = \frac{\sigma_{\bar{v}_i}}{\sqrt{1 - \bar{h}_i}\sqrt{1 - \bar{h}_i}} = \frac{\sigma_{\bar{v}_i}}{1 - \bar{h}_i}. \tag{36}$$

We see that $\sigma_{\hat{\bar{d}}_i}$ can be presented as a function of $\bar{h}_i$.

The test statistic w_i as presented in Eq. (15) can be rewritten as

$$k_i = \frac{\hat{\bar{d}}_i}{\sigma_{\hat{\bar{d}}_i}} = \frac{\hat{\bar{v}}_i}{1 - \bar{h}_i} / \frac{\sigma_{\bar{v}_i}}{1 - \bar{h}_i} = \frac{\hat{\bar{v}}_i}{\sigma_{\bar{v}_i}}. \tag{37}$$

This means that in the mixed adjustment model, the statistic w_i is the ratio of a LS residual to its standard error.

Placing $A = 0$ into Eq. (19) gives the condition model, and applying Lagrange's method leads to the same result, $k_i = \hat{\bar{v}}_i / \sigma_{\bar{v}}$. As might be expected, in the mixed adjustment model and the condition model we get the same ratio as in the observation model for the statistic k_i (Cross, 1983). The use of the normalized form allowed us to present the test statistic k_i even in cases of a non-diagonal weight matrix.

The data snooping method can be applied in the mixed adjustment model and condition model in a similar way as it is applied in the well-known observation model. Since data snooping allows detection of a single outlier, it can be applied in iterative mode (Teunissen, 2006).

4. Reliability concept in mixed adjustment model

Reliability is defined as the ability of an adjustment system to sense and identify gross errors in the measurements. Baarda (1968) distinguishes between internal reliability and external reliability. The internal reliability of a system "measures" the marginal undetectable gross errors in the measurements, while the external reliability "measures" the effect of undetected errors on the adjustment parameters and on quantities computed from them.

4.1. Internal reliability

If the observations are without gross errors, Baarda demonstrated that w_i is normally distributed with zero mean and unit variance. In the case of a gross error in observation i, the mean of the normal distribution is

$$\delta_i = \frac{\Delta_{\ell_i}}{\sigma_{\hat{d}_i}}. \tag{38}$$

We define the upper bound of δ_i as δ_i^u with probability levels α and β (α being the level of significance and β being the test power). Therefore, the maximum size of a gross error that could contaminate the i-th observation is

$$\Delta_i^u = \delta_i^u \sigma_{\hat{d}_i}. \tag{39}$$

As we see from Eq. (35), $\sigma_{\hat{d}_i}$ can be presented as a function of $\bar{h}_i$. Therefore, the maximum size of a gross error that could contaminate the *i*-th observation is

$$\Delta_i^u = \delta_i^u \sigma_0 \Big/ \sqrt{1-\bar{h}_i} \,. \tag{40}$$

Since σ_0 is not a random variable for a particular adjustment and δ_i^u is a constant that depends on α and β, the expression $1\Big/\sqrt{1-\bar{h}_i}$ is an index for internal reliability. As it decreases, the reliability increases and the ability of the adjustment system to identify outliers improves. Hence, the diagonal elements of $\bar{H}_{AB}$ serve as a primary tool in internal reliability analysis in the mixed adjustment model. It is obvious that the same is valid for matrixes $\bar{H}_A$ and $\bar{H}_B$, which can serve as a tool in internal reliability analysis in the observation equation model and in the condition equation model, respectively.

From Eq. (34) we have

$$\frac{\hat{\bar{v}}_i}{1-\bar{h}_i} = \hat{\bar{\ell}}_i^c - \bar{\ell}_i \,, \tag{41}$$

and since $\hat{\bar{v}}_i = \hat{\bar{\ell}}_i - \bar{\ell}_i$ we can get

$$\hat{\bar{\ell}}_i = (1-\bar{h}_i)\hat{\bar{\ell}}_i^c + \bar{h}_i \bar{\ell}_i \,. \tag{42}$$

The estimate of the adjusted measurement is a linear combination of the computed value and the observed value, with weights $1-\bar{h}_i$ and $\bar{h}_i$, respectively. If $\bar{h}_i = 0.5$ the influences of the calculated and observed values on the adjusted measurement are equal. For decreasing $\bar{h}_i$, the influence of the calculated value $\hat{\bar{\ell}}_i^c$ increases. In that case, the ability of the adjustment system to examine the measurement against gross error increases. Therefore, we should aim that the diagonal entries $\bar{h}_i$ be at least less than 0.5. Huber (1981), in his reference to the observation model, suggests that the size of $\bar{h}_i$ should be of the order of 0.2 to prevent the strong influence of a measurement on the evaluate solution. Let us define $\bar{h}_{max}$ as the maximum value of $\bar{h}_i$, then

$$\bar{h}_{max} = \max(\bar{h}_i) \geq \text{ave}(\bar{h}_i) = \frac{\text{tr}(\bar{H}_{AB})}{n} = \frac{n-r+u}{n} \,. \tag{43}$$

For the condition model $\text{tr}(\bar{H}_B) = n-r$; therefore, $\bar{h}_{max} \geq (n-r)/n$. For the observation model $\text{tr}(\bar{H}_A) = u$; therefore, $\bar{h}_{max} \geq u/n$. These expressions can give us a perspective on the expected diagonal values in any adjustment problem. Furthermore, $\bar{h}_i$ converges to zero if the ratio $(n-r+u)/n$ converges to zero in the mixed adjustment model. If we decrease the level of $\bar{h}_i$ we should increase the number of the measurements and the number of conditions or decrease the number of parameters.

4.2. External reliability

External reliability measures the influence of an undetected gross error on the estimation of parameters. Let an error in observation *i* be denoted as Δ_i^u and $\Delta_{\ell_i} = \begin{pmatrix} 0 & 0 & . & . & \Delta_i^u & . & . & 0 \end{pmatrix}^T$. For the undetected Δ_{ℓ_i} we compute the changes $\Delta\hat{X}_i$ of the adjusted parameters:

$$\Delta\hat{X}_i = -N^{-1}A^T M^{-1} B \Delta_{\ell_i} \,. \tag{44}$$

According to Baarda (1968) the global external reliability denotes the impact of a single outlier on the adjusted parameters, measured by

$$\lambda^2_{\Delta\hat{x}_i} = (\Delta\hat{X}_i)^T \Sigma_x^{-1} (\Delta\hat{X}_i) = \frac{1}{\sigma_0^2} (\Delta\hat{X}_i)^T N (\Delta\hat{X}_i) \,. \tag{45}$$

If we substitute Eq. (44) into Eq. (45) and consider that $\Delta_{\ell_i} = e_i \Delta_i^u$ we get

$$\lambda^2_{\Delta\hat{x}_i} = \frac{1}{\sigma_0^2} \Delta_{\ell_i}^T B^T M^{-1} A N^{-1} A^T M^{-1} B \Delta_{\ell_i} =$$

$$\frac{1}{\sigma_0^2} (\Delta_i^u)^2 e_i^T B^T M^{-1} A N^{-1} A^T M^{-1} B e_i \,. \tag{46}$$

Eq. (46) can assist us to specify the impact of a single blunder on the adjusted parameters.

Since $\Delta_i^u = \delta_i^u \sigma_0 \Big/ \sqrt{1-\bar{h}_i}$ as we get in Eq. (40), the normalized form of Eq. (46) is

$$\bar{\lambda}^2_{\Delta\hat{x}_i} = (\delta_i^u)^2 \frac{e_i^T \bar{B}^T M^{-1} A N^{-1} A^T M^{-1} \bar{B} e_i}{1-\bar{h}_i} \,. \tag{47}$$

The factor that multiplies $(\delta_i^u)^2$ defines the external reliability of the *i*-th measurement.

The smaller the factor, the greater the external reliability since the influence of the undetected gross error on the adjusted parameters decreases.

As $B = -I$ therefore $\bar{B} = \sqrt{P^{-1}}$ and $M^{-1} = P$ so we get Baarda's global external reliability, which relates to the observation equation model

$$\bar{\lambda}^2_{\Delta\hat{x}_i} = \frac{(\delta_i^u)^2}{1-\bar{h}_i} e_i^T \sqrt{P^{-1}}\, P A N^{-1} A^T P \sqrt{P^{-1}}\, e_i =$$

$$\frac{(\delta_i^u)^2}{1-\bar{h}_i} e_i^T \sqrt{P}\, A N^{-1} A^T \sqrt{P}\, e_i =$$

$$\frac{(\delta_i^u)^2}{1-\bar{h}_i} e_i^T \bar{H}_A e_i = (\delta_i^u)^2 \frac{\bar{h}_i}{1-\bar{h}_i} \,. \tag{48}$$

The result of the special case for an observation model as we get from the general case of a mixed adjustment model is expected. As presented by Even-Tzur (1999) both the internal and the external reliability are determined by $\bar{h}_i$, the *i*-th diagonal element of $\bar{H}_A$, for observation model. We can see that if $\bar{h}_i < 0.5$, the term $\bar{h}_i/(1-\bar{h}_i)$ is smaller than 1 and the global external reliability factor also becomes small. Therefore, it is essential to avoid measurements with $\bar{h}_i$ greater than 0.5.

We notice that using a normalized hat matrix allows to use it in defining the internal and external reliability of an adjustment system in a simple and efficient way.

5. Numerical example

Let us explore the proposed method on a numerical example of two parameters' transformation between two planar coordinate systems. The transformation of the coordinates (x, y) of point *i* to corresponding coordinates (u, v) is given by

$$\begin{aligned} u_i &= ax_i + by_i, \\ v_i &= -bx_i + ay_i, \end{aligned} \tag{49}$$

where a and b are the transformation parameters. To estimate the two parameters, four points of known coordinates in both systems are given. The data are provided in Table 1 and shown in Figure 1. Every point in the (x, y) coordinate system has a variance of $\sigma_{xx} = \sigma_{yy} = (2\ \text{cm})^2$ and covariance of $\sigma_{xy} = 0$, and a variance of $\sigma_{uu} = \sigma_{vv} = (4\ \text{cm})^2$ and covariance of $\sigma_{uv} = 0$ in the (u, v) coordinate system.

Table 1. The measured coordinates in both systems, in meters

Point #	x	y	u	v
1	521.48	115.38	529.76	69.57
2	58.37	445.36	96.94	438.68
3	153.69	567.13	202.62	551.75
4	532.18	501.12	574.00	452.96

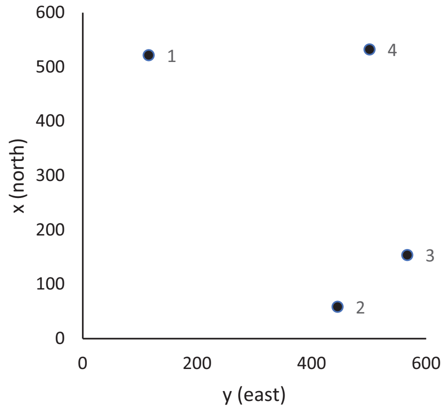

Figure 1. Location of the points in x, y coordinate system

Both sets of coordinates are observations with covariance matrices; therefore, it would be sensible to write condition equations with parameters; i.e., make use of the mixed adjustment model. There are two unknown parameters, thus u = 2. Because four points are included in the transformation, there are 16 measurements, n = 16. Each point produces two condition equations and therefore r = 8. There are 6 degrees of freedom.

The linearized condition equations for the adjustment of observations and parameters for the *i*-th point is

$$\underset{(2\times4)}{B_i}\ \underset{(4\times1)}{v_i} + \underset{(2\times2)}{A_i}\ \underset{(2\times1)}{x} + \underset{(2\times1)}{w_i} = 0, \tag{50}$$

where

$$B_i = \begin{bmatrix} a^0 & b^0 & -1 & 0 \\ -b^0 & a^0 & 0 & -1 \end{bmatrix}; \quad A_i = \begin{bmatrix} x_i & y_i \\ y_i & -x_i \end{bmatrix} \tag{51}$$

and

$$P_i = \begin{bmatrix} 2500 & & & \\ & 2500 & & \\ & & 625 & \\ & & & 625 \end{bmatrix}. \tag{52}$$

Eq. (50) is written four times for the given four points, so

$$\begin{bmatrix} B_1 & & & \\ & B_2 & & \\ & & B_3 & \\ & & & B_4 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} + \begin{bmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{bmatrix} x + \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = 0. \tag{53}$$

If the approximate values of the transformation parameters are $a^0 = 1$ and $b^0 = 0.1$, the solution is $x = \begin{bmatrix} -0.00349 & -0.01284 \end{bmatrix}^T$ and $v^T P v \quad 4.65$. Therefore, the adjusted parameters are $a^a = 0.9965$ and $b \quad = 0.0872$.

The diagonal elements of the hat matrix $\bar{H}_{AB}$ are presented in Table 2. The diagonal elements that refer to measurements in the (x, y) coordinate system are absolutely high and also high relative to the elements referring to measurements in the (u, v) coordinate system. The differences are due to the weight differences of the measurements. When the weight of a measurement is high it is expected that its corresponding $\bar{h}_i$ is high, and vice versa: when the weight of a measurement is low it is expected that its corresponding $\bar{h}_i$ is low. If, for example, $\alpha = 0.05$ and $\beta = 0.2$, we obtain $\delta_i^u = 2.80$ and can calculate the internal reliability by Eq. (40). The marginal undetectable gross errors in the measurements are in Table 2. The global external reliability of the measurements is calculated by Eq. (47) and presented in Table 3. All parameters are smaller than one, meaning that the external reliability is reasonable. The influence of the undetected gross error in each measured point is the same.

A look at Tables 2 and 3 shows that of the four participating points in the adjustment process of the transformation parameters, point number 4 has the strongest effect on the adjustment process. The internal reliability of point 4 is the lowest and its external reliability is the highest. The impact of an undetected error in the coordinate components of point number 4 on the adjusted parameters is high.

According to Eq. (43), $\bar{h}_{max} \ge (n - r + u)/n$; therefore, four points are involved in the transformation $\bar{h}_{max} \ge 0.625$ indicating low internal reliability. In general, where *q* points are involved, $\bar{h}_{max} \ge 0.5 + 1/(2q) = 0.5 + 1/r$; therefore, the maximum value of $\bar{h}_i$ converges to 0.5. This means that the ability to detect gross errors in the adjustment process is low and the addition of points to the adjustment cannot greatly improve the internal reliability. If the (u, v) coordinates are considered as constants the internal reliability will greatly improve with each addition of points.

Let us refer to the internal reliability in the adjustment of transformation parameters between two coordinate systems when both are considered as measurements. Let us define the dimension of the coordinate system as D, where $D=1,2,3$. In all, there are 2Dq measurements and Dq conditions, n = 2Dq, and r = Dq, therefore,

$$\bar{h}_{max} \geq (n-r+u)/n = (Dq+u)/2Dq = 1/2 + u/2Dq. \tag{54}$$

When we use the mixed adjustment model to estimate the transformation parameters between two coordinate systems, the diagonal elements of the hat matrix converge to 0.5. Therefore, the internal reliability in the adjustment of transformation parameters is not expected to be high.

Let us consider the possibility of using data snooping for outlier identification. The least squares residual vector $(\hat{\bar{v}})$ is estimated and Baarda's w-test statistic is computed by Eq. (37). For $\alpha = 0.05$ we obtain $\sqrt{F(0.05,1,\infty)} = 1.96$, so if $|k_i|$ > 1.96 we may reject H_0. We reject a measurement when it ought to have been accepted in 5% of the measurements. The absolute value of the test statistic k_i is presented in Table 4 for each of the measurements. Observing the test statistic k_i does not raise the suspicion of gross errors in the measurements because all values are smaller than 1.96.

Let us simulate a gross error in point number 2. Each time we add an error of 0.15 meters to a single component of the point. On the left side of Table 5 we can see the test statistic w_i when an error is added to the x component and on the right when an error is added to the y component. When there is an error in the x component of point 2, we notice that the statistic k_i for this measurement is greater than 1.96, $k_{2x} = 4.26 > 1.96$ as well as w_{2u}. An error in the x component is reflected in a high statistic k_i for x and for u as well. We realize that there is a problem, but it is not possible to determine if it is due to a gross error in the x component or u. We get similar results when the error is in the y component. The test statistic k_i when an error is added to the u and v components is presented in Table 6, which emphasizes the inability to distinguish between an error in x or u and y or v components.

Table 2. The internal reliability

Point #	$\bar{h}_i$				$\Delta^u_{i[m]}$			
	x	y	u	v	x	y	u	v
1	0.84	0.84	0.37	0.37	0.140	0.140	0.141	0.141
2	0.83	0.83	0.32	0.32	0.135	0.135	0.136	0.136
3	0.85	0.85	0.40	0.40	0.144	0.144	0.145	0.145
4	0.88	0.88	0.51	0.51	0.160	0.160	0.161	0.161

Note: left: The diagonal elements, $\bar{h}_i$, of the hat matrix $\bar{H}_{AB}$, right: The maximum size of a gross error that could contaminate the observations in meter units with probability levels $\alpha = 0.05$ and $\beta = 0.2$.

Table 3. The global external reliability. The values displayed are without multiplication by a coefficient $(\delta^u_i)^2$

Point #	$\bar{\lambda}^2_{\Delta\hat{x}_i}$			
	x	y	u	v
1	0.26	0.26	0.26	0.26
2	0.17	0.17	0.17	0.17
3	0.34	0.34	0.34	0.34
4	0.64	0.64	0.64	0.64

Table 4. The absolute value of the test statistic w_i for each of the measurements

Point #	$\lvert w_i \rvert$			
	x	y	u	v
1	1.00	1.24	−1.12	−1.13
2	−0.96	−1.00	1.06	0.90
3	0.93	−0.01	−0.92	0.10
4	0.11	−0.76	−0.04	0.76

Table 5. The absolute value of the test statistic w_i for each of the measurements with gross error in the (x, y) coordinate system

Point #	$\lvert w_i \rvert$							
	x	y	u	v	x	y	u	v
1	1.25	0.57	1.30	0.44	1.62	1.46	1.76	1.29
2	4.26	1.05	4.34	0.62	0.92	4.10	1.32	3.99
3	1.73	0.11	1.71	0.28	1.03	0.73	1.10	0.62
4	0.96	1.42	0.82	1.51	0.75	0.08	0.75	0.00

Note: left when there is a gross error of 0.15 meters in point 2, in the x component, right, in the y component.

Table 6. The absolute value of the test statistic w_i for each of the measurements with gross error in the (u, v) coordinate system

Point #	$\lvert w_i \rvert$							
	x	y	u	v	x	y	u	v
1	0.71	1.82	0.89	1.74	0.40	0.94	0.50	0.90
2	2.12	0.70	2.04	0.90	1.26	2.07	1.05	2.19
3	0.19	0.01	0.19	0.01	0.91	0.76	0.83	0.85
4	0.76	0.16	0.77	0.08	0.47	1.59	0.62	1.54

Note: left when there is a gross error of 0.15 meters in point 2, in the u component, right, in the v component.

We realize that it is not possible to separate the components x – u or y – v in the process of identifying gross errors, which is also reflected by the similar values of internal and external reliability for those components as seen in Table 2 and Table 3.

Conclusions and discussion

LS adjustment can be implemented in three main forms: the mixed adjustment model (GHM) and the two additional ones that can be derived from it, the condition equation model and the observation equation model (GMM). It is vital to identify and remove all outliers from the data used in the adjustment process, no matter which adjustment model is used. The concept of reliability is an important diagnostic tool for detecting outliers in the data and their influence on the adjusted parameters. We realize that the reliability concept is applicable to the mixed adjustment model. We can use reliability criteria not only in LS adjustment based on the observation equation model but also on the condition equation model and the mixed adjustment model.

For all adjustment models examined in this study, internal reliability can be defined by the diagonal elements of the hat matrix, as the diagonal elements reflect the reliability of the adjustment system. Large values of $\overline{\mathrm{h}}_{\mathrm{i}}$ should serve as a warning that the *i*-th measurement has a decisive influence on the adjustment process and it is difficult to check that measurement against outliers (Huber, 1981). Decreasing values of $\overline{\mathrm{h}}_{\mathrm{i}}$ cause increasing internal reliability of the adjustment system. The diagonal elements of the hat matrix play a rule in defining the external reliability as well, especially in determining the external reliability in the observation equation model. Since the estimate of the adjusted measurement is a linear combination of the computed value and the observed value with weights $1-\overline{\mathrm{h}}_{\mathrm{i}}$ and $\overline{\mathrm{h}}_{\mathrm{i}}$, respectively (see Eq. (42)) we should aim for diagonal entries less than 0.5 to ensure a reasonable level of reliability in the adjustment process. Therefore, it can be concluded that the reliability concept can serve efficiently in the mixed adjustment and condition equation models, in additional to its common use in the observation equation model.

The data snooping method for outlier identification serves as a basis for understanding and developing tools when determining the reliability of the adjustment process. It turns out that data snooping can be applied in the mixed adjustment model and condition model similarly to how it is applied in the well-known observation model.

Reliability in the observation equation model has been extensively researched and presented in geodetic literature but less has been regarding reliability criteria in the mixed and condition equation models. This paper has made a modest contribution to the study of reliability in other adjustment process models besides the observation equation model.

Data availability statement

All data, models, or code that support the findings of this study are available from the corresponding author upon reasonable request.

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