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Investigating the links of internal and external reliability with the system conditionality in Gauss-Markov models with uncorrelated observations

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Abstract: The relationship between internal response-based reliability and conditionality is investigated for Gauss-Markov (GM) models with uncorrelated observations. The models with design matrices of full rank and of incomplete rank are taken into consideration. The formulas based on the Singular Value Decomposition (SVD) of the design matrix are derived which clearly indicate that the investigated concepts are independent of each other. The methods are presented of constructing for a given design matrix the matrices equivalent with respect to internal response-based reliability as well as the matrices equivalent with respect to conditionality. To analyze conditionality of GM models, in general being inconsistent systems, a substitute for condition number commonly used in numerical linear algebra is developed, called a pseudo-conditionⁿnumber. Also on the basis of the SVD a formula for external reliability is proposed, being the 2-norm of a vector of parameter distortions induced by minimal detectable error in a particular observation. For systems with equal nonzero singular values of the design matrix, the formula can be expressed in terms of the index of internal response-based reliability and the pseudo-condition number. With these measures appearing in explicit form, the formula shows, although only for the above specific systems, the character of the impact of internal response-based reliability and conditionality of the model upon its external reliability. Proofs for complementary properties concerning the pseudo-conditionⁿumber and the 2-norm of parameter distortions in systems with minimal constraints are given in the Appendices. Numerical examples are provided to illustrate the theory.

Key words: internal reliability, external reliability, system conditionality, singular value decomposition, uncorrelated observations

1. Introduction

The internal and external reliability together with the system conditionality are the features that should all be taken into account in characterizing the quality of Gauss-Markov (GM) models. Since each of them is based on the properties of the design

matrix of a GM model, they are expected to be interrelated. The objective of the present paper is to investigate links between the above features, by establishing explicit relationships containing the corresponding measures. By this the paper aims at specifying closer links of the theory of reliability with the sensitivity analysis of linear systems established in numerical linear algebra.

In this paper the approach to "internal reliability" does not follow the traditional line of Baarda (1968), continued and developed by contributions from Wang and Chen (1994), Schaffrin (1997), Teunissen (1996), Knight et al. (2010) and others. It concentrates entirely on the properties of network responses to observation gross errors (Prószyński, 1994; 1997), characterized for uncorrelated observations by redundancy numbers. So, the approach does not operate with Minimal Detectable Biases (MDBs) for individual observations as the internal reliability measures. This corresponds to treating by Caspary (1988) the redundancy numbers (otherwise called the redundancy contributions) as measures of internal reliability. Therefore, for distinction from the traditional concept it is referred to as "internal response-based reliability" as used in Prószyński (2012). However, for saving space in the present paper the "response-based" specification will in most places be omitted. For external reliability Baarda's approach is followed, although the arbitrary vectors of observation disturbances are also taken into account.

The concept of conditionality of a linear system is well established in numerical linear algebra (e.g. Kiełbasiński and Schwetlick, 1992; Meyer 2000; Cheney and Kincaid, 2008; Kalitkin et al. 2010, and others). It describes sensitivity of the solution vector to disturbances in the input data. Such is also the sense of external reliability, so both the features are expected to have a direct connection. However, in the course of the present studies it turned out that the condition number commonly used as a measure of the system conditionality, is not applicable to inconsistent systems of equations. Therefore, a substitute measure called a pseudo-condition[^]number had to be developed for the purposes of the analysis.

The relationships between various types of measures of internal and external reliability have already been thoroughly studied by Caspary (1988). But to the knowledge of the present author, a relationship between the measures of internal response-based reliability and conditionality of the system as well as a relationship between the measures of external reliability and those of internal response-based reliability and conditionality have so far not been given a separate attention and reported in geodetic research publications. As regards the former relationship there are some implications that there may even be no dependence between the concepts. First of them is the fact that for systems with design matrices of full rank and of incomplete rank, the average reliability index depends only on the dimensions and rank of these matrices. Other implications are connected with invariance of the reliability matrix to the choice of minimal-constraint datum in observation systems with design matrices of incomplete rank. For every chosen datum we have the same reliability matrix but different magnitudes of eigenvalues of the covariance matrix for parameters, that decide about a level of the system conditionality.

In view of the above implications, the present paper seeks a theoretically grounded answer to the question of dependence between the internal response-based reliability and the conditionality of a system, both for the full-rank and rank-deficient systems. The author has not found any direct matrix operations that might provide answer to this question. That is why the analysis is based on the use of the SVD of a design matrix, since it discloses the inner structure of the matrix. Also with the use of SVD the relationship will be looked for, linking the external reliability with the measures of internal response-based reliability and the system conditionality.

A general objective of the present paper can be summed up as making an attempt to interrelate, in terms of the corresponding measures, the basic concepts that characterize quality of GM models with uncorrelated observations. It is also expected that this knowledge will help better understand and interpret the results of analyses of such models, especially in the course of their design.

2. Recalling basic concepts and auxiliary properties

We provide brief presentation of the concepts together with some auxiliary properties necessary for the analyses in the present paper. Some of the properties were developed deliberately for this purpose.

2.1. Observation model and basic formulas for least squares estimation of parameters

Let us consider a standardized Gauss-Markov model

$$\mathbf{A}\mathbf{x} + \mathbf{e} = \mathbf{y}; \quad \mathbf{e} \sim (\mathbf{0}, \mathbf{I}) \tag{1a}$$

and its form with minimal constraints

$$\mathbf{A}\mathbf{x} + \mathbf{e} = \mathbf{y}; \quad \mathbf{e} \sim (\mathbf{0}, \mathbf{I})$$
 (1b)
 $\mathbf{S}\mathbf{x} = \mathbf{0}$

where:

y – the $n \times 1$ vector of standardized uncorrelated observations;

A - the $n \times u$ design matrix; rank A = r; $r \le u$ for (1a), r < u for (1b);

x – the unknown $u \times 1$ vector of parameters;

e – the unknown $n \times 1$ vector of standardized random errors;

S – the $d \times u$ coefficient matrix in constraint equations,

 $d = u - \text{rank } \mathbf{A}$; rank $\mathbf{S} = d$; rank $\begin{bmatrix} \mathbf{A}^T & \mathbf{S}^T \end{bmatrix} = u$, i.e. each row-vector of \mathbf{S} belongs to the null-space of \mathbf{A} (Koch, 1999).

The least squares (LS) solutions of the system (1a) and (1b) will be denoted, respectively

$$\hat{\mathbf{x}} = \mathbf{A}^{\mathsf{T}} \mathbf{y}$$
 or equivalenly $\hat{\mathbf{x}} = (\mathbf{A}^{\mathsf{T}} \mathbf{A})^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{y}$

$$\hat{\mathbf{x}} = \mathbf{A}_{\mathbf{S}}^{\mathsf{T}} \mathbf{y}$$
 or equivalenly $\hat{\mathbf{x}} = (\mathbf{A}^{\mathsf{T}} \mathbf{A})_{\mathbf{S}}^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{y}$

where:

 $(\cdot)^+$ - the pseudo-inverse, $(\cdot)_S^-$ - a reflexive g - inverse, satisfying $S(\cdot)_S^- = 0$ (Rao and Mitra, 1971). The g - inverse $(A^TA)_S^-$ is a symmetrical matrix (Meyer 2000). With a specified S, A_S^- yields a unique solution.

The above cases are not disjoint, since with $S = S_0$, such that $AS_0^T = 0$, we have $A^+ \equiv A_{S_0}^-$.

2.2. Singular Value Decomposition of the design matrix

The SVD of the matrix A of incomplete rank, will be denoted by

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^{\mathrm{T}} \tag{2}$$

where:

 $U(n \times n)$, $V(u \times u)$ – orthogonal matrices containing the left-hand side and right-hand side singular vectors, respectively;

 $\Sigma(n \times u)$ – the matrix of singular values,

$$\sum_{n \times u} = \begin{bmatrix} \mathbf{\sigma} & \mathbf{0} \\ r \times r & r \times (u - r) \\ \mathbf{0} & \mathbf{0} \\ (n - r) \times r & (n - r) \times (u - r) \end{bmatrix}$$
(3)

 $\sigma(r \times r)$ – a diagonal matrix of nonzero singular values, i.e.

$$\sigma = \text{diag } (\sigma_1, \sigma_2, ..., \sigma_r), \text{ with } \sigma_i > 0 \ (i = 1, 2, ..., r)$$

Partitioning the matrices U and V according to the rank of A, as below

$$\mathbf{U} = \begin{bmatrix} \mathbf{U}_{r} & \mathbf{U}_{n-r} \end{bmatrix} \qquad \qquad \mathbf{V} = \begin{bmatrix} \mathbf{V}_{r} & \mathbf{V}_{u-r} \end{bmatrix}$$
 (4)

and substituting them into the formula (2), we get its equivalent reduced forms (see e.g. Golub and Reinsch, 1970)

$$\mathbf{A} = \mathbf{U}_{r} \boldsymbol{\sigma} \mathbf{V}_{r}^{T} \qquad \mathbf{A} = \begin{bmatrix} \mathbf{U}_{r} \boldsymbol{\sigma} & \mathbf{0} \end{bmatrix} \mathbf{V}^{T} \qquad \mathbf{A} = \mathbf{U} \begin{bmatrix} \boldsymbol{\sigma} \mathbf{V}_{r}^{T} \\ \mathbf{0} \end{bmatrix}$$
 (5)

2.3. A pseudo-condition^number developed for the purposes of analysis

The condition number as defined in numerical linear algebra (eg. Kiełbasiński and Schwetlick, 1992; Meyer, 2000), applies only to nonsingular systems of equations. Additionally, in (Meyer, 2000) a generalized condition number is introduced, that allows for the analysis of consistent systems with the design matrices being rectangular or singular. So, neither of the above condition numbers is applicable for the systems of the type (1a) and (1b) that are, in general, inconsistent, i.e. do not have exact solution. Although a generalized condition number could be used for singular normal equations, but we do not operate there with a vector of observation disturbances in explicit form, necessary for seeking the links between conditionality and external reliability.

For the purpose of the analysis undertaken in the present paper we introduce a substitute for conventional concept of conditionality, called here a "pseudoconditionality". We make an assumption that the model is exact, i.e. the matrices **A** or **A**, **S** are known exactly and all the disturbances reside only in the observation vector **y**.

We shall introduce a general form of unique solution for the systems (1a) and (1b), denoted by

$$\hat{\mathbf{x}} = \mathbf{A}^{\bullet} \mathbf{y} \tag{6}$$

where A^{\bullet} stands for either of A^{+} or A_{S}^{-} (with a specified S).

It follows from (6), that the disturbances in \mathbf{y} will cause distortions in $\hat{\mathbf{x}}$, as shown below

$$\Delta \hat{\mathbf{x}} = \mathbf{A}^{\bullet} \cdot \Delta \mathbf{y} \tag{7}$$

Expressing equation (7) in terms of the 2-norm and using the property given in (Meyer 2000), we get

$$\|\Delta \hat{\mathbf{x}}\| = \|\mathbf{A}^{\bullet} \cdot \Delta \mathbf{y}\| \le \|\mathbf{A}^{\bullet}\| \|\Delta \mathbf{y}\|$$
 (8)

where $\|\mathbf{A}^{\bullet}\|$ denotes the 2-norm of the matrix \mathbf{A}^{\bullet} .

Since it follows from (8) that

$$\left\| \mathbf{A}^{\bullet} \right\| = \left(\frac{\left\| \Delta \hat{\mathbf{x}} \right\|}{\left\| \Delta \mathbf{y} \right\|} \right)_{\text{max}} \tag{9}$$

we shall assume $\|\mathbf{A}^{\bullet}\|$ as a pseudo-conditionⁿnumber for inconsistent systems of linear equations (either rank-deficient or of full rank), and denote it by

$$k(\mathbf{A}^{\bullet}) = \|\mathbf{A}^{\bullet}\| \tag{10}$$

It serves here as a substitute for a condition number $k(\mathbf{A})$ used for consistent systems of equations. The condition number $k(\mathbf{A})$ is defined as a ratio of relative disturbances in solution and relative disturbances in observations, the former being referred to the exact solution. The pseudo-condition^number, due to the lack of exact solution, is defined as a ratio of absolute disturbances in solution and in observations, where the disturbances in solution are referred to the unique but approximate solution.

Moving the derivations to Appendix A, we present here the final detailed formulas for $k(\mathbf{A}^{\bullet})$, i.e.

$$k(\mathbf{A}^+) = \sqrt{\lambda_{\max} [(\mathbf{A}^T \mathbf{A})^+]} = [\sigma_{\min}(\mathbf{A})]^{-1}$$
 for all $\lambda_i > 0$ or $\sigma_i > 0$ (11a)

$$k(\mathbf{A}_{\mathbf{S}}^{-}) = \sqrt{\lambda_{\max} \left[(\mathbf{A}^{\mathrm{T}} \mathbf{A})_{\mathbf{S}}^{-} \right]}$$
 for all $\lambda_{i} > 0$ (11b)

For $S = S_0$, we have $A_{S_0}^- = A^+$ and hence, $k(A_{S_0}^-) = k(A^+)$

It follows from the derivations in Appendix B that for $S \neq S_o$, we have

$$k(\mathbf{A}_{\mathbf{S}}^{-}) > k(\mathbf{A}^{+}) \tag{12}$$

which means that the solution of the system 1b) is worse conditioned than that of the system 1a).

For the sake of simplicity, anywhere in the text when referring to a pseudo-condition number, we shall be using a general term "conditionality".

2.4. Internal response-based reliability of a model and its measures

The model internal reliability as presented in this paper, more properly termed the internal response-based reliability of a model, has as its basis the "disturbance/response relationship" (Prószyński, 1994; 1997), written as

$$\Delta \hat{\mathbf{v}} = -\mathbf{H} \cdot \Delta \mathbf{y} \tag{13}$$

where:

 Δy – the $n \times 1$ vector of the standardized observation disturbances (standardized gross errors),

 $\Delta \hat{\mathbf{v}}$ – the $n \times 1$ vector of increments in the standardized LS residuals,

 \mathbf{H} – the $n \times n$ reliability matrix, for a model with uncorrelated observations being an operator of orthogonal projection, given by the formula

$$\mathbf{H} = \mathbf{I} - \mathbf{A} (\mathbf{A}^{\mathrm{T}} \mathbf{A})^{+} \mathbf{A}^{\mathrm{T}}$$
 (14)

The expression (14) can be written in an equivalent generalized form

$$\mathbf{H} = \mathbf{I} - \mathbf{A} (\mathbf{A}^{\mathrm{T}} \mathbf{A})^{-} \mathbf{A}^{\mathrm{T}}$$
 (15)

which is invariant to the choice of generalized inverse $(\mathbf{A}^T \mathbf{A})^-$ (Rao, 1973), e.g. $(\mathbf{A}^T \mathbf{A})_{\mathbf{S}_0}^- \equiv (\mathbf{A}^T \mathbf{A})^+$, $(\mathbf{A}^T \mathbf{A})_{\mathbf{S}_1}^-$, $(\mathbf{A}^T \mathbf{A})_{\mathbf{S}_2}^-$,

The diagonal elements of \mathbf{H} , $h_{ii} < 0$, 1), i = 1, ..., n, known as redundancy numbers, are indices of the model internal reliability, their sum being Tr $\mathbf{H} = n - r$. The average index is $h_{ii} = 1 - r / n$. The reliability criterion for the case of a single outlier is $h_{ii} > 0.5$ (Prószyński, 1994).

3. SVD-based representation of reliability matrix and its invariance properties

Coming back to reliability matrix \mathbf{H} we derive other representation of the formula (14), basing on the SVD of the matrix \mathbf{A} as in (2).

The reliability matrix will take the form

$$\mathbf{H} = \mathbf{I} - \mathbf{A} (\mathbf{A}^{\mathrm{T}} \mathbf{A})^{+} \mathbf{A}^{\mathrm{T}} = \mathbf{I} - \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathrm{T}} (\mathbf{V} \mathbf{\Sigma}^{\mathrm{T}} \mathbf{U}^{\mathrm{T}} \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathrm{T}})^{+} \mathbf{V} \mathbf{\Sigma}^{\mathrm{T}} \mathbf{U}^{\mathrm{T}} =$$

$$= \mathbf{I} - \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathrm{T}} (\mathbf{V}^{\mathrm{T}})^{-1} (\mathbf{\Sigma}^{\mathrm{T}} \mathbf{\Sigma})^{+} \mathbf{V}^{-1} \mathbf{V} \mathbf{\Sigma}^{\mathrm{T}} \mathbf{U}^{\mathrm{T}} = \mathbf{I} - \mathbf{U} \mathbf{\Sigma} (\mathbf{\Sigma}^{\mathrm{T}} \mathbf{\Sigma})^{+} \mathbf{\Sigma}^{\mathrm{T}} \mathbf{U}^{\mathrm{T}} =$$

$$= \mathbf{I} - \mathbf{U} \begin{bmatrix} \mathbf{\sigma} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{\sigma}^{-2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{\sigma} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{U}^{\mathrm{T}} = \mathbf{I} - \mathbf{U} \begin{bmatrix} \mathbf{I}_{\mathrm{r}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0}_{\mathrm{n-r}} \end{bmatrix} \mathbf{U}^{\mathrm{T}}$$

$$(16)$$

Partitioning the matrix U as in (4) and substituting into the formula (16), we get

$$\mathbf{H} = \mathbf{I} - \begin{bmatrix} \mathbf{U}_{r} & \mathbf{U}_{n-r} \end{bmatrix} \begin{bmatrix} \mathbf{I}_{r} & \mathbf{0} \\ \mathbf{0} & \mathbf{0}_{n-r} \end{bmatrix} \begin{bmatrix} \mathbf{U}_{r}^{\mathrm{T}} \\ \mathbf{U}_{n-r}^{\mathrm{T}} \end{bmatrix} = \mathbf{I} - \mathbf{U}_{r} \mathbf{U}_{r}^{\mathrm{T}}$$
(17)

Since $\mathbf{H}\mathbf{U}_r = (\mathbf{I} - \mathbf{U}_r\mathbf{U}_r^T)\mathbf{U}_r = \mathbf{U}_r - \mathbf{U}_r = \mathbf{0}$, each column vector in \mathbf{U}_r belongs to $R(\mathbf{A})$ and therefore, we shall call \mathbf{U}_r the left active singular vectors of the matrix \mathbf{A} . Hence, we say that the operator \mathbf{H} depends entirely on the left active singular vectors of the matrix \mathbf{A} .

To create a basis for further analysis, we also recall a specific property of the reliability matrix **H** being, in the case that rank A = u, its invariance to non-

singular transformations. The property is extended here for rank $A \le u$ onto singular transformations that are non-singular in the subspace R(A).

The property reads, that for a transformed matrix A, denoted by A_{\bullet} , such that

$$\mathbf{A}_{\bullet} = \mathbf{A}\mathbf{G} \tag{18}$$

where $G(u \times u)$ is a singular matrix with SVD as below

$$\mathbf{G}_{u \times u} = \mathbf{V} \cdot \begin{bmatrix} \mathbf{\sigma}_{G} & \mathbf{0} \\ r \times r & r \times (u - r) \\ \mathbf{0} & \mathbf{0} \\ (u - r) \times r & (u - r) \times (u - r) \end{bmatrix} \cdot \mathbf{V}_{G}^{T}$$

$$(19)$$

with V being identical with that in (2),

we have $\mathbf{H}_{\bullet} = \mathbf{H}$.

The proof is as follows,

$$\mathbf{H}_{\bullet} = \mathbf{I} - \mathbf{A}_{\bullet} (\mathbf{A}_{\bullet}^{\mathsf{T}} \mathbf{A}_{\bullet})^{+} \mathbf{A}_{\bullet}^{\mathsf{T}} = \mathbf{I} - \mathbf{A} \mathbf{G} (\mathbf{G}^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{A} \mathbf{G})^{+} \mathbf{G}^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} =$$

$$= \mathbf{I} - \mathbf{A} \mathbf{G} \mathbf{G}^{\mathsf{T}} (\mathbf{A}^{\mathsf{T}} \mathbf{A})^{\mathsf{T}} \mathbf{G} \mathbf{G}^{\mathsf{T}} \mathbf{A}^{\mathsf{T}}$$
(20)

where GG⁺ is a symmetrical matrix.

Finding that

$$\begin{split} \mathbf{A}^{\mathrm{T}}\mathbf{A} &= \mathbf{V} \begin{bmatrix} \boldsymbol{\sigma}_{\mathrm{r}} \mathbf{U}_{\mathrm{r}}^{\mathrm{T}} \\ \boldsymbol{0} \end{bmatrix} \!\! \begin{bmatrix} \mathbf{U}_{\mathrm{r}} \boldsymbol{\sigma}_{\mathrm{r}} & \mathbf{0} \end{bmatrix} \!\! \mathbf{V}^{\mathrm{T}} = \mathbf{V} \begin{bmatrix} \boldsymbol{\sigma}_{\mathrm{r}}^{2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \!\! \mathbf{V}^{\mathrm{T}} \qquad (\mathbf{A}^{\mathrm{T}}\mathbf{A})^{+} = \mathbf{V} \begin{bmatrix} \boldsymbol{\sigma}_{\mathrm{r}}^{-2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \!\! \mathbf{V}^{\mathrm{T}} \\ \mathbf{G}\mathbf{G}^{+} &= \mathbf{V} \begin{bmatrix} \boldsymbol{\sigma}_{\mathrm{G}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \!\! \mathbf{V}_{\mathrm{G}}^{\mathrm{T}} \mathbf{V}_{\mathrm{G}} \begin{bmatrix} \boldsymbol{\sigma}_{\mathrm{G}}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \!\! \mathbf{V}^{\mathrm{T}} = \mathbf{V} \begin{bmatrix} \mathbf{I}_{\mathrm{r}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \!\! \mathbf{V}^{\mathrm{T}} \end{split}$$

and substituting into (20), we obtain

$$\mathbf{H}_{\bullet} = \mathbf{I} - \begin{bmatrix} \mathbf{U}_{r} \mathbf{\sigma}_{r}^{-1} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{\sigma}_{r} \mathbf{U}_{r}^{T} \\ \mathbf{0} \end{bmatrix} = \mathbf{I} - \mathbf{U}_{r} \mathbf{U}_{r}^{T} := \mathbf{H}$$

We can explain the above invariance property by stating that any singular transformation $A_{\bullet} = AG$, being non-singular in a subspace R(A) and compatible with A as regards the orientation of r – principal axes in a parameter space (R^u) , maintains the matrix of left active singular vectors \mathbf{U}_r .

The proof is immediate.

The transformed matrix takes the form

$$\mathbf{A}_{\bullet} = \mathbf{A}\mathbf{G} = \begin{bmatrix} \mathbf{U}_{\mathrm{T}}\mathbf{\sigma} & \mathbf{0} \end{bmatrix} \mathbf{V}^{\mathrm{T}} \cdot \mathbf{V} \begin{bmatrix} \mathbf{\sigma}_{\mathrm{G}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{V}_{\mathrm{G}}^{\mathrm{T}}$$

and we get

$$\boldsymbol{A}_{\bullet} = \begin{bmatrix} \boldsymbol{U}_r \boldsymbol{\sigma} \boldsymbol{\sigma}_G & \boldsymbol{0} \end{bmatrix} \boldsymbol{V}_G^T = \boldsymbol{U}_r (\boldsymbol{\sigma} \boldsymbol{\sigma}_G) \boldsymbol{V}_{G,r}^T$$

For matrices **A** of full rank the transformation matrix **G** can be any arbitrary non-singular matrix.

4. Generating reliability-equivalent and conditionality-equivalent matrices

The invariance property (18) enables one to generate for a given matrix A the matrices equivalent with respect to internal reliability. Using any transformation matrix G, we obtain a matrix A_{\bullet} having U_r as that in A, but the components σ and V of different values than those in A. Now, we show how to generate A_{\bullet} that has the a priori specified σ and V.

Denoting these elements by σ_{\bullet} and V_{\bullet} respectively, we write the required matrix A_{\bullet} in the SVD form

$$\mathbf{A}_{\bullet} = \mathbf{U} \cdot \begin{bmatrix} \mathbf{\sigma}_{\bullet} & \mathbf{0} \\ r \times r & r \times (u - r) \\ \mathbf{0} & \mathbf{0} \\ (n - r) \times r & (n - r) \times (u - r) \end{bmatrix} \cdot \mathbf{V}_{\bullet}^{\mathsf{T}} = \begin{bmatrix} \mathbf{U}_{\mathsf{T}} \mathbf{\sigma}_{\bullet} & \mathbf{0} \end{bmatrix} \cdot \mathbf{V}_{\bullet}^{\mathsf{T}}$$
(21)

Since we change the structural components of the initial matrix A, we denote the corresponding transformation matrix G as in (18) by G_A .

The derivation of the matrix G_A is as follows:

expressing the transformation formula $AG_A = A_{\bullet}$ in terms of the SVD, and assuming the structure of G_A as that of G in (19), we get

$$\mathbf{U} \begin{bmatrix} \boldsymbol{\sigma} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \mathbf{V}^{T} \mathbf{G}_{A} = \mathbf{U} \begin{bmatrix} \boldsymbol{\sigma}_{\bullet} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \cdot \mathbf{V}_{\bullet}^{T}$$

Then, premultiplying both sides by \mathbf{U}^T and decomposing \mathbf{V} and \mathbf{V}_{\bullet} as in (5), we obtain

$$\begin{bmatrix} \boldsymbol{\sigma} \boldsymbol{V}_{r}^{T} \\ \boldsymbol{0} \end{bmatrix} \boldsymbol{G}_{A} = \begin{bmatrix} \boldsymbol{\sigma}_{\bullet} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \boldsymbol{V}_{\bullet}^{T},$$

Finally, premultiplying both sides by $\begin{bmatrix} \mathbf{V}_r \mathbf{\sigma}^{-1} & \mathbf{0} \end{bmatrix}$, we get

$$\mathbf{G}_{\mathbf{A}} = \begin{bmatrix} \mathbf{V}_{\mathbf{r}} \mathbf{\sigma}^{-1} \mathbf{\sigma}_{\bullet} & \mathbf{0} \end{bmatrix} \mathbf{V}_{\bullet}^{\mathrm{T}}$$
 (22)

This, after taking into account the eigenvectors V_{u-r} complementary to V_r , can be considered as an equivalent reduced form of the matrix

$$\mathbf{G}_{\mathbf{A}} = \mathbf{V} \begin{bmatrix} \mathbf{\sigma}^{-1} \mathbf{\sigma}_{\bullet} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{V}_{\bullet}^{\mathrm{T}}$$
 (23)

In the case that r = u, we have

$$\mathbf{G}_{\mathbf{A}} = \mathbf{V} \mathbf{\sigma}^{-1} \mathbf{\sigma}_{\bullet} \mathbf{V}_{\bullet}^{\mathrm{T}} \tag{24}$$

Substituting into (24) $\sigma_{\bullet} = I_r$ and $V_{\bullet} = I_u$, we get G_A that generates the matrix A_{\bullet} with unit singular values, i.e.

$$\mathbf{G}_{A} = \mathbf{V} \mathbf{\sigma}^{-1}$$
 and hence, $\mathbf{A}_{\bullet} = \mathbf{U}_{r} \mathbf{\sigma} \mathbf{V}^{T} \mathbf{V} \mathbf{\sigma}^{-1} = \mathbf{U}_{r}$ (25)

We can see that the matrix A_{\bullet} is equivalent to A with respect to internal reliability, being equal to that structural component of A which determines the internal reliability of the system.

To extend the analysis we shall consider the transformation carried out on the rows of the matrix A, i.e.

$$\mathbf{A}_{\bullet} = \mathbf{K}\mathbf{A} \tag{26}$$

where \mathbf{K} is an arbitrary nonsingular matrix.

We can check that in general we have $\sigma(A_*) \neq \sigma(A)$ and $H_{\bullet} \neq H$. However, for **K** being orthogonal, we get

$$\mathbf{A}_{\bullet} = \mathbf{K}\mathbf{U} \cdot \begin{bmatrix} \boldsymbol{\sigma} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \cdot \mathbf{V}^{\mathrm{T}} = \mathbf{U}_{\mathbf{K}} \cdot \begin{bmatrix} \boldsymbol{\sigma} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \cdot \mathbf{V}^{\mathrm{T}} = \mathbf{U}_{\mathbf{K},r} \boldsymbol{\sigma} \mathbf{V}_{r}^{\mathrm{T}}$$

where: $U_K = KU$ (orthogonal); $U_{K,r} = KU_{r}$.

Since $\mathbf{U}_{\mathbf{K},r}\mathbf{U}_{\mathbf{K},r}^{\mathrm{T}} = \mathbf{K}\mathbf{U}_{r}\mathbf{U}_{r}^{\mathrm{T}}\mathbf{K}^{\mathrm{T}} \neq \mathbf{U}_{r}\mathbf{U}_{r}^{\mathrm{T}}$, we have $\mathbf{H}_{\bullet} \neq \mathbf{H}$. But, since $\mathbf{A}_{\bullet}^{\mathrm{T}}\mathbf{A}_{\bullet} = \mathbf{A}^{\mathrm{T}}\mathbf{K}^{\mathrm{T}}\mathbf{K}\mathbf{A} = \mathbf{A}^{\mathrm{T}}\mathbf{A}$, therefore $\sigma(\mathbf{A}_{\bullet}) = \sigma(\mathbf{A})$ and hence, $k(\mathbf{A}_{\bullet}^{+}) = k(\mathbf{A}^{+})$

We notice that the resulting matrix A_{\bullet} is of different internal reliability but the same conditionality as the initial matrix A.

Therefore, using orthogonal transformation matrices K, we can generate the conditionality-equivalent matrices of different reliability characteristics.

The structure of matrices equivalent to a given design matrix **A** with respect to internal reliability or with respect to conditionality is shown in Fig. 1.

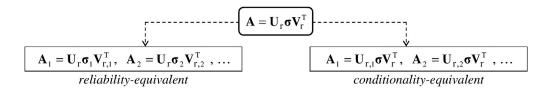


Fig. 1. The SVD structure of reliability-equivalent and conditionality-equivalent matrices

As the reliability characteristics contained in the matrix \mathbf{H} can be obtained for an infinite number of systems with different conditionality characteristics (i.e. $\sigma(\mathbf{A})$, $k(\mathbf{A}^+)$, and reversely, the specified conditionality characteristics can be obtained for an infinite number of systems with different reliability characteristics, we may conclude, that in terms of the above characteristics the concepts of internal reliability and conditionality are not interrelated. It is shown on a scheme in Fig.2, by referring the SVD of the design matrix \mathbf{A} to that of the coefficient matrix $\mathbf{A}^{T}\mathbf{A}$ in normal equations.

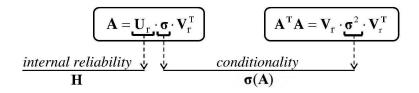


Fig. 2. Lack of interrelation between the concepts of internal response-based reliability and conditionality of the system

The measures of system conditionality are, in general, based on the eigenvalues of the matrix $\mathbf{A}^T\mathbf{A}$, each being a square of the corresponding singular value of the design matrix \mathbf{A} . Instead, the measures of internal reliability are determined on the basis of the matrix \mathbf{U}_r , being the component of \mathbf{A} which disappears when passing to $\mathbf{A}^T\mathbf{A}$. Since passing to normal equations means transforming the initial inconsistent system of observation equations into a consistent system of normal equations, the internal reliability is not covered by the existing definition of a condition number.

The above considerations can be summarized as follows:

 in GM models the internal reliability and conditionality are defined on different components of the SVD of a design matrix, so these features are not interrelated. Hence, a GM model may have low internal reliability and also be well—conditioned, and reversely, may have a high internal reliability and also be ill-conditioned;

- since adding or removing an observation in a GM model changes the structure of the design matrix and hence, affects both the internal reliability and the conditionality, we have to check each feature in the design separately;
- it can be proved that the transformations AG_A and KA of the design matrix, can be applied to a GM model so that we get its modified forms being equivalent with respect to the LS estimation. However, it was not investigated in the present research whether the transformed models can be helpful in the design of networks.

5. Seeking links of external reliability with the internal reliability and conditionality of a model

We shall try to determine the relationship linking external reliability of a model with its internal reliability and conditionality. As in the preceding sections, for derivation of the relationship we shall use the SVD of the design matrix \mathbf{A} .

The Baarda concept of external reliability as applied to the system (1a) is based on a formula

$$\Delta \hat{\mathbf{x}} = (\mathbf{A}^{\mathrm{T}} \mathbf{A})^{+} \mathbf{A}^{\mathrm{T}} \cdot \Delta \mathbf{y}$$
 (27)

where:

 Δy – the vector of standardized observation disturbances as in (13)

 $\Delta \hat{\mathbf{x}}$ – the vector of distortions in the LS solution $\hat{\mathbf{x}}$, induced by the disturbances $\Delta \mathbf{y}$.

In the case of a single disturbance, (27) takes the form

$$\Delta \hat{\mathbf{x}}_{(i)} = (\mathbf{A}^{\mathrm{T}} \mathbf{A})^{+} \mathbf{A}^{\mathrm{T}} \cdot \Delta \mathbf{y}_{(i)}$$
(28)

where $\Delta \mathbf{y}_{(i)} = \begin{bmatrix} 0 & \dots & 0 & \Delta y_i & 0 & \dots & 0 \end{bmatrix}^T$.

Baarda considers a specific single disturbance case, i.e.

$$\Delta y_i = \frac{1}{\sigma_i} MDB_i = \sqrt{\frac{\delta}{h_{ii}}}; \qquad (29)$$

where:

 MDB_i – Minimal Detectable Bias in the i-th observation, σ_i – standard deviation of the i-th observation, δ – the non-centrality parameter.

In this specific case the corresponding vector $\Delta \hat{\mathbf{x}}_{(i)}$ as in (28) will be denoted by $\Delta \hat{\mathbf{x}}_{(B_i)}$.

Applying the SVD of A, we get (27) in the form

$$\Delta \hat{\mathbf{x}} = \mathbf{V}_{r} \mathbf{\sigma}^{-2} \mathbf{V}_{r}^{\mathrm{T}} \mathbf{V}_{r} \mathbf{\sigma} \mathbf{U}_{r}^{\mathrm{T}} \cdot \Delta \mathbf{y}$$
(30)

and finally

$$\Delta \hat{\mathbf{x}} = \mathbf{V}_{\mathbf{r}} \mathbf{\sigma}^{-1} \mathbf{U}_{\mathbf{r}}^{\mathrm{T}} \cdot \Delta \mathbf{y} \tag{31}$$

As could be expected, the formula (31) shows that the vector of distortions $\Delta \hat{\mathbf{x}}$ depends on all the structural components of the matrix \mathbf{A} , and hence, on the internal reliability (\mathbf{U}_r) and conditionality ($\boldsymbol{\sigma}$) of the system. We can also notice that the greater are the singular values, the smaller are the distortions in the parameters. In a single disturbance case (see (28)), where Δy_i is as in (29), we get in (31) another component containing internal reliability, i.e. h_{ii} .

Since formula (31) does not precisely indicate, i.e. in terms of specified measures, the character of the influence of internal reliability and conditionality of the system upon $\Delta \hat{\mathbf{x}}$, we shall consider the 2-norm instead, i.e.

$$\left\|\Delta \hat{\mathbf{x}}\right\|^2 = \Delta \mathbf{y}^{\mathrm{T}} \mathbf{U}_{\mathrm{r}} \mathbf{\sigma}^{-2} \mathbf{U}_{\mathrm{r}}^{\mathrm{T}} \Delta \mathbf{y} = \left\|\mathbf{\sigma}^{-1} \mathbf{U}_{\mathrm{r}}^{\mathrm{T}} \Delta \mathbf{y}\right\|^2$$
(32)

In a specific case of systems with equal nonzero singular values, we get $\mathbf{\sigma} = \mathbf{\sigma} \cdot \mathbf{I}_{r}$, and the formula (32) will take a simplified form

$$\|\Delta \hat{\mathbf{x}}\|^2 = \sigma^{-2} \|\mathbf{U}_r^T \Delta \mathbf{y}\|^2 = \sigma^{-2} \Delta \mathbf{y}^T \mathbf{U}_r \mathbf{U}_r^T \Delta \mathbf{y} = \sigma^{-2} (\|\Delta \mathbf{y}\|^2 - \|\mathbf{H} \cdot \Delta \mathbf{y}\|^2)$$
(33)

In the above derivation the equation (17) was used, i.e. $\mathbf{U}_r \mathbf{U}_r^T = \mathbf{I} - \mathbf{H}$. Hence

$$\|\Delta \hat{\mathbf{x}}\| = \frac{1}{\sigma} \sqrt{\|\Delta \mathbf{y}\|^2 - \|\mathbf{H} \cdot \Delta \mathbf{y}\|^2}$$
(34)

Assuming a single disturbance, we have $\|\Delta \mathbf{y}\|^2 = (\Delta y_i)^2$, $\|\mathbf{H} \cdot \Delta \mathbf{y}\|^2 = h_{ii} \cdot (\Delta y_i)^2$, and the formula (34) takes the form

$$\left\| \Delta \hat{\mathbf{x}}_{(i)} \right\| = \left| \Delta \mathbf{y}_{i} \right| \cdot \frac{1}{\sigma} \sqrt{(1 - \mathbf{h}_{ii})}$$
 (35)

Putting $\Delta y_i = \sqrt{\frac{\delta}{h_{ii}}}$ as in (29), we obtain for such systems the exact formula for external reliability

$$\left\| \Delta \hat{\mathbf{x}}_{(\mathrm{B}_{\mathrm{i}})} \right\| = \sqrt{\delta} \cdot \frac{1}{\sigma} \sqrt{\frac{1}{\mathrm{h}_{\mathrm{ii}}} - 1} \tag{36}$$

The analyzed specific case of equal singular values allows one to introduce into the formula (36) a pseudo-condition^number $k(\mathbf{A}^{\bullet})$ (here $k(\mathbf{A}^{+})$), by substituting $\frac{1}{\sigma} = k(\mathbf{A}^{\bullet})$, i.e.

$$\left\| \Delta \hat{\mathbf{x}}_{(B_i)} \right\| = \sqrt{\delta} \cdot k(\mathbf{A}^{\bullet}) \sqrt{\frac{1}{h_{ii}} - 1}$$
(37)

By this we get, although for a specific case, a formula with a clear separation of the influence of conditionality and internal reliability, expressed in terms of the corresponding measures. The formula (37) can be considered as an approximate formula for the systems (1a) that have small variation in nonzero singular values.

As regards internal reliability, each of the formulas discussed above, i.e. (35), (36), (37), indicates that the greater the reliability index for the i–th observation, the smaller is the norm of parameter distortions. From the formula (36) or (37) we can see that the internal reliability, at any value of its index h_{ii} , except $h_{ii} = 0$, decreases the norm of parameter distortions. The formula (37) shows that for a disturbance being the MDB_i, the decrease in that norm occurs for $h_{ii} > 0.5$, i.e. when satisfying the reliability criterion. We may thus conclude that both the appropriately high level of internal reliability and a good conditionality of a system are advantageous for external reliability.

In spite of the approximate character of the formulas (35), (36) or (37) when applied for systems with $\sigma_{min} \neq \sigma_{max}$, we may, without a further loss of accuracy, analyze the impact of internal reliability level h_{ii} upon $\left\|\Delta\hat{\mathbf{x}}_{(B_i)}\right\|$ with respect to that upon $\left\|\Delta\hat{\mathbf{x}}_{(i)}\right\|$. We shall therefore compare the following influencing factors appearing in the formulas (29), (35) and (36), respectively

$$\eta_{(1)} = \sqrt{\frac{1}{h_{ii}}}$$
, due to MDB_i; $\eta_{(2)} = \sqrt{1 - h_{ii}}$, due to the structure of **A**,

$$\eta_{(1,2)}=\eta_{(1)}\cdot\eta_{(2)}=\sqrt{\frac{1}{h_{ii}}-1}$$
 , due to the joint influence

The corresponding graphs are shown in Fig. 3. It is only within the interval $0.5 < h_{ii} < 1$, that the joint influence of internal reliability upon $\left\| \Delta \hat{\mathbf{x}}_{(B_i)} \right\|$ is advantageous $(\eta_{(1,2)} < 1)$, and the greater are the values of h_{ii} , the greater is the reduction in $\left\| \Delta \hat{\mathbf{x}}_{(B_i)} \right\|$.

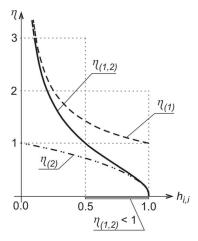


Fig. 3. Relibility-dependent factors influencing the norm of parameter distortions

For the models (1b) with $S \neq S_0$, the formula analogous to (27) takes the form

$$\Delta \hat{\mathbf{x}}_{(S)} = (\mathbf{A}^{\mathrm{T}} \mathbf{A})_{S}^{-} \mathbf{A}^{\mathrm{T}} \cdot \Delta \mathbf{y}$$
(38)

and, after applying the SVD of the factors and carrying out several matrix operations (see appendix B), we get

$$\left\| \Delta \hat{\mathbf{x}}_{(\mathbf{s})} \right\| = \left\| (\mathbf{V}_{r}^{\mathsf{T}} \mathbf{V}_{*,r})^{-1} \mathbf{\sigma}^{-1} \mathbf{U}_{r}^{\mathsf{T}} \cdot \Delta \mathbf{y} \right\|$$
(39)

where V_r and $V_{*,r}$ are the matrices of active eigenvectors of A^TA and $(A^TA)_S^-$ respectively.

Comparing the formulas (39) and (32), we can see that the factor $(\mathbf{V}_r^T \mathbf{V}_{*,r})^{-1}$ reflects the influence of the constraints used. For $\mathbf{S} = \mathbf{S}_0$, we get $\mathbf{V}_r^T \mathbf{V}_r = \mathbf{I}_r$, and (39) becomes identical with (32).

Finally, since $\|\Delta \hat{\mathbf{x}}_{(s)}\| > \|\Delta \hat{\mathbf{x}}\|$, where $\Delta \hat{\mathbf{x}}$ is as in (27), we obtain the inequality (see Appendix C)

$$\left\| \Delta \hat{\mathbf{x}}_{(\mathbf{s})} \right\| > \left\| \mathbf{\sigma}^{-1} \mathbf{U}_{\mathbf{r}}^{\mathrm{T}} \cdot \Delta \mathbf{y} \right\| \tag{40}$$

By noticing structural analogy in the formulas (39) and (32), we get a link between the analyses of external reliability for the systems 1b) and 1a). The analogy enables us to follow in the analyses of the systems 1b) a final general conclusion drawn for the systems 1a), that the better the internal reliability and the conditionality of a system, the smaller is the norm of parameter distortions induced by observation disturbances. The relations between the analyzed concepts, shown by indicating the involved SVD components of the design matrix \mathbf{A} , are presented on a scheme in Fig. 4. The scheme takes into account that the external reliability can be expressed either in terms of the vector of parameter distortions $(\mathbf{U}_r \mathbf{\sigma} \mathbf{V}_r^T)$ or in terms of the 2-norm of this vector $(\mathbf{U}_r \mathbf{\sigma})$.

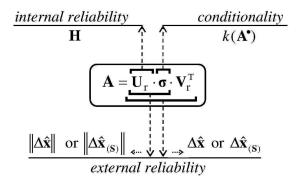


Fig. 4. Links between the concepts of external reliability, internal reliability and conditionality of a system

6. Numerical examples

Example 1. For a given design matrix A (3×2) of full rank, find a matrix equivalent to A with respect to internal reliability, having equal singular values and a matrix equivalent to A with respect to conditionality, obtained with the use of an arbitrary orthogonal transformation matrix. Make a graphical presentation of the systems generated by the 3 matrices.

$$\mathbf{A} = \begin{bmatrix} 1 & -1 \\ 1 & -0.9 \\ 1.1 & -0.95 \end{bmatrix}$$

We get for this matrix:

$$\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathrm{T}} = \begin{bmatrix} \mathbf{0.58088} & -\mathbf{0.78464} & -0.21662 \\ \mathbf{0.55306} & \mathbf{0.18519} & 0.81230 \\ \mathbf{0.59724} & \mathbf{0.59165} & -0.54153 \end{bmatrix} \cdot \begin{bmatrix} 2.43243 & 0 \\ 0 & 0.075916 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} 0.73626 & -0.67670 \\ 0.67670 & 0.73626 \end{bmatrix}$$

(left active singular vectors are marked in bold); pseudo-condition^number $k(\mathbf{A}^{\bullet}) = k(\mathbf{A}^{+}) = 13.2$; indices of internal reliability: $h_{11} = 0.047$; $h_{22} = 0.660$; $h_{33} = 0.293$

Solution

Option 1. Assuming $\sigma_G = I_2$, $V_G = I_2$ we get on the basis of formula (25) (for r = u) the following transformation matrix G_A

$$\mathbf{G}_{A} = \mathbf{V} \mathbf{\sigma}^{-1} = \begin{bmatrix} 0.73626 & 0.67670 \\ -0.67670 & 0.73626 \end{bmatrix} \cdot \begin{bmatrix} 2.43243 & 0 \\ 0 & 0.075916 \end{bmatrix}^{-1} = \begin{bmatrix} 0.30269 & 8.91375 \\ -0.27820 & 9.69839 \end{bmatrix}$$

and hence,

$$\mathbf{A}_{(1)} = \mathbf{AG}_{A} = \begin{bmatrix} 0.58088 & -0.78464 \\ 0.55306 & 0.18519 \\ 0.59724 & 0.59165 \end{bmatrix}$$

which, according to formula (25), is a matrix of left active singular vectors of the initial matrix \mathbf{A} , i.e. \mathbf{U}_{r} . Due to the assumptions, we have $k(\mathbf{A}_{(1)}^{\bullet}) = 1$.

Applying the formula (17) we get the reliability indices, being the same as those for the initial matrix A.

Option 2. Assuming an arbitrary orthogonal matrix K, we transform A as in (26), i.e.

$$\mathbf{A}_{(2)} = \mathbf{K}\mathbf{A} = \begin{bmatrix} 0.83391 & 0.01562 & -0.55168 \\ -0.15162 & 0.96762 & -0.20180 \\ 0.53067 & 0.25193 & 0.80927 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 1 & -0.9 \\ 1.1 & -0.95 \end{bmatrix} = \begin{bmatrix} 0.24267 & -0.32386 \\ 0.59403 & -0.52753 \\ 1.67280 & -1.52621 \end{bmatrix}$$

We can readily check that the resulting matrix $\mathbf{A}_{(2)}$ is conditionality-equivalent to the initial matrix \mathbf{A} , i.e. $k(\mathbf{A}_{(2)}^{\bullet}) = 13.2$, but of different internal reliability (h₁₁ = 0.017; h₂₂ = 0.861; h₃₃ = 0.122).

Graphical presentation of the results is given in Fig. 5. For each of the analyzed cases an ellipse representing $(A^TA)^{-1}$ and the gradients of positional lines are shown.

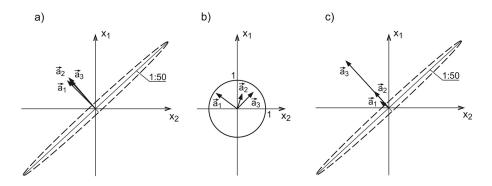


Fig. 5. Graphical presentation of the results: a) initial matrix, b) a matrix reliability-equivalent to that in a), a matrix, conditionality-equivalent to that in a); (major axis in a) and c) is shown at scale 1:50)

As could be expected, both the lengths and the orientation of the gradients in the case b) vary considerably from those in the case a). The lengths of the gradients in c) vary considerably from those in a), whereas their orientation is roughly maintained.

Example 2. For a given matrix A (6×5) of incomplete rank (r = 4), being a design matrix for a simple local levelling network,

$$\mathbf{A} = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 1 \end{bmatrix}$$

and the following options of coefficient matrices S ($S \neq S_o$) in constraint equations as in a system (1b), i.e.

$$\mathbf{S}_{1} = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$
; $\mathbf{S}_{2} = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \end{bmatrix}$; $\mathbf{S}_{3} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \end{bmatrix}$,

find the nonzero eigenvalues and pseudo-conditionⁿumbers for a system 1a) and a system 1b).

Solution

For a system 1a)

$$\lambda_1 = 4.618$$
; $\lambda_2 = 3.618$; $\lambda_3 = 2.382$; $\lambda_4 = 1.382$; $k(\mathbf{A}^{\bullet}) = k(\mathbf{A}^{+}) = 0.85$

For a system 1b)

To verify the property $\lambda_i(\mathbf{A}^T\mathbf{A})_S^- \ge \lambda_i(\mathbf{A}^T\mathbf{A})^+$ and hence $k(\mathbf{A}_S^-) \ge k(\mathbf{A}^+)$ (see Appendix B), we precede the eigenvalues of $(\mathbf{A}^T\mathbf{A})_S^-$ with those of $(\mathbf{A}^T\mathbf{A})^+$, denoted by λ_i and λ_i^+ respectively:

$$\lambda_{1}^{+} = 0.724 \; ; \; \lambda_{2}^{+} = 0.420 \; ; \; \lambda_{3}^{+} = 0.276 \; ; \; \lambda_{4}^{+} = 0.216 \; ; \qquad k(\mathbf{A}^{+}) = 0.85$$

$$\lambda_{1} = 0.734 \; ; \; \lambda_{2} = 0.443 \; ; \; \lambda_{3} = 0.302 \; ; \; \lambda_{4} = 0.232 \; ; \qquad k(\mathbf{A}_{\mathbf{S}_{1}}^{-}) = 0.86$$

$$\lambda_{1} = 1.456 \; ; \; \lambda_{2} = 0.446 \; ; \; \lambda_{3} = 0.281 \; ; \; \lambda_{4} = 0.250 \; ; \qquad k(\mathbf{A}_{\mathbf{S}_{2}}^{-}) = 1.21$$

$$\lambda_{1} = 4.217 \; ; \; \lambda_{2} = 2.618 \; ; \; \lambda_{3} = 0.420 \; ; \; \lambda_{4} = 0.382 \; ; \qquad k(\mathbf{A}_{\mathbf{S}_{3}}^{-}) = 2.05$$

The above listing of eigenvalues and the corresponding pseudo-condition[^]numbers verifies the property in Appendix B.

7. Conclusions

The SVD of the design matrix proved to be useful in seeking the relationships between the measures of internal reliability, external reliability and conditionality of GM models with uncorrelated observations. The analysis concerning the model conditionality had to be based on a substitute measure called pseudo-condition[^]number, developed in this paper for inconsistent systems of linear equations.

And so, the following properties of GM models with respect to interrelations between the above mentioned concepts could be established, covering both the case of the full-rank and the rank-deficient design matrices:

- the concepts of internal response-based reliability and conditionality of a model are not interrelated. Hence, in the design of observation systems each feature can be considered independently of each other. The design operations such as adding or removing observations change both the features, so the lack of interrelation between these features does not seem to offer advantage for the design process, at least at this state of research,
- as could be expected, the external reliability, expressed either as a vector of parameter distortions (as in Baarda definition) or in the form of the 2-norm of this vector (as in this paper), depends on both the conditionality and the internal reliability of a model. The newly derived auxiliary formula for external reliability, although being exact only for the systems with the design matrices having equal singular values, contains the measures of internal reliability and the conditionality in explicit form. It shows in terms of these measures that the appropriately high level of internal reliability and a good conditionality of a system are advantageous for external reliability. Such a general conclusion applies also to systems with minimal constraints on parameters, however the detailed analysis based on the measures of internal reliability and conditionality did not prove possible for such systems.

It seems to the present author that research in this area is worth continuing and should cover the systems with correlated observations. The approach to reliability measures for the systems with singular both the design matrices and the covariance matrices as in Wang and Chen (1999), paves the way for further extension of the research.

Acknowledgments

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APPENDIX A

Derivation of the formulas (11a) and (11b)

By definition of the 2-norm of the matrix A^{\bullet} , we get

$$\left\| \mathbf{A}^{\bullet} \right\| = \sqrt{\lambda_{\text{max}} \left[(\mathbf{A}^{\bullet})^{\text{T}} \mathbf{A}^{\bullet} \right]}$$
 (41)

Using the equality as below (e.g. Kiełbasiński and Schwetlick 1992)

$$\lambda_{\max} \left[(\mathbf{A}^{\bullet})^{\mathrm{T}} \mathbf{A}^{\bullet} \right] = \lambda_{\max} \left[\mathbf{A}^{\bullet} (\mathbf{A}^{\bullet})^{\mathrm{T}} \right]$$
 (42)

we may express (41) in the equivalent form

$$\|\mathbf{A}^{\bullet}\| = \sqrt{\lambda_{\max} [\mathbf{A}^{\bullet} (\mathbf{A}^{\bullet})^{\mathrm{T}}]}$$
 (43)

Applying (43) for each of the two types of the inverse A^{\bullet} , i.e. A^{+} and A_{S}^{-} , we get after several operations

$$\|\mathbf{A}^{+}\| = \sqrt{\lambda_{\max}} [\mathbf{A}^{+} (\mathbf{A}^{+})^{\mathrm{T}}] = \sqrt{\lambda_{\max}} [(\mathbf{A}^{\mathrm{T}} \mathbf{A})^{+} \mathbf{A}^{\mathrm{T}} \mathbf{A} (\mathbf{A}^{\mathrm{T}} \mathbf{A})^{+}] =$$

$$= \sqrt{\lambda_{\max}} [(\mathbf{A}^{\mathrm{T}} \mathbf{A})^{+}] = \sqrt{\left[\lambda_{\min} [(\mathbf{A}^{\mathrm{T}} \mathbf{A})^{+}]\right]^{-1}} = [\sigma_{\min} (\mathbf{A})]^{-1}$$
for all $\lambda_{i} > 0$ or $\sigma_{i} > 0$ (43a)

$$\|\mathbf{A}_{\mathbf{S}}^{-}\| = \sqrt{\lambda_{\max}} [\mathbf{A}_{\mathbf{S}}^{-} (\mathbf{A}_{\mathbf{S}}^{-})^{\mathrm{T}}] = \sqrt{\lambda_{\max}} [(\mathbf{A}^{\mathrm{T}} \mathbf{A})_{\mathbf{S}}^{-} \mathbf{A}^{\mathrm{T}} \mathbf{A} (\mathbf{A}^{\mathrm{T}} \mathbf{A})_{\mathbf{S}}^{-}] = \sqrt{\lambda_{\max}} [(\mathbf{A}^{\mathrm{T}} \mathbf{A})_{\mathbf{S}}^{-}]$$
for all $\lambda_{i} > 0$ (43b)

This ends the derivations.

APPENDIX B

<u>Derivation</u> of the relationship between the eigenvalues of $(\mathbf{A}^T \mathbf{A})_{\mathbf{S}}^-$ and $(\mathbf{A}^T \mathbf{A})^+$ Applying to $(\mathbf{A}^T \mathbf{A})_{\mathbf{S}}^-$ a basic property of generalized inverses, i.e.

$$\mathbf{A}^{\mathrm{T}}\mathbf{A}(\mathbf{A}^{\mathrm{T}}\mathbf{A})_{\mathbf{S}}^{\mathrm{T}}\mathbf{A} = \mathbf{A}^{\mathrm{T}}\mathbf{A} \tag{44}$$

and expressing it in terms of SVD, we shall write

$$\mathbf{V} \begin{bmatrix} \boldsymbol{\lambda} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \mathbf{V}^{\mathrm{T}} \mathbf{V}_{*} \begin{bmatrix} \boldsymbol{\lambda}_{*} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \mathbf{V}_{*}^{\mathrm{T}} \mathbf{V} \begin{bmatrix} \boldsymbol{\lambda} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \mathbf{V}^{\mathrm{T}} = \mathbf{V} \begin{bmatrix} \boldsymbol{\lambda} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \mathbf{V}^{\mathrm{T}}$$

and, since det $\mathbf{V} \neq 0$

$$\begin{bmatrix} \lambda & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{V}^{\mathsf{T}} \mathbf{V}_{*} \begin{bmatrix} \lambda_{*} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{V}_{*}^{\mathsf{T}} \mathbf{V} \begin{bmatrix} \lambda & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \lambda & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$$
(45)

Partitioning V and V_* as in (4), we get

$$\mathbf{V}^{T}\mathbf{V}_{*} = \begin{bmatrix} \mathbf{V}_{r}^{T}\mathbf{V}_{*,r} & \mathbf{V}_{r}^{T}\mathbf{V}_{*,u-r} \\ \mathbf{V}_{u-r}^{T}\mathbf{V}_{*,r} & \mathbf{V}_{u-r}^{T}\mathbf{V}_{*,u-r} \end{bmatrix}$$

and after substituting it into (45) and considering the $r \times r$ blocks only, we obtain the equality

$$\lambda \mathbf{V}_{r}^{\mathsf{T}} \mathbf{V}_{* r} \lambda_{* \mathsf{V}} \mathbf{V}_{* r}^{\mathsf{T}} \mathbf{V}_{r} \lambda = \lambda \tag{46}$$

After a simple modification of (46), we get

$$\mathbf{V}_{r}^{T}\mathbf{V}_{*,r}\boldsymbol{\lambda}_{*}\mathbf{V}_{*,r}^{T}\mathbf{V}_{r} = \boldsymbol{\lambda}^{+} \tag{47}$$

where $\lambda^+ = \lambda^{-1}$ denotes the matrix of eigenvalues of the pseudo-inverse $(\mathbf{A}^T \mathbf{A})^+$.

The matrix $\mathbf{V}_{r}^{T}\mathbf{V}_{*,r}$ can be expressed with the use of its *i,j*-th element (Meyer 2000), as

$$\mathbf{V}_{r}^{T} \mathbf{V}_{*,r} = \left[\cos \alpha(\mathbf{v}_{r,i}, \mathbf{v}_{*r,j}) \right] \quad i, j = 1, 2, \dots, r$$
 (48)

where:

 $v_{r,i},~v_{*r,j}$ – the column-vectors of $\mathbf{V}_{r},~\mathbf{V}_{*,r}$ respectively,

 $\alpha-$ the angle between the column-vectors $v_{r,i},\,v_{*r,j}.$

Applying the simplified notation $\mathbf{V}_{r}^{T}\mathbf{V}_{*,r} = [c_{ij}]$ in (48) and substituting it into (47), we obtain after carrying out several operations a consistent system of r equations in r unknowns, i.e. $\lambda_{*,1}, \lambda_{*,2}, ..., \lambda_{*,-}$

$$c_{11}^{2}\lambda_{*,1} + c_{12}^{2}\lambda_{*,2} + \dots + c_{1r}^{2}\lambda_{*,\mathbf{r}} = \lambda_{1}^{+}$$

$$c_{21}^{2}\lambda_{*,1} + c_{22}^{2}\lambda_{*,2} + \dots + c_{2r}^{2}\lambda_{*,\mathbf{r}} = \lambda_{2}^{+}$$

$$\dots$$

$$c_{r1}^{2}\lambda_{*,1} + c_{r2}^{2}\lambda_{*,2} + \dots + c_{rr}^{2}\lambda_{*,\mathbf{r}} = \lambda_{r}^{+}$$

$$(49)$$

where:

$$\lambda_{*,i} > 0, \ \lambda_{i}^{+} > 0; \ 0 \le c_{ij}^{2} \le 1, \ \sum c_{i \bullet}^{2} \le 1, \ \sum c_{\bullet i}^{2} \le 1, \ i,j = 1,2,...,r,$$

(i•), (•j) indicate that summation runs in a column or a row of the coefficient matrix, respectively.

It can be proved that with the limitations for the values of coefficients, the unknowns and the free terms as listed above, the solution of the system satisfies the inequalities

$$\lambda_{*,i} \ge \lambda_i^+, \qquad i = 1, ..., r,$$
 excluding $\lambda_{*,i} = \lambda_i^+$ for all " i " and $(\lambda_*)_{\max} = (\lambda^+)_{\max}$

To verify the appropriateness of excluding the equality $(\lambda_*)_{max} = (\lambda^+)_{max}$, we carry out the reasoning presented below.

Since $\Delta \hat{\mathbf{x}}$ as in (27) is a minimum norm solution, we have for $\mathbf{S} \neq \mathbf{S}_0 \quad \left\| \Delta \hat{\mathbf{x}}_{(\mathbf{s})} \right\| > \left\| \Delta \hat{\mathbf{x}} \right\|$, and hence

$$\left(\frac{\left\|\Delta\hat{\mathbf{x}}_{(\mathbf{S})}\right\|}{\left\|\Delta\mathbf{y}\right\|}\right)_{\max} > \left(\frac{\left\|\Delta\hat{\mathbf{x}}\right\|}{\left\|\Delta\mathbf{y}\right\|}\right)_{\max}$$

Taking into account (9) and (43a), (43b) we get

$$\lambda_{\text{max}}(\mathbf{A}^{\mathsf{T}}\mathbf{A})_{\mathbf{S}}^{-} > \lambda_{\text{max}}(\mathbf{A}^{\mathsf{T}}\mathbf{A})^{+}$$

which verifies the above exclusion.

Due to (11a) and (11b), we get $k(\mathbf{A}_{\mathbf{S}}^{-}) > k(\mathbf{A}^{+})$, which ends the derivations.

APPENDIX C

Proof for the property (40)

For the systems 1b) we shall write (27) in the form

$$\Delta \hat{\mathbf{x}}_{(s)} = (\mathbf{A}^{\mathsf{T}} \mathbf{A})_{s}^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \cdot \Delta \mathbf{y} \quad \text{where } \mathbf{S} \neq \mathbf{S}_{0}$$
 (50)

Expressing the formula (50) in terms of the 2-norm and applying SVD for the components, we obtain

$$\left\|\Delta\hat{\mathbf{x}}_{(s)}\right\|^{2} = \Delta\mathbf{y}^{\mathrm{T}}\mathbf{A}(\mathbf{A}^{\mathrm{T}}\mathbf{A})_{s}^{\mathrm{T}}(\mathbf{A}^{\mathrm{T}}\mathbf{A})_{s}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}} \cdot \Delta\mathbf{y} =$$

$$= \Delta \mathbf{y}^{\mathrm{T}} \mathbf{U} \begin{bmatrix} \mathbf{\sigma} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{V}^{\mathrm{T}} \mathbf{V}_{*} \begin{bmatrix} \boldsymbol{\lambda}_{*} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{V}_{*}^{\mathrm{T}} \mathbf{V}_{*} \begin{bmatrix} \boldsymbol{\lambda}_{*} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{V}_{*}^{\mathrm{T}} \mathbf{V} \begin{bmatrix} \mathbf{\sigma} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{U}^{\mathrm{T}} \cdot \Delta \mathbf{y}$$

Partitioning U, V and V_* as in (4) and carrying out several simple operations, we obtain

$$\left\|\Delta \hat{\mathbf{x}}_{(s)}\right\|^{2} = \Delta \mathbf{y}^{\mathrm{T}} \mathbf{U}_{\mathrm{r}} \mathbf{\sigma} \mathbf{V}_{\mathrm{r}}^{\mathrm{T}} \mathbf{V}_{*,\mathrm{r}} \lambda_{*}^{2} \mathbf{V}_{*,\mathrm{r}}^{\mathrm{T}} \mathbf{V}_{\mathrm{r}} \mathbf{\sigma} \mathbf{U}_{\mathrm{r}}^{\mathrm{T}} \cdot \Delta \mathbf{y}$$

Taking into account the property (47) and realizing that $\lambda^+ = \sigma^{-2}$, we get

$$\left\|\Delta \hat{\mathbf{x}}_{(s)}\right\|^{2} = \Delta \mathbf{y}^{\mathrm{T}} \mathbf{U}_{\mathrm{r}} \mathbf{\sigma}^{-1} (\mathbf{V}_{*,\mathrm{r}}^{\mathrm{T}} \mathbf{V}_{\mathrm{r}})^{-1} (\mathbf{V}_{\mathrm{r}}^{\mathrm{T}} \mathbf{V}_{*,\mathrm{r}})^{-1} \mathbf{\sigma}^{-1} \mathbf{U}_{\mathrm{r}}^{\mathrm{T}} \cdot \Delta \mathbf{y}$$

and hence

$$\left\|\Delta \hat{\mathbf{x}}_{(\mathbf{s})}\right\|^2 = \left\| (\mathbf{V}_r^T \mathbf{V}_{*,r})^{-1} \mathbf{\sigma}^{-1} \mathbf{U}_r^T \cdot \Delta \mathbf{y} \right\|^2$$
 (51)

which, for a system 1a) where $\mathbf{V}_{r}^{T}\mathbf{V}_{*,r} = \mathbf{I}$, is consistent with (32).

Using a well known property, that $\|\Delta \hat{\mathbf{x}}_{(s)}\| > \|\Delta \hat{\mathbf{x}}_{(s_0)}\|$ for any nonzero vector $\Delta \mathbf{y}$, we get on the basis of (32) the inequality

$$\left\|\Delta \hat{\mathbf{x}}_{(\mathbf{s})}\right\| > \left\|\mathbf{\sigma}^{-1}\mathbf{U}_{r}^{T} \cdot \Delta \mathbf{y}\right\|$$

which proves the property.

Badanie związków między niezawodnością wewnętrzną i zewnętrzną a uwarunkowaniem układu w modelach Gaussa-Markova z nieskorelowanymi obserwacjami

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Streszczenie

Badany jest związek między niezawodnością wewnętrzną bazującą na odpowiedziach modelu a uwarunkowaniem układu dla modeli Gaussa-Markova z obserwacjami nieskorelowanymi. Rozpatrywane są przy tym modele z macierzami projektu pełnego i niepełnego rzędu. Wzory wyprowadzone przy użyciu rozkładu macierzy ze względu na wartości szczególne (SVD) wskazują wyraźnie, że te dwa badane pojęcia są wzajemnie niezależne. Przedstawione są metody konstruowania dla danej macierzy projektu macierzy równoważnych pod względem niezawodności wewnętrznej oraz macierzy równoważnych pod względem uwarunkowania. Aby umożliwić analizę uwarunkowania modeli GM stanowiących w ogólności układy sprzeczne, wyprowadzono pseudo-wskaźnik zastępujący wskaźnik uwarunkowania układu powszechnie stosowany w numerycznej algebrze liniowej. Także na podstawie rozkładu SVD zaproponowano wzór określający niezawodność zewnętrzną bazujący na 2-giej normie wektora zniekształceń parametrów indukowanych przez minimalny wykrywalny bład w danej obserwacji. Dla układów z jednakowymi niezerowymi wartościami szczególnymi wzór ten może być wyrażony poprzez wskaźnik niezawodności wewnętrznej oraz pseudo-wskaźnik uwarunkowania. Z tymi miarami występującymi w postaci jawnej, wzór ukazuje, chociaż jedynie dla powyższych specyficznych układów, charakter wpływu niezawodności wewnętrznej i uwarunkowania modelu na jego niezawodność zewnętrzną. Dowody uzupełniających własności dotyczących pseudo-wskaźnika uwarunkowania oraz 2-giej normy wektora zniekształceń parametrów w układach z minimalnymi ograniczeniami, zamieszczone są w Dodatkach. Teoria ilustrowana jest na przykładach numerycznych.