On the Unified Approach of the Least Squares Method

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Abstract

In the adjustment of observations by the Least Squares Method the variance covariance matrix (of observations) is usually a positive definite matrix. In cases such as the derived observations, e.g. in the sequential approach (stepwise adjustment) for the assessment and interpretation of the geodetic data for the detection of possible spatial displacements and the estimation of deformation parameters, the covariance matrix may be singular. In this case the problem is the choice of a g-inverse matrix as a weight matrix that leads to the Best Linear Unbiased Estimation. Several attempts have been presented which finally end up in the Rao-Mitra approach of Unified Least Squares.

1. Introduction

In the standard linear model being used in geodetic data analysis, the observation equations are written as

$$\mathbf{b} = \mathbf{A}\ \mathbf{x} + \mathbf{v} \tag{1}$$

where $\mathbf{b} = \mathbf{y}^b - \mathbf{y}^o$ is the $\mathrm{n} \times 1$ vector of the observables, $\mathbf{A}$ is the $\mathrm{n} \times \mathrm{m}$ matrix of known coefficients (design matrix) of the unknown parameters $\mathbf{x}$ and $\mathbf{v}$ the unknown observational errors. The relations

$$\begin{aligned} &E\{\mathbf{v}\} = \mathbf{0} \\ &E\{\mathbf{v}\mathbf{v}^T\} = \mathbf{C} = \sigma^2\ \mathbf{Q} \end{aligned} \tag{2}$$

describe the stochastic model, where σ^2 is the unknown variance of unit weight and $\mathbf{C}$ is the $\mathrm{n} \times \mathrm{n}$ covariance matrix of observations. The cofactor or weight coefficients matrix $\mathbf{Q}$ is usually positive definite.

In case $\mathbf{Q} = \mathbf{I}$ and matrix $\mathbf{A}$ is full of rank in (1), Adrien-Marie Legendre (1752-1833) in 1806 and Carl-Friedrich Gauss (1777-1855) in 1809 propounded the famous theory of Least Squares which postulates that the Best Linear Unbiased Estimates of $\mathbf{x}$ is obtained by minimizing the sum of squares $\mathbf{v}^T\mathbf{v}$. At the beginning of 20 century Andrei Markov (1856-1922) was credited with justifying the method of least squares without superfluous assumptions of normality. Because of this contribution the key theorem in the theory of least squares is often refer to as Gauss-Markov theorem. If $\mathbf{Q} \neq \mathbf{I}$, but nonsingular, Alexander Craig Aitken (1895-1967), one of New-Zealand's greater mathematicians, proposed to minimize the sum of weighed least squares $\mathbf{v}^T \mathbf{P}\, \mathbf{v}$, which leads to the Best Linear Unbiased Estimate of $\mathbf{x}$ when $\mathbf{P} = \mathbf{Q}^{-1}$.

When the rank of **A** is not full, a situation which was first formulated by the Indian mathematician and statistician Raj Chandra Bose (1901-1987), Rao (1945, 1962) showed that the theory of least squares is still applicable. He was first led to the pseudo-inverse of **N** and to the concept that any solution of the normal equations $\mathbf{N}\,\hat{\mathbf{x}} = \mathbf{u}$ is the best linear unbiased estimate of $\mathbf{x}$. He showed that in the discussion of least squares theory one needs the so called Moore-Penrose inverse only in the weak sense of non-estimable parameters. The concept of pseudo-inverse was introduced by Erik Ivar Fredholm (1866-1927) in 1903 and the pseudo-inverse matrix was independently described by Eliakim Hastings Moore (1862-1932) in 1920, Arne Bjerhammar in 1951 and Roger Penrose in 1955.

In the case of geodetic networks the rank deficiency of matrix **A** is related to the reference frame definition problem, the well known datum problem or zero order design problem in the geodetic literature. The reference frame definition problem has received considerable attention in the geodetic world since the pioneering work of Meissl (1969) and its popularization by Blaha (1971). The nature of the problem has been clarified in two important papers by Grafarend and Schaffrin (1974, 1976) while the relation of various solutions to Meissl's inner solution has been established with the introduction of the S-transformation by Baarda (1973). This problem dominated the geodetic literature in the 70s, although it still remains opportune in GNSS applications, as well as in the assessment of geodetic data for the detection of possible displacements and the estimation of deformation parameters.

If the observation vector consists of original observations, the cofactor matrix **Q** will be always positive definite. In cases, however, of derived observations it may be singular. If an unknown vector $\mathbf{x}$ resulting from an adjustment of incomplete observations will be used in a second adjustment, the cofactor matrix $\mathbf{Q}_\mathbf{x}$ is singular and has no ordinary inverse. Rao and Mitra (1971b) suggested one unified method of least squares which holds good whether **Q** is singular or not. Related works have been provided by Bjerhammer (1973), Uotila (1974), Pelzer (1974), Wolf (1979), Niemeir (1979), Perelmuter (1981), Caspary (1983), Sjöberg (1985), Nkuite (1998) and Nkuite and Mierlo (1998).

2. The weight matrix

The Least Squares Estimation is equivalent to the Best Linear Unbiased Estimation in the case that the variance-covariance matrix **Q** of observations is nonsingular and the weight matrix is the regular inverse $\mathbf{P} = \mathbf{Q}^{-1}$. In the case that the variance-covariance matrix of observations is singular, a general inverse $\mathbf{Q}^{g}$ can be used as the weight matrix **P**, therefore the pseudo-inverse matrix $\mathbf{P} = \mathbf{Q}^{+}$ itself. In this case the best linear unbiased estimation of the parameters **x** doesn't depend on the choice of the g-inverse $\mathbf{Q}^{g}$ (Mitra and Rao, 1968).

The question that arises is the following: *Does there exists a weight matrix* **P** *that can be used in least squares estimation to get the best linear unbiased estimation of parameters* **x** *in any case, regardless of the rank of matrix* **Q**? The answer is that such a matrix exists and emerges as g-inverse of the matrix $\mathbf{M} = (\mathbf{Q} + \mathbf{AUA}^{T})$

$$\mathbf{P} = \mathbf{M}^{g} = (\mathbf{Q} + \mathbf{AUA}^{T})^{g} \tag{3}$$

where **U** is a symmetric matrix, such that the number of rank of $\mathbf{Q} + \mathbf{AUA}^{T}$ is equal to the rank of [**Q A**]. This solution was given by Rao and Mitra (1971b) and Rao (1971, 1972) where a generalized method called "unified theory of least squares" has been developed which doesn't depend on the rank of matrix **Q**. This solution has also been proposed in geodetic literature by Bjerhammer (1973) and Uotila (1974).

From the observation equations (1), satisfying the minimum criterion

$$\mathbf{v}^{T}\mathbf{P}\ \mathbf{v} = \mathbf{v}^{T}(\mathbf{Q} + \mathbf{AUA}^{T})^{g}\mathbf{v} = \min. \tag{4}$$

where $\mathbf{P} = \mathbf{M}^{g}$, the system of normal equations is obtained

$$\mathbf{N}\ \hat{\mathbf{x}} = \mathbf{u} \tag{5}$$

where $\mathbf{N} = \mathbf{A}^{T}\mathbf{P}\ \mathbf{A} = \mathbf{A}^{T}(\mathbf{Q} + \mathbf{AUA}^{T})^{g}\mathbf{A}$ and $\mathbf{u} = \mathbf{A}^{T}\mathbf{P}\ \mathbf{b} = \mathbf{A}^{T}(\mathbf{Q} + \mathbf{AUA}^{T})^{g}\mathbf{b}$.

There are three key notes that should be mentioned:

1. The weight matrix (3) can be considered as a general solution since, when **Q** is regular, it is proved that the solution obtained with this choice is equivalent to the solution where $\mathbf{P} = \mathbf{Q}^{-1}$. The proof of this proposal is simple (Uotila, 1974): The expressions bellow are valid

$$\left[\mathbf{A}^{T}(\mathbf{Q} + \mathbf{AUA}^{T})^{-1}\mathbf{A}\right]\hat{\mathbf{x}} = \mathbf{A}^{T}(\mathbf{Q} + \mathbf{AUA}^{T})^{-1}\mathbf{b}$$

or

$$\begin{aligned}&\left[\mathbf{I} - \mathbf{A}^{T}\mathbf{Q}^{-1}\mathbf{A}(\mathbf{A}^{T}\mathbf{Q}^{-1}\mathbf{A} + \mathbf{U}^{-1})^{-1}\right]\mathbf{A}^{T}\mathbf{Q}^{-1}\mathbf{A}\ \hat{\mathbf{x}} = \\ &\qquad = \left[\mathbf{I} - \mathbf{A}^{T}\mathbf{Q}^{-1}\mathbf{A}(\mathbf{A}^{T}\mathbf{Q}^{-1}\mathbf{A} + \mathbf{U}^{-1})^{-1}\right]\mathbf{A}^{T}\mathbf{Q}^{-1}\mathbf{b}\end{aligned} \tag{6}$$

Due to the fact that matrix $\mathbf{I}-\mathbf{A}^T\mathbf{Q}^{-1}\mathbf{A}(\mathbf{A}^T\mathbf{Q}^{-1}\mathbf{A}+\mathbf{U}^{-1})^{-1}$ is regular, the expression above becomes $(\mathbf{A}^T\mathbf{Q}^{-1}\mathbf{A})\,\hat{\mathbf{x}}=\mathbf{A}^T\mathbf{Q}^{-1}\mathbf{b}$.

2. The least squares criterion $\mathbf{v}^T\mathbf{P}\,\mathbf{v}$ doesn't depend on the choice of the g-inverse $\mathbf{M}^g=(\mathbf{Q}+\mathbf{AUA}^T)^g$ and generally, under appropriate conditions (Rao, 1972) that usually are fulfilled in the geodetic applications (Nkuite and Mierlo, 1998), it doesn't depend on any choice of g-inverse $\mathbf{Q}^g$. The expression bellow is valid

$$\mathbf{v}^T\mathbf{Q}^g\,\mathbf{v}=\mathbf{v}^T(\mathbf{Q}+\mathbf{AUA}^T)^g\,\mathbf{v} \tag{7}$$

3. Although $\mathbf{Q}$ may be singular, there is a possibility of $\mathbf{M}=(\mathbf{Q}+\mathbf{AUA}^T)$ being non-singular, in which case the weight matrix $\mathbf{P}$ would be the regular inverse $\mathbf{P}=\mathbf{M}^{-1}$.

A simple choice of $\mathbf{U}$ in all situations is $\mathbf{U}=\delta^2\,\mathbf{I}$ and $\mathbf{P}=(\mathbf{Q}+\delta^2\mathbf{AA}^T)^g$, where the coefficient δ^2 ($\delta\neq 0$) regulates the magnitude of the elements of the matrix $\mathbf{AA}^T$ compared to the elements of matrix $\mathbf{Q}$. This choice of $\mathbf{U}$ seems to have some advantages. Even if $\mathbf{Q}$ is singular, it may so happen that $\mathbf{M}$ is nonsingular, in which case $\mathbf{P}$ can result as a regular inverse ($\mathbf{P}=\mathbf{M}^{-1}$). In case that $\mathbf{Q}$ is nonsingular but ill-conditioned, the computation of $(\mathbf{Q}+\delta^2\mathbf{AA}^T)^{-1}$ may be more stable than $\mathbf{Q}^{-1}$.

3. Computation of adjusted parameters and a-posteriori errors

The solution of the normal equations (5), with constraints $\mathbf{H\,x}=\mathbf{z}$, doesn't depend on the choice of the weight matrix $\mathbf{P}$ ($\mathbf{P}=\mathbf{Q}^{-1}$ when $\mathbf{Q}$ is nonsingular, $\mathbf{P}=\mathbf{Q}^g$ when $\mathbf{Q}$ is singular, or generally $\mathbf{P}=\mathbf{M}^g$ when $\mathbf{Q}$ may be whether singular or not), and can be summarized as below (Dermanis, 1986):

a. Minimal constraints solution:

$$\hat{\mathbf{x}}=\mathbf{N}^g\mathbf{u}+\mathbf{E}^T(\mathbf{HE}^T)^{-1}\mathbf{z}=\mathbf{R}^{-1}\mathbf{u}+\mathbf{E}^T(\mathbf{HE}^T)^{-1}\mathbf{z} \tag{8}$$

where

$$\mathbf{N}^g=(\mathbf{N}+\mathbf{H}^T\mathbf{H})^{-1}-\mathbf{E}^T(\mathbf{HE}^T)^{-1}(\mathbf{EH}^T)^{-1}\mathbf{E} \quad \text{and} \quad \mathbf{R}=\mathbf{N}+\mathbf{H}^T\mathbf{H} \tag{9}$$

and the rank of $\mathbf{H}$ is equal to the number of rank defects of $\mathbf{A}$. The inner constraints solution ($\mathbf{E\,x}=\mathbf{0}$) is

$$\hat{\mathbf{x}}=\mathbf{N}^+\,\mathbf{u}=(\mathbf{N}+\mathbf{E}^T\mathbf{E})^{-1}\mathbf{u} \tag{10}$$

where $\mathbf{N}^+$ is the pseudo-inverse matrix of $\mathbf{N}$,

$$\mathbf{N}^+=(\mathbf{N}+\mathbf{E}^T\mathbf{E})^{-1}-\mathbf{E}^T(\mathbf{EE}^T)^{-1}(\mathbf{EE}^T)^{-1}\mathbf{E}\quad . \tag{11}$$

b. Redundant constraints solution:

$$\hat{\mathbf{x}} = [\mathbf{R}^{-1} - \mathbf{R}^{-1}\mathbf{H}^T(\mathbf{H}\,\mathbf{R}^{-1}\mathbf{H}^T)^{-1}\mathbf{H}\,\mathbf{R}^{-1}]\,\mathbf{u} + \mathbf{R}^{-1}\mathbf{H}^T(\mathbf{H}\,\mathbf{R}^{-1}\mathbf{H}^T)^{-1}\mathbf{z} = \\ = \hat{\mathbf{x}}_R - \mathbf{R}^{-1}\mathbf{H}^T(\mathbf{H}\,\mathbf{R}^{-1}\mathbf{H}^T)^{-1}(\mathbf{H}\,\hat{\mathbf{x}}_R - \mathbf{z}) = \hat{\mathbf{x}}_R - \delta\hat{\mathbf{x}} \tag{12}$$

where

$$\mathbf{R} = \mathbf{N} + \mathbf{H}^T\mathbf{H}\,, \quad \hat{\mathbf{x}}_R = \mathbf{R}^{-1}\,\mathbf{u} \tag{13}$$

and the g-inverse is $\mathbf{N}^g = \mathbf{R}^{-1} - \mathbf{R}^{-1}\mathbf{H}^T(\mathbf{H}\,\mathbf{R}^{-1}\mathbf{H}^T)^{-1}\mathbf{H}\,\mathbf{R}^{-1}$.

The adjusted residuals and the a-posteriori variance of unit weight are evaluated as

$$\hat{\mathbf{v}} = \mathbf{b} - \mathbf{A}\,\hat{\mathbf{x}}\,, \quad \hat{\sigma}^2 = \frac{1}{f}\,\hat{\mathbf{v}}^T\mathbf{P}\,\hat{\mathbf{v}} \tag{14}$$

where $f = tr(\mathbf{WQ})$ are the degrees of freedom and the adjusted residuals $\hat{\mathbf{v}}$ corresponds to $\mathbf{v}$ through the matrix $\mathbf{W}$

$$\hat{\mathbf{v}} = \mathbf{Q}(\mathbf{P} - \mathbf{P}\,\mathbf{A}\,\mathbf{N}^g\mathbf{A}^T\mathbf{P}) = \mathbf{QW}\,\mathbf{v} \tag{15}$$

The Minimum Norm Quadratic Unbiased Estimation (MINQUE) of the variance of unit weight σ^2 and its variance (under the assumption of normally distributed observations), for $\mathbf{P} = \mathbf{M}^g$, are given by

$$\hat{\sigma}^2 = \frac{1}{f}\,\hat{\mathbf{v}}^T(\mathbf{Q} + \mathbf{AUA}^T)^g\,\hat{\mathbf{v}} \quad \text{and} \quad \sigma^2(\hat{\sigma}^2) = \frac{2\hat{\sigma}^4}{f}\ . \tag{16}$$

The covariance matrices of the adjusted parameters $\hat{\mathbf{x}}$, the residuals $\hat{\mathbf{v}}$ and the observations $\hat{\mathbf{y}}$, for the general choice $\mathbf{P} = \mathbf{M}^g$, follow by

$$\hat{\mathbf{C}}_{\hat{\mathbf{x}}} = \hat{\sigma}^2\mathbf{Q}_{\hat{\mathbf{x}}} = \hat{\sigma}^2\left(\{\mathbf{A}^T(\mathbf{Q} + \mathbf{AUA}^T)^g\,\mathbf{A}\}^g - \mathbf{U}\right) \tag{17}$$

$$\hat{\mathbf{C}}_{\hat{\mathbf{v}}} = \hat{\sigma}^2\mathbf{Q}_{\hat{\mathbf{v}}} = \hat{\sigma}^2\left(\mathbf{Q} - \mathbf{AQ}_{\hat{\mathbf{x}}}\mathbf{A}^T\right) \tag{18}$$

and

$$\hat{\mathbf{C}}_{\hat{\mathbf{y}}} = \hat{\sigma}^2\mathbf{Q}_{\hat{\mathbf{y}}} = \hat{\sigma}^2\mathbf{AQ}_{\hat{\mathbf{x}}}\mathbf{A}^T\ . \tag{19}$$

If the cofactor matrix $\mathbf{Q}$ is nonsingular, the relation

$$[\mathbf{A}^T(\mathbf{Q} + \mathbf{AUA}^T)^{-1}\mathbf{A}]^g = (\mathbf{A}^T\mathbf{Q}^{-1}\mathbf{A})^g + \mathbf{U} \tag{20}$$

being in effect, it is proved that the cofactor matrix of adjusted parameters becomes $\mathbf{Q}_{\hat{\mathbf{x}}} = (\mathbf{A}^T\mathbf{Q}^{-1}\mathbf{A})^g$.

4. Statistical evaluation of the results

A general check on the overall validity of the Gauss-Markov model is based on the a-posteriori variance of unit weight $\hat{\sigma}^2$. The null hypothesis $H_o : \sigma^2 = \sigma_o^2$ for the value of unit weight σ^2, where σ_o^2 is its a-priori value, is tested against the alternative hypothesis $H_a : \sigma^2 \neq \sigma_o^2$ using the statistics

$$\chi = \frac{f\,\hat{\sigma}^2}{\sigma_o^2} = \frac{\hat{\mathbf{v}}^T (\mathbf{Q} + \mathbf{AUA}^T)^g\ \hat{\mathbf{v}}}{\sigma_o^2} \sim \chi_f^2 \tag{21}$$

or, alternatively

$$F = \frac{\hat{\sigma}^2}{\sigma_o^2} = \frac{\hat{\mathbf{v}}^T (\mathbf{Q} + \mathbf{AUA}^T)^g\ \hat{\mathbf{v}}}{f\,\sigma_o^2} \sim F_{f,\infty}\ . \tag{22}$$

For the purposes of data snooping in the case of correlated observations, the modified errors are calculated as

$$\hat{\hat{\mathbf{v}}} = \mathbf{P}\ \hat{\mathbf{v}}\,,\ \ \mathbf{Q}_{\hat{\hat{\mathbf{v}}}} = \mathbf{P}\ \mathbf{Q}_{\hat{\mathbf{v}}}\mathbf{P} \tag{23}$$

where $\mathbf{P} = \mathbf{Q}^{-1}$ when $\mathbf{Q}$ is nonsingular, $\mathbf{P} = \mathbf{Q}^g$ when $\mathbf{Q}$ is singular, or generally $\mathbf{P} = (\mathbf{Q} + \mathbf{AUA}^T)^g$ when $\mathbf{Q}$ may be either singular or not. The test statistic is

$$t_i = \tau_i \sqrt{\frac{f-1}{f-\tau_i^2}} \sim t_{f-1} \tag{24}$$

where the standardized residual is

$$\tau_i = \frac{\hat{\hat{v}}_i}{\hat{\sigma}(\hat{\hat{v}}_i)} = \frac{\hat{\hat{v}}_i}{\hat{\sigma}\ \bar{q}_{ii}} = \frac{(\mathbf{P}\ \hat{\mathbf{v}})_i}{\hat{\sigma}\ \sqrt{(\mathbf{P}\ \mathbf{Q}_{\hat{\mathbf{v}}}\mathbf{P})_{ii}}} \tag{25}$$

and $\bar{q}_{ii}^2 = q^2(\hat{\hat{v}}_i) = (\mathbf{P}\mathbf{Q}_{\hat{\mathbf{v}}}\mathbf{P})_{ii}$ (26)

is the weight coefficient of the modified error $\hat{\hat{v}}_i = (\mathbf{P}\hat{\mathbf{v}})_i$.

A test for many outliers is obtained if the null hypothesis $H_o : \mathbf{v}_2 = \mathbf{0}$, that all outliers (of n_2 observations) are equal to zero, is tested against the alternative hypothesis $H_2 : \mathbf{v}_2 \neq \mathbf{0}$ that the outliers are present. The test statistic is

$$T = \frac{\hat{\mathbf{v}}_2^T (\mathbf{P}_2 - \mathbf{A}_2\mathbf{N}^g\mathbf{A}_2^T)^{-1}\hat{\mathbf{v}}_2}{n_2\,\hat{\sigma}^2}\ \ ,\ \ F = T\frac{f-n_2}{f-n_2\,T} \sim F_{n_2, f-n_2} \tag{27}$$

where the indicator (2) corresponds to n_2 observations which are tested.

For the general linear hypothesis, the hypothesis to be tested involves *k* relations on the m parameters **x**. The general hypothesis H_o: $\mathbf{H\,x} = \mathbf{z}$, is tested against the alternative H_a: $\mathbf{H\,x} \neq \mathbf{z}$ and the test statistic, which follows the F distribution, is

$$F = \frac{(\mathbf{H}\,\hat{\mathbf{x}} - \mathbf{z})^T (\mathbf{H}\,\mathbf{Q}_{\hat{\mathbf{x}}} \mathbf{H}^T)^g (\mathbf{H}\,\hat{\mathbf{x}} - \mathbf{z})}{k\,\hat{\sigma}^2} = \frac{\hat{\mathbf{e}}^T \mathbf{S}^g\,\hat{\mathbf{e}}}{k\,\hat{\sigma}^2} \sim F_{k,f} \tag{28}$$

where $\hat{\mathbf{e}} = \mathbf{H}\,\hat{\mathbf{x}} - \mathbf{z}$ and $\mathbf{S} = \mathbf{H}\,\mathbf{Q}_{\hat{\mathbf{x}}} \mathbf{H}^T = \mathbf{H}\left(\{\mathbf{A}^T (\mathbf{Q} + \mathbf{AUA}^T)^g \mathbf{A}\}^g - \mathbf{U}\right)\mathbf{H}^T$. (29)

The alternative form of the above test

$$F = \frac{f}{k} \frac{\delta\hat{\varphi}}{\hat{\varphi}} = \frac{f}{k} \frac{\delta\hat{\varphi}}{\hat{\varphi}_H - \delta\hat{\varphi}} \sim F_{k,f} \tag{30}$$

is valid only for the case $\mathbf{P} = \mathbf{Q}^{-1}$ and $\mathbf{P} = \mathbf{Q}^g$. When the weight matrix is a g-inverse of $\mathbf{M} = \mathbf{Q} + \mathbf{AUA}^T$, the quantity $\hat{\mathbf{e}}^T \mathbf{S}^g\,\hat{\mathbf{e}}$ cannot be obtained as the difference $\delta\hat{\varphi} = \hat{\varphi}_H - \hat{\varphi}$, where $\hat{\varphi}_H = \hat{\mathbf{v}}_H^T\,\mathbf{P}\,\hat{\mathbf{v}}_H$ is the least squares criterion which corresponds to the adjustment with constraints $\mathbf{H}\,\mathbf{x} = \mathbf{z}$ and $\hat{\varphi} = \hat{\mathbf{v}}^T\,\mathbf{P}\,\hat{\mathbf{v}}$ is the least squares criterion of the simple model without constraints.

5. Conclusions

The Least Squares Estimation is equivalent to the Best Linear Unbiased Estimation in the case that the variance-covariance matrix **Q** of observations is nonsingular and the weight matrix is the regular inverse $\mathbf{P} = \mathbf{Q}^{-1}$.

In case the variance-covariance matrix of the observations is singular, and under appropriate conditions (that usually are fulfilled in the geodetic applications), a general inverse $\mathbf{Q}^g$ can be used as the weight matrix **P**, as well as the pseudo-inverse matrix ($\mathbf{P} = \mathbf{Q}^+$). In this case the best linear unbiased estimation doesn't depend on the choice of the g-inverse.

According to Rao and Mitra (1971b) a unified theory of least squares, with the simple choice for the weight matrix $\mathbf{P} = \mathbf{M}^g = (\mathbf{Q} + \mathbf{AUA}^T)^g$, valid for all situations whether the variance-covariance matrix of observations **Q** is non-singular or not, whether there are constraints on the parameters or not and whatever may be the rank of the design matrix **A**. It must be noted that we do not need to choose a general inversion of **M**, as all the expressions involved are invariant for any choice of $\mathbf{M}^g$.

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