

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/225446169>

An iterative solution of weighted total least-squares adjustment

Article in *Journal of Geodesy* · April 2010

DOI: 10.1007/s00190-010-0431-1

CITATIONS

122

READS

844

3 authors, including:



Yunzhong Shen

Tongji University

149 PUBLICATIONS 1,782 CITATIONS

[SEE PROFILE](#)



Bofeng Li

Tongji University

177 PUBLICATIONS 2,024 CITATIONS

[SEE PROFILE](#)

Some of the authors of this publication are also working on these related projects:



GNSS precise orbit determination [View project](#)



PostDoc Job in GNSS group of Tongji University [View project](#)

An iterative solution of weighted total least-squares adjustment

Yunzhong Shen · Bofeng Li · Yi Chen

Received: 31 December 2008 / Accepted: 22 November 2010 / Published online: 9 December 2010
© Springer-Verlag 2010

Abstract Total least-squares (TLS) adjustment is used to estimate the parameters in the errors-in-variables (EIV) model. However, its exact solution is rather complicated, and the accuracies of estimated parameters are too difficult to analytically compute. Since the EIV model is essentially a non-linear model, it can be solved according to the theory of non-linear least-squares adjustment. In this contribution, we will propose an iterative method of weighted TLS (WTLS) adjustment to solve EIV model based on Newton–Gauss approach of non-linear weighted least-squares (WLS) adjustment. Then the WLS solution to linearly approximated EIV model is derived and its discrepancy is investigated by comparing with WTLS solution. In addition, a numerical method is developed to compute the unbiased variance component estimate and the covariance matrix of the WTLS estimates. Finally, the real and simulation experiments are implemented to demonstrate the performance and efficiency of the presented iterative method and its linearly approximated version as well as the numerical method. The results show that the proposed iterative method can obtain such good solution as WTLS solution of Schaffrin and Wieser (J Geod 82:415–421, 2008) and the presented numerical method can be reasonably applied to evaluate the accuracy of WTLS solution.

Y. Shen (✉) · B. Li · Y. Chen
Department of Surveying and Geo-informatics, Tongji University,
1239 Siping Road, Shanghai 200092, People's Republic of China
e-mail: yzshen@tongji.edu.cn

B. Li
e-mail: bofeng_li@163.com

Y. Shen · Y. Chen
Key Laboratory of Advanced Surveying Engineering of State Bureau
of Surveying and Mapping, Shanghai, People's Republic of China

Y. Chen
e-mail: chenyl@tongji.edu.cn

Keywords Errors-in-variables model · Total least-squares adjustment · Iterative least-squares adjustment · Unbiased variance component estimate

1 Introduction

Since the total least-squares (TLS) approach was introduced by Golub and Van Loan (1980) to estimate the parameters in the error-in-variables (EIV) model where the design matrix besides the observations is affected by random errors, extensive studies have been made towards extending its application areas, such as remote sensing (Felus and Schaffrin 2005), geodetic datum transformation (Schaffrin and Felus 2008) and linear regression (Neri et al. 1989; Schaffrin and Wieser 2008).

From a theoretical point of view, a great number of algorithms have been developed to solve the homoscedastic (Schaffrin et al. 2006; Schaffrin and Felus 2008), weighted (Van Huffel and Vandewalle 1989; Markovsky et al. 2006; Schaffrin and Wieser 2008), constrained (Schaffrin and Felus 2005; Schaffrin 2006) and regularized (Golub et al. 1999) TLS problems. For the methodology aspect, a class of methods is based on solving the eigenvalues problem, such as singular value decomposition (see e.g. Van Huffel and Vandewalle 1991; Golub and Van Loan 1980; Golub and van Loan 1996; Schaffrin and Felus 2008). Another class of methods is based on a non-linear Lagrange function approach in the cases of identity or fairly general covariance matrices (see e.g., Schaffrin et al. 2006; Schaffrin and Wieser 2008). For more information about the development of TLS approach, one can refer to the textbooks (Van Huffel and Vandewalle 1991; Van Huffel 1997; Van Huffel and Lemmerling 2002) and the latest literature (Van Huffel et al. 2007).

Although a quite number of methods as mentioned above have been proposed to solve the EIV models with the different cases, such as homoscedastic or heteroscedastic and correlated covariance matrices, the solutions are in general rather complicated and the issue about the accuracy assessment of estimated parameters is still problematic and the variance component estimate is computed in bias, as also recognized by Schaffrin and Wieser (2008). If the bias can be numerically estimated and then removed, the unbiased accuracy estimate is achievable.

The EIV observation model is essentially a kind of non-linear model, thus it can be solved by employing the theory of non-linear least-squares (LS) adjustment, which has been intensively investigated between 1970s and 1990s (see e.g. Pope 1972, 1974; Teunissen 1990). Nevertheless, most of these works focus only on the solution, and the problem about the unbiased variance component estimate and the accuracy assessment of estimated parameters is not yet solved in non-linear LS adjustment. Another method widely used in geodetic literatures is that a non-linear observation model is linearly approximated and then solved by standard LS adjustment (see e.g. Mikhail 1976; Dermanis 1987; Koch 1999).

The objective of this contribution is twofold. First, an iterative method of weighted TLS (WTLS) adjustment to the EIV model is derived based on the theory of general non-linear LS adjustment, e.g., Newton–Gauss approach. Moreover, we will propose a numerical method to compute the unbiased variance component and the covariance matrix of WTLS estimates.

The rest of the paper is organized as follows. In Sect. 2, we will derive the iterative formulae to solve the EIV model by using the Newton–Gauss approach of non-linear LS adjustment. Then the weighted LS (WLS) solution of linearly approximated EIV model is derived. Furthermore, the difference of the WLS solution from the WTLS solution of Schaffrin and Wieser (2008) is examined. In Sect. 3, a numerical method will be developed to compute the unbiased variance component estimate and the covariance matrix of WTLS parameters. The real and simulation experiments are carried out in Sect. 4 to demonstrate the performance and efficiency of developed iterative method and numerical technique. Finally, some concluding remarks are given from theoretical and practical aspects.

2 Iterative solution of WTLS adjustment and its approximation

The EIV observation model is conceptually symbolized as

$$\mathbf{y} - \mathbf{e}_y = (\mathbf{A} - \mathbf{E}_A) \boldsymbol{\xi} \quad (1)$$

where \mathbf{y} is an $m \times 1$ observation vector affected by an $m \times 1$ random vector \mathbf{e}_y ; \mathbf{A} is an $m \times n$ design matrix with full

column rank affected by an $m \times n$ random matrix \mathbf{E}_A , which is different from the traditional model where \mathbf{A} is free of contamination of random error; $\boldsymbol{\xi}$ is an $n \times 1$ unknown parameter vector. Due to the existence of a product term $\mathbf{E}_A \boldsymbol{\xi}$, Eq. 1 is essentially a non-linear model. The stochastic properties of the error vectors \mathbf{e}_y and \mathbf{e}_A are characterized by

$$\begin{bmatrix} \mathbf{e}_y \\ \mathbf{e}_A \end{bmatrix} \sim \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \sigma_0^2 \begin{bmatrix} \mathbf{Q}_y & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_A \end{bmatrix} \right) \quad (2)$$

where $\mathbf{e}_A = \text{vec}(\mathbf{E}_A)$, the symbol “vec” denotes the operator that converts a matrix to a column vector by stacking one column of this matrix underneath the previous one. σ_0^2 is an (unknown) variance scalar, \mathbf{Q}_y and \mathbf{Q}_A are non negative-definite and symmetric matrices with sizes $m \times m$ and $mn \times mn$, respectively.

The target function of solving the EIV model is

$$\mathbf{e}_y^T \mathbf{Q}_y^{-1} \mathbf{e}_y + \mathbf{e}_A^T \mathbf{Q}_A^{-1} \mathbf{e}_A = \min \quad (3)$$

The product term $\mathbf{E}_A \boldsymbol{\xi}$ is represented in linear form of \mathbf{e}_A using the following identity

$$\mathbf{E}_A \boldsymbol{\xi} = (\boldsymbol{\xi}^T \otimes \mathbf{I}_m) \mathbf{e}_A \quad (4)$$

with \otimes the Kronecker product of two matrices. According to the definition of the Kronecker product, $(\boldsymbol{\xi}^T \otimes \mathbf{I}_m)$ is an $m \times mn$ matrix.

2.1 Iterative formulae derived from Newton–Gauss algorithm of non-linear LS adjustment

A number of methods have been developed to solve the EIV model (1) with weighted strategy (2) (Van Huffel and Vandewalle 1989; Markovsky et al. 2006; Schaffrin and Wieser 2008), of which Schaffrin and Wieser (2008) derived the exact WTLS solution by minimizing the target function (3) subject to (1). However, the derived formulae of these methods are in general complicated. In this section, we will propose an iterative method based on the Newton–Gauss algorithm of non-linear LS adjustment.

If the parameter vector $\boldsymbol{\xi}$ is iteratively computed in terms of Newton–Gauss algorithm of the non-linear LS adjustment proposed by Pope (1974), the EIV model is expressed at the i th iteration as

$$\mathbf{y} - \mathbf{e}_y = \mathbf{A} \boldsymbol{\xi}_{(i)} + \mathbf{A}_{(i)} \delta \boldsymbol{\xi} - \mathbf{E}_A \boldsymbol{\xi}_{(i)} \quad (5)$$

where the subscript (i) indicates the quantity updated at the i th iteration, and

$$\mathbf{A}_{(i)} = \mathbf{A} - \tilde{\mathbf{E}}_{A(i)}, \quad (6)$$

$$\boldsymbol{\xi} = \boldsymbol{\xi}_{(i)} + \delta \boldsymbol{\xi}, \quad (7)$$

where $\delta \boldsymbol{\xi}$ is generally a small quantity to be solved in the coming iteration, and $\tilde{\mathbf{E}}_{A(i)}$ is the predicted residual matrix at the i th iteration. It is noticed that the coefficient matrix $\mathbf{A}_{(i)}$ is not

allowed to be replaced by A , otherwise, the Newton–Gauss algorithm may converge to a wrong stationary point, recognized by Pope (1972) as one of the pitfalls in the iterative adjustment of non-linear problems. More recently, Schaffrin et al. (2009) dealt with the empirical similarity transformation of TLS adjustment, in which the pitfalls are avoided using the same way as used in Pope (1972).

In contrast to Schaffrin and Wieser (2008), we minimize the target function of classical Lagrange approach to solve the EIV model subject to the linear Eq. 5 instead of the non-linear Eq. 1 with considering the identity of Eq. 4 as

$$\Phi(e_y, e_A, \lambda, \xi) = e_y^T Q_y^{-1} e_y + e_A^T Q_A^{-1} e_A + 2\lambda^T (y - A\xi_{(i)} - A_{(i)}\delta\xi - e_y + (\xi_{(i)}^T \otimes I_m) e_A) \quad (8)$$

where λ denotes an $m \times 1$ vector of “Lagrange multipliers”. The solution of this target function is derived via the Euler-Lagrange necessary conditions, namely,

$$\left. \frac{1}{2} \frac{\partial \Phi}{\partial e_y} \right|_{\tilde{e}_y, \tilde{e}_A, \hat{\lambda}, \delta\hat{\xi}} = Q_y^{-1} \tilde{e}_y - \hat{\lambda} = 0 \quad (9a)$$

$$\left. \frac{1}{2} \frac{\partial \Phi}{\partial e_A} \right|_{\tilde{e}_y, \tilde{e}_A, \hat{\lambda}, \delta\hat{\xi}} = Q_A^{-1} \tilde{e}_A + (\xi_{(i)} \otimes I_m) \hat{\lambda} = 0 \quad (9b)$$

$$\left. \frac{1}{2} \frac{\partial \Phi}{\partial \lambda} \right|_{\tilde{e}_y, \tilde{e}_A, \hat{\lambda}, \delta\hat{\xi}} = y - A\xi_{(i)} - A_{(i)}\delta\hat{\xi} - \tilde{e}_y + (\xi_{(i)}^T \otimes I_m) \tilde{e}_A = 0 \quad (9c)$$

$$\left. \frac{1}{2} \frac{\partial \Phi}{\partial \delta\xi} \right|_{\tilde{e}_y, \tilde{e}_A, \hat{\lambda}, \delta\hat{\xi}} = -A_{(i)}^T \hat{\lambda} = 0 \quad (9d)$$

where tildes indicate “predicted” vectors, and hats indicate “estimated” ones. Referring to Schaffrin and Wieser (2008), it is rather easy to prove that the Hessian matrix of second-order derivatives of the target function with respect to e_y and e_A is positive-definite. Thus the solution to Eqs. 9a–d indeed gives us the minimum of target function (3).

From the Eqs. 9a, b, we readily derive the residual vectors \tilde{e}_y and \tilde{e}_A in form of $\hat{\lambda}$ as

$$\tilde{e}_y = Q_y \hat{\lambda} \quad (10a)$$

$$\tilde{e}_A = -Q_A (\xi_{(i)} \otimes I_m) \hat{\lambda} \quad (10b)$$

Inserting Eqs. 10a, b into Eq. 9c, we derive

$$\begin{aligned} \hat{\lambda} &= (Q_y + (\xi_{(i)}^T \otimes I_m) Q_A (\xi_{(i)} \otimes I_m))^{-1} \\ &\quad \times (y - A\xi_{(i)} - A_{(i)}\delta\hat{\xi}) \\ &= Q_{l(i)}^{-1} (y - A\xi_{(i)} - A_{(i)}\delta\hat{\xi}) \end{aligned} \quad (11)$$

with

$$Q_{l(i)} = Q_y + (\xi_{(i)}^T \otimes I_m) Q_A (\xi_{(i)} \otimes I_m) \quad (12)$$

Inserting Eq. 11 into Eq. 9d, we derive the solution to $\delta\hat{\xi}$ at the $(i + 1)$ th iteration as

$$\delta\hat{\xi}_{(i+1)} = (A_{(i)}^T Q_{l(i)}^{-1} A_{(i)})^{-1} A_{(i)}^T Q_{l(i)}^{-1} (y - A\xi_{(i)}) \quad (13)$$

Thereby, the updated parameter vector after the $(i + 1)$ th iteration is

$$\begin{aligned} \hat{\xi}_{(i+1)} &= \hat{\xi}_{(i)} + \delta\hat{\xi}_{(i+1)} \\ &= (A_{(i)}^T Q_{l(i)}^{-1} A_{(i)})^{-1} A_{(i)}^T Q_{l(i)}^{-1} (y - \tilde{E}_{A(i)} \xi_{(i)}) \end{aligned} \quad (14)$$

Substituting Eq. 13 into Eq. 11 and then into Eqs. 10a, b, we finally obtain the predicted error vectors at the $(i + 1)$ th iteration as

$$\tilde{e}_{y(i+1)} = Q_y Q_{l(i)}^{-1} (y - A\hat{\xi}_{(i)} - A_{(i)}\delta\hat{\xi}_{(i+1)}) \quad (15a)$$

$$\tilde{e}_{A(i+1)} = -Q_A (\hat{\xi}_{(i)} \otimes I_m) Q_{l(i)}^{-1} (y - A\hat{\xi}_{(i)} - A_{(i)}\delta\hat{\xi}_{(i+1)}) \quad (15b)$$

The iterative procedure specified by Eqs. 13–15b can be implemented starting from the standard LS solution. The suitable threshold ε_0 should be primarily given to stop the iteration until $\|\delta\hat{\xi}_{(i+1)}\| < \varepsilon_0$. Obviously, if the starting point is within the convergence radius, the iteration procedure will converge to the exact solution.

If the cofactor matrix Q_A is decomposed as that in Schaffrin and Wieser (2008), i.e.,

$$Q_A = Q_0 \otimes Q_x \quad (16)$$

where Q_0 has size $n \times n$, and Q_x has size $m \times m$, the individual cofactor matrices Q_0 could be singular.

2.2 Approximation of the iterative method and its discrepancy analysis

Omitting the second-order smaller quantity $\tilde{E}_{A(i)}\delta\hat{\xi}$ in Eq. 5 yields the following linearly approximated EIV model,

$$y - e_y = A\xi_{(i)} + A\delta\xi - E_A \xi_{(i)} \quad (17)$$

Its solution is derived from the target function (3) subject to Eq. 17 in the similar way in Sect. 2.1,

$$\hat{\xi}_{(i+1)}^{\text{WLS}} = (A^T Q_{l(i)}^{-1} A)^{-1} A^T Q_{l(i)}^{-1} y \quad (18)$$

where the superscript WLS indicates the WLS solution for the linearly approximate model (17). For the brevity of expressions, we omit the subscript of iteration count and rewrite Eq. 18 as

$$(A^T Q_l^{-1} A) \hat{\xi}^{\text{WLS}} = A^T Q_l^{-1} y \quad (19)$$

The WTLS solution derived by Schaffrin and Wieser (2008) is

$$\hat{\xi} = (A^T Q_l^{-1} A - \hat{v} Q_0)^{-1} A^T Q_l^{-1} y \quad (20)$$

with the scalar \hat{v} being

$$\hat{v} = (y - A\hat{\xi})^T Q_l^{-1} Q_x Q_l^{-1} (y - A\hat{\xi}) \quad (21)$$

where Q_0 and Q_x are defined in Eq. 16. Since both Q_l and the scalar \hat{v} are the function of parameter vector ξ , Eq. 20 also needs the iterative computation. If we neglect the difference of computing Q_l with $\hat{\xi}^{\text{WLS}}$ and $\hat{\xi}$, we have the equation

$$\begin{aligned} \hat{\xi} &= (A^T Q_l^{-1} A - \hat{v} Q_0)^{-1} (A^T Q_l^{-1} A) \hat{\xi}^{\text{WLS}} \\ &= \hat{\xi}^{\text{WLS}} + \hat{v} (A^T Q_l^{-1} A - \hat{v} Q_0)^{-1} Q_0 \hat{\xi}^{\text{WLS}} \end{aligned} \quad (22a)$$

by substituting Eq. 19 into Eq. 20. Analogously,

$$\begin{aligned} \hat{\xi}^{\text{WLS}} &= (A^T Q_l^{-1} A)^{-1} (A^T Q_l^{-1} A - \hat{v} Q_0) \hat{\xi} \\ &= \hat{\xi} - \hat{v} (A^T Q_l^{-1} A)^{-1} Q_0 \hat{\xi} \end{aligned} \quad (22b)$$

Therefore, the difference of solutions between Eqs. 18 and 20 is

$$\Delta \hat{\xi} = \hat{\xi} - \hat{\xi}^{\text{WLS}} = \hat{v} (A^T Q_l^{-1} A - \hat{v} Q_0)^{-1} Q_0 \hat{\xi}^{\text{WLS}} \quad (23a)$$

or, in complete analogy,

$$\Delta \hat{\xi} = \hat{v} (A^T Q_l^{-1} A)^{-1} Q_0 \hat{\xi} \quad (23b)$$

3 Numerical method for accuracy assessment of WTLS solution

Although the EIV models have been solved by different methods, the issue about the precision assessment of estimates is still problematic and the variance component estimate is computed in bias, as also recognized by Schaffrin and Wieser (2008). In this section, we will develop a numerical method to compute and correct the bias from the biased variance component estimate, and then the unbiased variance component is obtained.

If a sufficiently small threshold ε_0 is chosen to terminate the iteration procedure, i.e., $\|\delta \hat{\xi}_{(i+1)}\| < \varepsilon_0 \rightarrow 0$, Eqs. 15a, b can be simplified as

$$\tilde{e}_y = Q_y Q_l^{-1} (y - A\hat{\xi}) \quad (24a)$$

$$\tilde{e}_A = -Q_A (\hat{\xi} \otimes I_m) Q_l^{-1} (y - A\hat{\xi}) \quad (24b)$$

Consequently, the variance component estimate is computed as

$$\begin{aligned} \hat{\sigma}_0^2 &= \frac{\tilde{e}_y^T Q_y^{-1} \tilde{e}_y + \tilde{e}_A^T Q_A^{-1} \tilde{e}_A}{r} \\ &= \frac{(y - A\hat{\xi})^T Q_l^{-1} (y - A\hat{\xi})}{r} \end{aligned} \quad (25)$$

where r denotes the redundancy determined as

$$r = rk([Q_y, Q_x]) - rk(A) = m - n \quad (26)$$

with $rk(\cdot)$ being the operator of computing the rank of matrix. The same formula of variance component estimate is given by Schaffrin and Wieser (2008). It is trivial to prove that the variance estimate of Eq. 25 is unbiased for the WLS solution (18) of linearly approximated EIV model (17). However, as declared by Schaffrin and Wieser (2008), the estimate of Eq. 25 is biased for the WTLS solution, since the WTLS solution is biased itself.

In order to compute the unbiased variance component estimate of WTLS solution, the bias term must be reasonably estimated and removed from the quadratic quantity in the numerator of Eq. 25, because Eq. 26 indeed represents the degree of freedom of the EIV model as claimed by Schaffrin and Wieser (2008). Introducing a bias term δb to correct Eq. 25, the unbiased variance estimate is computed as

$$\hat{\sigma}_0^2 = \frac{(y - A\hat{\xi})^T Q_l^{-1} (y - A\hat{\xi}) - \delta b}{r} \quad (27)$$

Obviously the analytical expression of δb is too difficult to be derived. Therefore, we propose a numerical method to compute δb with the following steps:

The first step compute the predicted error vectors \tilde{e}_y and \tilde{e}_A with WTLS solution and the biased variance estimate $\hat{\sigma}_{0,b}^2$ by Eqs. 24a, b and Eq. 25, respectively. Here subscript b indicates the biased estimate. Then recover the residual matrix \tilde{E}_A from \tilde{e}_A by reshaping a vector to a square matrix.

The second step correct the observation vector y and coefficient matrix A using the computed residual vector \tilde{e}_y and residual matrix \tilde{E}_A , respectively. The corrected observation vector and coefficient matrix are $\tilde{y} = y - \tilde{e}_y$ and $\tilde{A} = A - \tilde{E}_A$. After this correction, the parameter vector of WTLS solution newly denoted as $\tilde{\xi}$ holds exactly true for the equations

$$\tilde{y} = \tilde{A} \tilde{\xi} \quad (28)$$

The third step simulate random errors of normal distribution with zero-mean and covariance $\hat{\sigma}_{0,b}^2 Q_y$ and $\hat{\sigma}_{0,b}^2 Q_A$ to vector \tilde{y} and matrix \tilde{A} , respectively. Then compute the parameter vector estimate $\hat{\xi}_b$ iteratively as well as its quadratic term s as

$$s = (y - A\hat{\xi}_b)^T Q_l^{-1} (y - A\hat{\xi}_b) \quad (29)$$

This random simulation is repeated by N times, such that the mean of the quadratic quantity \bar{s} is of statistic meaning.

The fourth step estimate the bias δb as

$$\delta b = \bar{s} - r\hat{\sigma}_{0,b}^2 \quad (30)$$

Then substitute the estimated δb into Eq. 27 to compute the unbiased variance estimate

$$\hat{\sigma}_0^2 = \hat{\sigma}_{0,b}^2 - \delta b/r \quad (31)$$

We would like to give comments on the numerical method for variance component estimate. In theory, the variance estimate (31) is not an unbiased variance component. It is observed from Eq. 27 that the bias δb is specified to the given unbiased variance $\hat{\sigma}_0^2$. In other words, the different variance components correspond to the different biases δb in the same WTLS model although they are very close. Therefore, to recover the unbiased variance component, the unbiased variance component should be used instead of biased variance $\hat{\sigma}_{0,b}^2$ in the third step of numerical method. As a result, the computed bias by Eq. 30 is the exact bias associated to the unbiased variance component. However, it is impossible to know the unbiased variance. Otherwise we do not need to compute it anymore. Fortunately, the difference between the biases with respect to the unbiased variance $\hat{\sigma}_0^2$ (we never know) and the biased variance $\hat{\sigma}_{0,b}^2$ is very small. Therefore the bias computed by Eq. 30 with respect to $\hat{\sigma}_{0,b}^2$ can be used as the bias with respect to $\hat{\sigma}_0^2$, and then recover $\hat{\sigma}_0^2$ by Eq. 31. If $\hat{\sigma}_0^2$ is different from $\hat{\sigma}_{0,b}^2$ significantly, one can recover the unbiased variance by iteratively conducting the third and fourth steps, because after each iteration, the bias-corrected variance in Eq. 31 becomes closer to the unbiased variance. In addition, it is emphasized that the number of simulations N must be sufficient to guarantee the reliable bias estimate δb . Anyway, it is more precise to call variance estimate computed in Eq. 31 as bias-corrected variance component rather than the unbiased one. We claim the unbiased variance component only to highlight its sufficient approximation to the unbiased estimate.

Once the unbiased variance estimate is obtained, we can simulate the random errors of normal distribution with zero-mean and covariance $\hat{\sigma}_0^2 \mathbf{Q}_y$ and $\hat{\sigma}_0^2 \mathbf{Q}_A$ to vector $\tilde{\mathbf{y}}$ and matrix $\tilde{\mathbf{A}}$, respectively. We repeat the random simulation by N times. For each simulation we run the iterative computation of WTLS adjustment presented in Sect. 2.1 of this paper or in Schaffrin and Wieser (2008) starting from $\tilde{\xi}$. The i th WTLS solution is denoted as $\hat{\xi}_i$. Since $\tilde{\xi}$ exactly fulfills Eq. 28, the difference $\hat{\xi}_i - \tilde{\xi}$ includes the errors caused by both the observation errors and the non-linear characteristics of the EIV model. Thereby, the matrix of mean-squared error $(\hat{\xi}_i - \tilde{\xi})(\hat{\xi}_i - \tilde{\xi})^T$ is a reasonable measure for the precision of the i th WTLS solution. Using total N simulations, we get

the averaged mean-squared error \mathbf{M}_{ξ} as

$$\mathbf{M}_{\xi} = \frac{1}{N} \sum_{i=1}^N \left\{ (\hat{\xi}_i - \tilde{\xi})(\hat{\xi}_i - \tilde{\xi})^T \right\}, \quad (32)$$

which can adequately reveal the precisions of estimates and their correlations. Admittedly, the mean-squared error of the estimates can be computed via non-linear error propagation as presented in e.g. Xu (1986) where the high-order derivatives are necessary. As well known by geodesists, it is complicated to compute the high-order derivatives, thus it is favor to numerically compute the mean-squared errors. It is important to notice that the presented numerical technique can be used to evaluate the accuracy of estimate in any non-linear models, not only for WTLS solution.

The formula of approximately computing the mean-squared error $\mathbf{D}_{\hat{\xi}}$, called covariance matrix, of the WTLS solution can be derived via linear error propagation to Eq. 13 as

$$\mathbf{D}_{\hat{\xi}} = \hat{\sigma}_0^2 (\tilde{\mathbf{A}}^T \mathbf{Q}_l^{-1} \tilde{\mathbf{A}})^{-1} \quad (33)$$

Here $\hat{\sigma}_0^2$ is the bias-corrected variance component. For the solution (18) of the linearly approximated EIV model, its unbiased covariance matrix $\mathbf{D}_{\hat{\xi}}$ is computed with the well-known formula

$$\mathbf{D}_{\hat{\xi}}^{\text{WLS}} = \hat{\sigma}_0^2 (\mathbf{A}^T \mathbf{Q}_l^{-1} \mathbf{A})^{-1} \quad (34)$$

where $\hat{\sigma}_0^2$ is the variance estimated directly by Eq. 25 using the WLS solution.

4 Experiment and analysis

The experiments are designed in this section to examine the proposed iterative method and its linear approximation, as well as the performance and efficiency of numerical method for accuracy assessment of WTLS solution. For distinguishing from the WTLS solution of Schaffrin and Wieser (2008), we call the presented iterative method as iterative method in the following context, although it is essentially an alternative algorithm of WTLS adjustment.

4.1 Solution of iterative method and its approximation for straight-line fit

We compute a straight-line fit problem where both variables have been observed and, thus EIV are involved. We use the data and the exact solution presented in Neri et al. (1989), see columns 2 to 5 of Table 1, and try to estimate the intercept

Table 1 Observed data and corresponding weights taken from Neri et al. (1989) as well as their residuals and corresponding true values

i	Observed data		Weights		Residuals		True data	
	x_i	y_i	W_{xi}	W_{yi}	e_A	e_y	\bar{x}_i	\bar{y}_i
1	0.0	5.9	1,000.0	1.0	0.000202	0.419993	0.000202	5.480007
2	0.9	5.4	1,000.0	1.8	0.000305	0.352423	0.899695	5.047577
3	1.8	4.4	500.0	4.0	0.000825	0.214554	1.800825	4.614554
4	2.6	4.6	800.0	8.0	0.001771	0.368625	2.598229	4.231375
5	3.3	3.5	200.0	20.0	0.018513	0.385254	3.318513	3.885254
6	4.4	3.7	80.0	20.0	0.037984	0.316184	4.362016	3.383816
7	5.2	2.8	60.0	70.0	0.079998	0.142695	5.279998	2.942695
8	6.1	2.8	20.0	70.0	0.233784	0.139003	5.866216	2.660997
9	6.5	2.4	1.8	100.0	0.084088	0.003150	6.415912	2.396850
10	7.4	1.5	1.0	500.0	0.874700	0.003641	8.274700	1.503641

Table 2 Results of straight-line fit to the observed data of Table 1

Parameter estimate	Exact solution (Neri et al.)	WTLS solution	GLS (using W_{xi})	TLS solution	New iterative solution	WLS approximate solution
$\hat{\xi}_1$	5.47991022	5.479910224	6.100	5.784	5.479910224	5.3960523
$\hat{\xi}_2$	0.480533407	0.480533407	0.611	0.546	0.480533407	0.4634489

and slope regression parameters, ξ_1 and ξ_2 , in the regression line

$$y_i - e_{y_i} = \xi_2 \times (x_i - e_{x_i}) + \xi_1 \quad (35)$$

using the proposed iterative method and its linear approximation, respectively. In Table 1, the observations are in columns 2 and 3, and their corresponding weights in columns 4 and 5. We define the parameter vector as $\xi = [\xi_1 \ \xi_2]^T$ and, the second column of the coefficient matrix A in Eq. 1 is associated with random errors, while all the values in the first column are fixed to 1. We compose the cofactor matrices as $Q_y = (\text{diag}[W_{y_i}])^{-1}$, $Q_x = (\text{diag}[W_{x_i}])^{-1}$ and $Q_A = Q_0 \otimes Q_x$ with $Q_0 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$, where “diag” denotes the operator that converts a vector into a diagonal matrix with the vector’s elements representing the diagonal entries of the matrix. This coincides with the model used by Schaffrin and Wieser (2008) for the same data set.

First of all, we examine the solution of iterative method and the degree of approximation of the WLS approximate solution, namely, how close the solutions from iterative method and its approximation are to the exact one. Choosing the same threshold $\varepsilon_0 = 10^{-10}$ as in Schaffrin and Wieser (2008), we compute the regression parameters using the iterative method in Sect. 2.1 and its approximation in Sect. 2.2, respectively. The results are presented in the last two columns of Table 2, comparing with the exact solution reported by Neri et al. (1989) and WTLS, GLS as well as TLS solutions provided by Schaffrin and Wieser (2008).

Here, WTLS solution is computed according to the algorithm of Schaffrin and Wieser (2008), the GLS represents the ordinary LS algorithm when only considering the weight matrix of the y data, while TLS is the standard TLS method when disregarding the weight matrix for both x and y data. It is observed from Table 2 that the solution of our iterative method is the same as WTLS solution, matching the exact one very well, which means that the presented iterative method is indeed an alternative WTLS method. The WLS approximate solution is much closer to exact solution than both the GLS and TLS solutions, and the relative errors for two regression parameters are 1.53 and 3.56%, respectively.

Moreover, the differences between WLS approximate solution and WTLS solution estimated by Eq. 23a for the presented example are 0.0914 and 0.0185, which are consistent with the actual differences, 0.0839 and 0.0171, computed from their solutions in Table 2. It is important to notice that the approximation method is rather simple and thus ease the implementation. The more important benefit of the WLS approximate solution is that it can compute an unbiased variance component estimate by Eq. 25 and the reasonable covariance matrix of the estimated parameter vector by Eq. 34 in the sense of the proposed linear approximation model. However, the variance estimate computed by Eq. 25 using WTLS solution or new iterative solution is biased. Table 3 presents the estimated variance components for three different solutions, respectively, and covariance matrix for WLS approximate solution by Eq. 34 based on the observed data of Table 1.

Table 3 Estimated variances of unit weight for three methods and covariance matrix for WLS approximation method

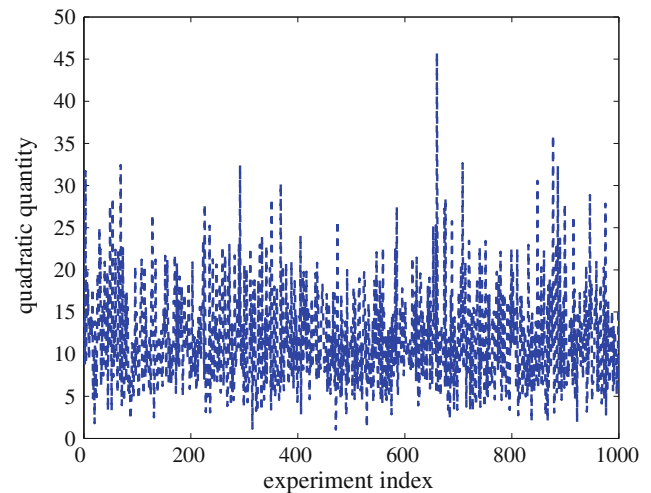
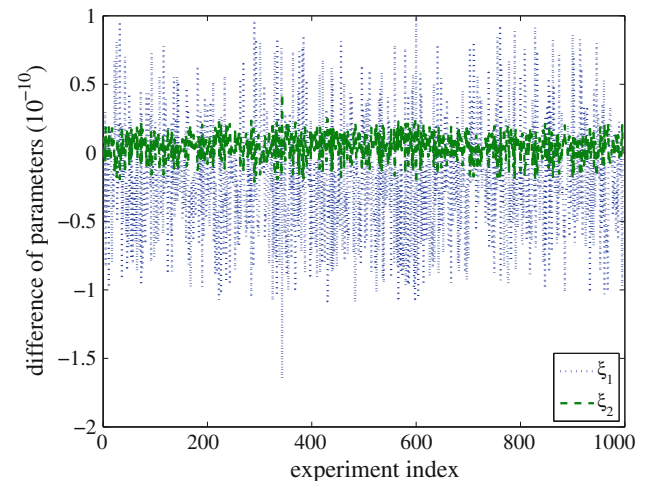
Methods	Variance of unit weight	Covariance matrix		
		$\hat{\sigma}_{\xi_1}^2$	$\hat{\sigma}_{\xi_2}^2$	$\hat{\sigma}_{\xi_1, \xi_2}^2$
WTLS solution	1.21791 ²			
New iterative solution	1.21791 ²			
WLS approximate solution	1.22252 ²	0.13065217	0.00499322	−0.02462112

4.2 Numerical method for accuracy assessment

We use the numerical method presented in Sect. 3 to compute the unbiased variance estimate and covariance matrix of WTLS solution. In addition, the approximate formula (33) for covariance matrix of WTLS solution is evaluated, and the unbiased characteristics of variance component and covariance matrix estimated by the WLS approximation method are exhibited.

According to the presented numerical method, we first compute the residuals of the observed data by the rigorous Eqs. 15a, b or simplified Eqs. 24a, b with the iterative solution or WTLS solution in Table 1, and then recover the “true” values, \bar{x}_i and \bar{y}_i , via correcting the residuals to the observed data, see i.e., the last two columns of Table 1. To date, we have completed the second step of numerical method, and we have the “true” values and exact Eq. (28) with iterative solution in hand. We use the biased variance component of iterative solution, $\hat{\sigma}_{0,b} = 1.21791$, in Table 3 and the same weights as in Table 1 to simulate normally distributed random noises $e_{x_i} = \hat{\sigma}_{0,b} \times W_{x_i}^{-1/2}$ and $e_{y_i} = \hat{\sigma}_{0,b} \times W_{y_i}^{-1/2}$ that associate to \bar{x}_i and \bar{y}_i , respectively. Thus the simulated observations are determined as $x_i = \bar{x}_i + e_{x_i}$ and $y_i = \bar{y}_i + e_{y_i}$. Based on the simulated data set, we compute regression parameters using iterative method and their quadratic term s as described in the third step of numerical method. A total of 1,000 simulations were carried out to achieve reliable results from the statistic point of view. The quadratic quantities for 1,000 simulations are illustrated in Fig. 1. The mean of quadratic quantities, the bias and the unbiased variance estimate computed by Eqs. 30 and 31 are $\bar{s} = 11.70748$, $\delta b = -0.15887$ and $\hat{\sigma}_0 = 1.22603$. Comparing the variance estimates in Table 3 with this unbiased estimate, the relative biases are 1.32% for WTLS and iterative solutions, and 0.57% for WLS approximation. Apparently, the variance estimate from the WLS approximation method is much closer to the computed unbiased one than the WTLS solution.

According to the proposed numerical method, we measure the approximation degree of three different solutions to the exact solution. We simulate the random errors of normal distribution with zero-mean and covariance $\hat{\sigma}_0^2 Q_y$ and $\hat{\sigma}_0^2 Q_A$ to vector \tilde{y} and matrix \tilde{A} , respectively. The 1,000 simulations are implemented, and for each simulation we run our iterative method, WTLS adjustment of Schaffrin and Wieser

**Fig. 1** The computed quadratic quantities for 1,000 simulations**Fig. 2** The difference of parameters between new iterative method and WTLS of Schaffrin and Wieser (2008)

(2008) and WLS approximation method all starting from $\tilde{\xi}$. Their estimates at i th simulation are denoted as $\hat{\xi}_i^{\text{New}}$, $\hat{\xi}_i^{\text{WTLS}}$ and $\hat{\xi}_i^{\text{WLS}}$, respectively. Figure 2 illustrates the difference between our iterative solution and WTLS solution for two regression parameters. The scale in y-axis is 10^{-10} which is the same level as the threshold. Thus, the estimates from our iterative method and WTLS adjustment are considered same. The difference between iterative solution and exact

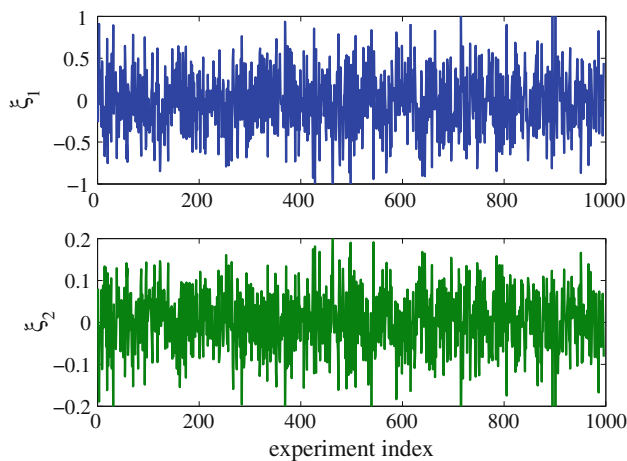


Fig. 3 The difference between new iterative solution and exact ones

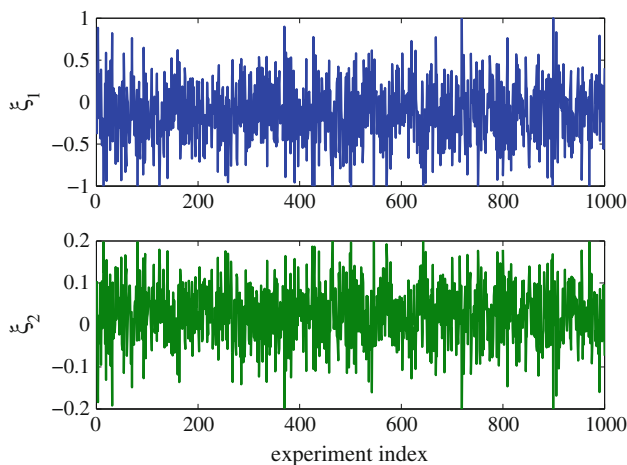


Fig. 4 Difference between WLS approximate solution and the exact ones

solution is shown in Fig. 3, and their means are 0.02934 and -0.00720 , namely, relative errors are 0.54 and 1.50%. The difference between WLS approximate solution and exact one are presented in Fig. 4. Their means are -0.078303 and 0.01462 , i.e., relative errors are 1.43 and 3.04%. Apparently, the iterative method can indeed achieve more accurate solution than the WLS approximation method. However, the difference is so small that WLS approximation method can be applied in real applications.

Table 4 Estimated variance components of two regression parameters and their covariance in simulation experiments

Variance and covariance	WTLS solution Eq. 32	New iterative method by Eq. 32	Approximate covariance by Eq. 33	WLS approximation method by Eq. 34
$\hat{\sigma}_{\xi_1}^2$	0.1383039	0.1383039	0.1309128	0.1244961
$\hat{\sigma}_{\xi_2}^2$	0.0052724	0.0052724	0.0050754	0.0047924
$\hat{\sigma}_{\xi_1, \xi_2}^2$	-0.0259858	-0.0259858	-0.0248147	-0.0234807

To evaluate the unbiased characteristics of the variance estimate by WLS approximation method and measure the bias degree of variance estimates by iterative method and WTLS method, we compute 1,000 variance component estimates $\hat{\sigma}_{i, \text{New}}^2$, $\hat{\sigma}_{i, \text{WTLS}}^2$, $\hat{\sigma}_{i, \text{WLS}}^2$ by Eq. 25 with $\hat{\xi}_i^{\text{New}}$, $\hat{\xi}_i^{\text{WTLS}}$ and $\hat{\xi}_i^{\text{WLS}}$, respectively. The mean relative biases for 1,000 simulations with respect to the unbiased variance $\hat{\sigma}_0^2$ used as prior one in simulation are computed to be 1.43% for our iterative method and WTLS solution, and 0.76% for WLS approximation method. The variance estimate from WLS approximation method is much closer to the prior variance estimate than the others, although they are all very small. It means that the variance estimate from WLS approximation method is, to a great extent, unbiased in the sense of the proposed linear approximation model and can thus be employed to reasonably assess the accuracy of the WTLS solution.

We compute the covariance matrix of estimated regression parameters via substituting the estimates, $\hat{\xi}_i^{\text{New}}$ and $\hat{\xi}_i^{\text{WTLS}}$, into Eq. 32. The mean covariance matrices of 1,000 simulations for our iterative method and WTLS are shown in Table 4. They are same due to the equal parameter estimates, which are regarded as the actual covariance matrix of regression parameters to assess the covariance matrices from linearly approximate error propagation law specified by Eq. 33 and WLS solution computed by Eq. 34. Obviously the covariance matrix computed by Eq. 33 is closer than the actual one than that computed by Eq. 34, and the relative differences of three elements in Table 4 are 5.34, 3.74 and 4.51% for Eq. 33, and 9.98, 9.10 and 9.64% for Eq. 34. Therefore, the covariance matrix from linearly approximate error propagation law can be used reasonably assess the accuracies of WTLS estimates.

5 Concluding remarks

We have developed an iterative method based on Newton–Gauss algorithm of non-linear LS adjustment to solve WTLS problems. Its linear approximation version has been investigated as well. Because it is rather difficult to derive an analytical formula for exact accuracy assessment in the context of WTLS theory, we have proposed a numerical method to compute the unbiased variance component estimate and mean-squared error matrix of the WTLS param-

eters. Moreover a formula for approximately assessing the accuracy of WTLS solution was derived by using linearly approximate error propagation law. The conclusions are summarized from the theoretical point of view as follows:

1. The proposed iterative method is very convenient to implement and the exact solution can be achievable. Thus, the presented iterative method can be totally deemed as an alternative method for exact WTLS solution. The WLS solution in the sense of the proposed linear approximation model is generally close to the exact WTLS solution, which can be used in real application considering its simplest formulae and superior computation;
2. The presented numerical method can compute the unbiased variance component estimate and reasonable covariance matrix of WTLS estimates, which can be analogously applied to the other non-linear problems;
3. The covariance matrix of WTLS estimates computed from the linearly approximate error propagation law is a good approximation to the actual covariance matrix. In WLS approximate method, the unbiased variance estimate and covariance matrix of estimates can be directly computed, which can also be used as an approximated covariance matrix to WTLS solution.

Furthermore, some more conclusions are obtained from the presented experiments.

4. The same solution to exact WTLS solution given by Schaffrin and Wieser (2008) was computed by iterative method. Thus, the iterative method can be indeed used as an alternative method to WTLS adjustment. The linearly approximated WLS solution is very close to the WTLS one. The relative differences are 1.43% and 3.04% with respect to two regression parameters, which are significantly smaller than those of the TLS and GLS solutions and acceptable in real applications;
5. The variance estimate from WLS approximation method is so close to the prior variance estimate with relative difference 0.76% that it can be employed to assess the accuracy of the WTLS solution without bias. The covariance matrix from the linearly approximate error propagation law is compatible with actual one from the numerical method (relative differences for three elements are 5.34, 3.74 and 4.51%) and, thus it can be used to assess the accuracies of WTLS estimates and their correlations.

On all accounts, the presented iterative method can be used as an alternative WTLS method to compute the exact solution. The numerical method is applied to compute unbiased variance component estimate and reasonable covariance matrix of WTLS estimates. It is also applicable for the accu-

racy assessment of the other non-linear problems. The WLS solution in the sense of the proposed linear approximation model is worthy to be used to deal with the WTLS problems due to its benefits that the estimates have the smaller difference from the exact ones and the unbiased variance estimate can be employed to evaluate the WTLS solution. The covariance matrix from the linearly approximate error propagation law can be used to assess the accuracies of WTLS estimates and their correlations.

Acknowledgments This paper is sponsored by the Natural Science Foundation of China (Grant No. 41074018, 40874016). Three anonymous reviewers are appreciated for their constructive comments, which helped to improve the manuscript significantly.

References

- Dermanis A (1987) Geodetic applications of interpolation and prediction. Lecture presented at the international school of geodesy "A. Marussi", 4th course: applied and basic geodesy: present and future trends. Ettore Majorana Centre for Scientific Culture, Erice-Sicily, 15–25 June 1987
- Felus Y, Schaffrin B (2005) Performing similarity transformations using the error-in-variables model. American society for photogrammetry and remote sensing (ASPRS) annual meeting on CD, Baltimore, Maryland
- Golub H, Van Loan Ch (1980) An analysis of the total least squares problem. *SIAM J Numer Anal* 17(6):883–893
- Golub G, van Loan Ch (1996) Matrix computations, 3rd edn. Johns Hopkins University Press, Baltimore
- Golub G, Hansen P, O'Leary D (1999) Tikhonov regularization and total least squares. *SIAM J Matrix Anal* 21, 185–194
- Koch K (1999) Parameter estimation and hypothesis testing in linear models, 2nd edn. Springer, Berlin
- Markovsky I, Rastello M, Premoli A, Kukush A, Van Huffel S (2006) The element-wise weighted total least-squares problem. *Comput Stat Data Anal* 50:181–209
- Mikhail E (1976) Observations & least squares. Harper&Row, New York
- Neri F, Saitta G, Chiofalo S (1989) An accurate and straightforward approach to line regression analysis of error-affected experimental data. *J Phys Ser E Sci Instr* 22:215–217
- Pope A (1972) Some pitfalls to be avoided in the iterative adjustment of nonlinear problems. In: Proceedings of 38th annual meeting of the American society photogrammetry, Washington, DC, pp 449–473
- Pope A (1974) Two approaches to nonlinear least squares adjustments. *Can Surv* 28(5):663–669
- Schaffrin B, Felus Y (2005) On total least-squares adjustment with constraints. In: A window on the future of Geodesy, IAG-Symposium, vol 128. Springer, Berlin, pp 417–421
- Schaffrin B (2006) A note on constrained total least-squares estimation. *Linear Algebra Appl* 417(1):245–258
- Schaffrin B, Felus Y (2008) Multivariate total-least squares adjustment for empirical affine transformations. In: Xu P, Liu J, Sermanis A (eds) International association of geodesy symposia: VI Hotine-Marussi symposium on theoretical and computational Geodesy, 29 May–2 June 2006, Wuhan, China, vol 132. Springer, Berlin, pp 238–242
- Schaffrin B, Lee I, Felus Y, Choi Y (2006) Total least-squares for geodetic straight-line and plane adjustment. *Boll Geod Sci Aff* 65:141–168

- Schaffrin B, Felus Y (2008) On the multivariate total least-squares approach to empirical coordinate transformations. three algorithms. *J Geod* 82:373–383
- Schaffrin B, Wieser A (2008) On weighted total least-squares adjustment for linear regression. *J Geod* 82:415–421
- Schaffrin B, Neitzel F, Uzun S (2009) Empirical similarity transformation via TLS-adjustment: exact solution vs. Cadzow's approximation. *International Geomatics Forum*, 28–30 May 2009, Qingdao, People's Republic of China
- Teunissen PJG (1990) Nonlinear least squares. *Manuscr Geod* 15:137–150
- Van Huffel S (ed) (1997) Recent advances in total least squares techniques and errors-in-variables modeling. *SIAM proceedings series*, SIAM, Philadelphia
- Van Huffel S, Cheng C, Mastronardi N, Paige C, Kukush A (2007) Total least squares and errors-in-variables modeling. *Comput Stat Data Anal* 52:1076–1079
- Van Huffel S, Lemmerling P (eds) (2002) Total least squares and errors-in-variables modeling: analysis, algorithms and applications. Kluwer Academic Publishers, Dordrecht
- Van Huffel S, Vandewalle J (1989) Analysis and properties of the generalized total least-squares problem $AX \approx B$ when some or all columns of A are subject to error. *SIAM J Matrix Anal Appl* 10:294–315
- Van Huffel S, Vandewalle J (1991) The total least Squares problem: computational aspects and analysis. SIAM, Philadelphia
- Xu P (1986) Variance-covariance propagation for a non-linear function. *J Wuhan Techn Uni Surv Mapp* 11(2):92–99 (in Chinese with an English abstract)