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Multivariate Weighted Total Least Squares Based on the Standard Least-Squares Theory

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Abstract: The weighted total least squares (WTLS) has been widely used in many geodetic problems to solve the error-in-variable (EIV) models in which both the observation vector and the design matrix contain random errors. This method is widely applied in its univariate form, where the observations and unknown coefficients appear in vector forms. However, in some geodetic problems, data sets appear in more than one dimension, and the vector representation of the univariate model may not be suitable to efficiently solve the problem. The observation and unknown parameter vectors can then be replaced with their counterparts in matrix representations in a multivariate model. In this paper, we propose a simple, fast, and flexible procedure for solving the multivariate WTLS (MWTLS) problem using the standard least squares theory. The method has the capability of applying to large-size and high-dimensional data sets. Our numerical experiments on both simulated and real datasets demonstrate the high performance of the proposed method for solving multivariate WTLS problems. In terms of computational complexity, our method outperforms the existing state-of-the-art methods, both numerically and analytically. **DOI:** 10.1061/JSUED2.SUENG-1424.

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Introduction

The least squares (LS) method is widely used in many geodetic problems to estimate unknown parameters based on the Gauss-Markov model. In this method, the observational errors are only attributed to the so-called vector of observations. There are however applications where the design (or coefficient) matrix is not error-free, and, therefore, it is only suboptimal to consider it as a fixed matrix. Golub and Van Loan (1980) proposed the total least squares (TLS) method, applied to the error-in-variable (EIV) model, to simultaneously consider errors in both the observation vector and design matrix. Since then, many developments on the formulations and applications of TLS have taken place, in the statistics literature in general and in the geodetic literature in particular.

In geodetic and geomatics studies, different versions of TLS were applied, especially in the field of coordinate system transformation (Felus 2004; Akyilmaz 2007; Schaffrin and Wieser 2007; Felus and Burtch 2008; Neitzel 2010; Shen et al. 2010; Amiri-Simkooei et al. 2016a; Amiri-Simkooei 2018a). Moreover, an immense range of studies introduced several extensions of the TLS solutions for equally and quadratically constrained problems. An iterative algorithm was proposed by Schaffrin (2006) for solving the TLS problem with linear stochastic constraints. A solution for TLS with quadratic constraints was also provided in Sima et al. (2004) to investigate the regularized TLS problem. Furthermore, TLS adjustment through a second-order approximation function was examined by Wang and Zhao (2019). Two algorithms including the adaptive two-stage Monte Carlo (ATMC) and adaptive two-stage quasi-Monte Carlo (ATQMC) algorithms were also introduced for the accuracy estimation of the TLS and calculation of the expected bias in parameter estimates (Wang and Luo 2023). Regularized and structured TLS methods were also two wide categories of the studies.

In addition to the above-mentioned studies, one of the most important extensions of the TLS method is the weighted TLS (WTLS) method, which originated from the study of Schaffrin and Wieser (2007), where WTLS was presented for the linear regression based on the traditional Lagrange function. WTLS can be considered as a generalized version of the unweighted TLS algorithm, where the weight matrices of the observations and design matrix are unequal and nonidentity. Although the original TLS problem can be solved by using the singular value decomposition (SVD) theorem without iteration, a general WTLS problem can only be solved through an iterative procedure (Amiri-Simkooei et al. 2016a).

Since the development of the WTLS, different variants of the WTLS problems have been presented of which we name a few contributions. To estimate the parameters in a structured EIV model, with linear and quadratic constraints, Fang (2013) proposed a constrained WTLS in which functionally independent random errors and their functional relationship were explored. In another study, Fang provided a solution for the inequality-constrained WTLS based on a set of Euler-Lagrange conditions (Fang 2014). To enhance the numerical efficiency of the WTLS for the mixed EIV model, where there are some fixed columns in the design matrix, Zhou and Fang provided a combinatorial method using the weighted least squares (WLS) and WTLS. Their motivation was to reduce the computational complexity of the WTLS procedure while preserving its accuracy (Zhou and Fang 2016). Wang et al. (2021) also proposed a computationally efficient method to reduce the time and memory consumption during the WTLS procedure in large-size problems.

In 2012, Amiri-Simkooei and Jazaeri (2012) proposed a new formulation of WTLS based on the standard LS, which was more

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applicable and implementable than the original formulation. This formulation allows applying the existing body of knowledge of the least squares theory to the EIV models, which are briefly explained as follows. The least squares variance component estimation (LS-VCE) theory was adopted to deal with the estimation of different variance components in an EIV model (Amiri-Simkooei 2013). Jazaeri et al. (2013) introduced an iterative algorithm based on the complete description of the variance-covariance matrices of the vector of observations errors and the design matrix. Estimation of the covariance matrix of the WTLS outputs through the direct conversion of the normal matrix was investigated in Amiri-Simkooei et al. (2016b). Amiri-Simkooei (2017) provided the formulations of the WTLS problem subject to weighted or hard linear(ized) equality constraints on the unknown parameters. He also presented an alternative derivation without using Lagrange multipliers for the same problem in Amiri-Simkooei (2018b). A Tikhonov regularized WTLS method is proposed by Kariminejad et al. (2021), which was a generalized form of the classical nonlinear Gauss-Helmert model.

All of the above-mentioned versions of the WTLS have been applied to the one-dimensional problems. In other words, in these problems, observations and unknown parameters were presented in the form of a vector. However, in many cases, the samples have more than one dimension, and consequently, the observations and unknowns are represented in the form of a matrix. In these cases, the initial solution is to convert matrices into vectors and use the univariate mode of the EIV model. But, a proper alternative that can be used is to use the multivariate EIV model. In this regard, in various studies, several versions of multivariate EIV-based methods have been presented, which are highlighted as follows. Two methods based on the singular value decomposition (SVD) and on the nonlinear Euler-Lagrange condition equations, were proposed by Schaffrin and Felus (2008) to solve the multivariate TLS problem. In another study, Schaffrin and Wieser (2009) successfully applied multivariate WTLS on the 2D affine transformation problem. Another method was also presented by Fang (2011), in which the Lagrange approach was utilized to solve the multivariate WTLS. Wang et al. (2016) exhibited the Newton algorithm for the multivariate WTLS problem, which was too complicated to implement.

Among different methods provided to solve the multivariate WTLS problem, the multivariate error-in-variable (MEIV) (Wang et al. 2019) method was recently introduced. This method has two versions, named MEIV1 and MEIV2, of which MEIV2 outperforms MEIV1 in terms of simplicity and convergence. Despite the efficiency of both MEIV1 and MEIV2, they cannot be considered as high-speed methods due to the use of a Kronecker product in their formulation, especially in the case of large-size data. In addition to the computational burden, applying the Kronecker product may practically lead to calculation problems when dealing with a large number of features and *out of memory* limitation.

Regarding the aforementioned problems, a simple, fast, and efficient method is proposed in this study to handle the problem of multivariate WTLS. This method, called multivariate WTLS (MWTLS), is based on the standard LS method and can be applied in a wide range of geodetic applications with various types of constraints. On the other hand, using the LS formulation guarantees its simple implementation and execution.

The remainder of this paper is organized as follows. In the next section, we first review the available standard least squares theory applied to the multivariate weighted least squares (MWLS) and WTLS. A subsequent subsection will then use this background to present the multivariate WTLS (MWTLS) theory, continued by computational complexity analysis. Experiments, conducted to illustrate the efficiency of the proposed MWTLS, are described in the section "Experiments." Finally, we conclude this study in the section "Conclusion."

Background and Methodology

This section, presenting the methodology, consists of three subsections. The first subsection reviews the available standard least squares theory applied to the MWLS. The second subsection briefly presents the univariate WTLS described in detail. The third subsection uses these backgrounds to present the multivariate WTLS (MWTLS) theory.

Multivariate WLS Formulation

Having k groups of data, each with m observations, the following linear models of observation equations can be considered for such a multivariate model (Amiri-Simkooei 2007):

$$\mathrm{E}\{y_i\} = Ax_i; \qquad D\{y_i, y_j\} = \sigma_{ij}Q; \qquad i, j = 1, \ldots, k \quad (1)$$

where $y_i \in \mathbb{R}^m$ = vector of observations in the ith group; $x_i \in \mathbb{R}^n$ = corresponding unknown vector, $A \in \mathbb{R}^{m\times n}$ = design matrix; and $Q \in \mathbb{R}^{m\times m}$ = symmetric positive-definite cofactor matrix. $\sigma_{ij}(i, j = 1, \ldots, k)$ are also variance and covariance components, expressing the variances and covariances among the different groups. The matrices A and Q are assumed to be identical for all observation groups.

By aggregating all the unknown vectors x_i into the matrix $X \in \mathbb{R}^{n\times k}$, and correspondingly the observation vectors into $Y \in \mathbb{R}^{m\times k}$ we can write

$$\begin{aligned} X &= [x_1, x_2, \ldots, x_k] \\ Y &= [y_1, y_2, \ldots, y_k] \end{aligned} \quad (2)$$

The functional part in Eq. (1) can then be rewritten as $\mathrm{E}\{Y\} = AX$. Then, using the vec operator, the vector representation of this model can be written through the Kronecker product as

$$\mathrm{E}\{\mathrm{vec}(Y)\} = (I \otimes A)\mathrm{vec}(X); \qquad Q_{\mathrm{vec}(Y)} = \Sigma \otimes Q \quad (3)$$

where $\otimes$ denotes the Kronecker product and $\Sigma \in \mathbb{R}^{k\times k}$, containing $\sigma_{ij}, i, j = 1, \ldots, k$, is the cross-covariance matrix among different y_i's.

The best linear unbiased estimation (BLUE) of the unknown matrix X is (Amiri-Simkooei 2007):

$$\hat{X} = (A^TQ^{-1}A)^{-1}A^TQ^{-1}Y \quad (4)$$

Moreover, the BLUE of the observation matrix Y and the residuals matrix E can be obtained as follows:

$$\hat{Y} = P_AY, \qquad \hat{E} = Y - \hat{Y} = P_A^\perp Y \quad (5)$$

where $P_A = A(A^TQ^{-1}A)^{-1}A^TQ^{-1}$ and $P_A^\perp = I_m - P_A$ = two orthogonal projectors (Teunissen 2000). The covariance matrices of $\mathrm{vec}(\hat{X})$, $\mathrm{vec}(\hat{Y})$, and $\mathrm{vec}(\hat{E})$ are obtained as:

$$\begin{aligned} Q_{\mathrm{vec}(\hat{X})} &= \Sigma \otimes (A^TQ^{-1}A)^{-1} \\ Q_{\mathrm{vec}(\hat{Y})} &= \Sigma \otimes P_AQ \\ Q_{\mathrm{vec}(\hat{E})} &= \Sigma \otimes P_A^\perp Q \end{aligned} \quad (6)$$

For further details, the readers can refer to Amiri-Simkooei (2007).

Univariate WTLS Formulation

The traditional univariate error-in-variable (EIV) model is expressed as (Golub and Van Loan 1980):

$$y = (A - E_A)x + e_y \tag{7}$$

with the following stochastic properties:

$$e = \begin{bmatrix} e_y \\ e_A \end{bmatrix} = \begin{bmatrix} e_y \\ \mathrm{vec}(E_A) \end{bmatrix} \sim \left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \sigma_0^2 \begin{bmatrix} Q_y & 0 \\ 0 & Q_A \end{bmatrix} \right) \tag{8}$$

where $y \in \mathbb{R}^m$, $A \in \mathbb{R}^{m\times n}$, and $x \in \mathbb{R}^n$ are, respectively, the observation vector, design (or coefficient) matrix, and unknown vector of parameters to be estimated. Furthermore, $E_A \in \mathbb{R}^{m\times n}$ and $e_y \in \mathbb{R}^m$ = corresponding random error of the design matrix and of the observation vector. $Q_y \in \mathbb{R}^{m\times m}$ and $Q_A \in \mathbb{R}^{mn\times mn}$ = covariance matrices corresponding to the observations vector and the design matrix, respectively. Moreover, σ_0^2 = (un)known variance factor of the unit weight, which is set to one for brevity.

The minimization problem to obtain the unknown parameters of Eq. (7) is based on the following least squares principle:

$$\begin{aligned} &\min_x e_y^T Q_y^{-1} e_y + e_A^T Q_A^{-1} e_A \\ &\text{subject to } y - e_y = (A - E_A)x \end{aligned} \tag{9}$$

Considering the identity $\mathrm{vec}(UVS) = (S^T \otimes U)\mathrm{vec}(V)$, as stated in Amiri-Simkooei and Jazaeri (2012), the target Lagrange function is formulated as

$$\phi = e_y^T Q_y^{-1} e_y + e_A^T Q_A^{-1} e_A + 2\lambda^T (y - Ax - e_y + (x^T \otimes I_m)e_A) \tag{10}$$

where $I_m = m \times m$ identity matrix and $\lambda \in \mathbb{R}^m$ = vector of unknown Lagrange multipliers. After calculating some partial derivatives of the above objective function with respect to its unknown parameters and applying a few simple mathematical operations, $\hat{x}$ is obtained as follows (Amiri-Simkooei and Jazaeri 2012):

$$\hat{x} = ((A - \tilde{E}_A)^T Q_{\tilde{y}}^{-1} A)^{-1} (A - \tilde{E}_A)^T Q_{\tilde{y}}^{-1} y \tag{11}$$

where $Q_{\tilde{y}}$ = covariance matrix of the predicted observations, $\tilde{y} = y - \tilde{E}_A \hat{x}$, defined as:

$$Q_{\tilde{y}} = Q_y + (\hat{x}^T \otimes I_m) Q_A (\hat{x} \otimes I_m) \tag{12}$$

Moreover, in Eq. (11), $\tilde{E}_A$ is obtained as:

$$\tilde{E}_A = \mathrm{ivec}(\tilde{e}_A) = \mathrm{ivec}(-Q_A(\hat{x} \otimes I_m)\hat{\lambda}) \tag{13}$$

where ivec = inverse of vec operator, and

$$\hat{\lambda} = Q_{\tilde{y}}^{-1}(y - A\hat{x}) \tag{14}$$

The drawback of the formulation of $\hat{x}$ in Eq. (11) is that the normal matrix is not symmetric and positive-definite. To establish such a normal matrix (in analogy with the standard least squares), considering $A = \tilde{A} + \tilde{E}_A$, $\hat{x}$ can be reformulated as:

$$\hat{x} = (\tilde{A}^T Q_{\tilde{y}}^{-1} \tilde{A})^{-1} \tilde{A}^T Q_{\tilde{y}}^{-1} \tilde{y} \tag{15}$$

and therefore, the first approximation of the covariance matrix of the estimated parameters $\hat{x}$ is obtained as follows:

$$Q_{\hat{x}} = (\tilde{A}^T Q_{\tilde{y}}^{-1} \tilde{A})^{-1} \tag{16}$$

which provides measures for the precision of $\hat{x}$. The posterior variance component is obtained as follows:

$$\hat{\sigma}_0^2 = \frac{\hat{e}^T Q_{\tilde{y}}^{-1} \hat{e}}{m - n} \tag{17}$$

where $\hat{e} = y - A\hat{x}$ = least squares residuals.

Multivariate WTLS Formulation

The results and derivations of the two previous subsections are used to present the multivariate weighted total least squares (MWTLS) theory. The combination consists of the terms *multivariate weighted least squares* and *weighted total least squares*. In a multivariate model, multiple observation vectors can be formulated in an EIV model, which is of the following form:

$$Y - E_Y = (A - E_A)X \tag{18}$$

where $Y \in \mathbb{R}^{m\times k}$, $X \in \mathbb{R}^{n\times k}$, and $E_Y \in \mathbb{R}^{m\times k}$ are same as those introduced in subsection "Multivariate WLS Formulation." In this case, the covariance matrix of $y = \mathrm{vec}(Y)$ is $Q_{\mathrm{vec}(Y)} \in \mathbb{R}^{mk\times mk}$. Accordingly, to estimate the unknown parameters, the minimization problem is as follows:

$$\begin{aligned} &\min_X e_y^T Q_Y^{-1} e_y + e_a^T Q_A^{-1} e_a \\ &\text{s.t. } Y = (A - E_A)X + E_Y \end{aligned} \tag{19}$$

where $e_y = e_{\mathrm{vec}(Y)} \in \mathbb{R}^{mk}$ and $e_a = \mathrm{vec}(E_A) = e_{\mathrm{vec}(A)} \in \mathbb{R}^{mn}$. The Lagrange function of the above optimization problem is

$$\phi = e_y^T Q_Y^{-1} e_y + e_a^T Q_A^{-1} e_a + 2\mathrm{tr}(\Lambda^T (Y - AX - E_Y + E_A X)) \tag{20}$$

where $\Lambda = m \times k$ matrix of Lagrange multipliers. Let us assume $a = \mathrm{vec}(A)$, $y = \mathrm{vec}(Y)$, $x = \mathrm{vec}(X)$, and $\lambda = \mathrm{vec}(\Lambda)$. Using the identities $\mathrm{vec}(UVS) = (S^T \otimes U)\mathrm{vec}(V)$ and $\mathrm{tr}(UV^T) = \mathrm{vec}(U)^T \mathrm{vec}(V)$, the Lagrange function in Eq. (20) can be reformulated to the following two equivalent representations:

$$\begin{aligned} \phi &= e_y^T Q_Y^{-1} e_y + e_a^T Q_A^{-1} e_a + 2\lambda^T (y - \mathrm{vec}(AX) \\ &\quad - e_y + \mathrm{vec}(I_m E_A X)) \\ &= e_y^T Q_Y^{-1} e_y + e_a^T Q_A^{-1} e_a + 2\lambda^T (y - \mathrm{vec}(AX) \\ &\quad - e_y + (X^T \otimes I_m) e_a) \end{aligned} \tag{21}$$

Based on the Euler-Lagrange necessary conditions, the partial derivatives of the above function should satisfy the following equations:

$$\frac{1}{2}\frac{d\phi}{de_y^T} = Q_Y^{-1}\tilde{e}_y - \hat{\lambda} = 0 \rightarrow \tilde{e}_y = Q_Y \hat{\lambda} \tag{22a}$$

$$\frac{1}{2}\frac{d\phi}{de_a^T} = Q_A^{-1}\tilde{e}_a + (\hat{X} \otimes I_m)\hat{\lambda} = 0 \rightarrow \tilde{e}_a = -Q_A(\hat{X} \otimes I_m)\hat{\lambda} \tag{22b}$$

$$\frac{1}{2}\frac{d\phi}{d\lambda^T} = y - \mathrm{vec}(A\hat{X}) - \tilde{e}_y + (\hat{X}^T \otimes I_m)\tilde{e}_a = 0 \tag{22c}$$

$$\frac{1}{2}\frac{d\phi}{dX^T} = (-A^T + \tilde{E}_A^T)\hat{\Lambda} = (A^T - \tilde{E}_A^T)\hat{\Lambda} = 0 \tag{22d}$$

Substituting $\tilde{e}_y$ and $\tilde{e}_a$ from Eqs. (22a) and (22b) into Eq. (22c), we get

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$$y - \text{vec}(A\hat{X}) - Q_Y\hat{\lambda} - (\hat{X}^T \otimes I)Q_A(\hat{X} \otimes I_m)\hat{\lambda} = 0 \tag{23}$$

and then

$$\text{vec}(\hat{E}) = (Q_Y + (\hat{X}^T \otimes I_m)Q_A(\hat{X} \otimes I_m))\hat{\lambda} \tag{24}$$

where $\hat{E} = Y - A\hat{X}$ = estimated total residuals matrix. From the above equation, $\hat{\lambda}$ can be calculated as:

$$\hat{\lambda} = Q_{\tilde{Y}}^{-1}\text{vec}(\hat{E}) = Q_{\tilde{Y}}^{-1}\hat{e} \tag{25}$$

where $\hat{e} = \text{vec}(\hat{E})$, and

$$Q_{\tilde{Y}} = Q_Y + (\hat{X}^T \otimes I_m)Q_A(\hat{X} \otimes I_m) \tag{26}$$

Substituting $\hat{\lambda}$ from Eq. (25) into Eqs. (22*a*) and (22*b*), respectively, yields

$$\hat{e}_y = Q_Y Q_{\tilde{Y}}^{-1}\hat{e} \tag{27}$$

and

$$\hat{e}_a = -Q_A(\hat{X} \otimes I_m)Q_{\tilde{Y}}^{-1}\hat{e} \tag{28}$$

Although the above formulation can directly be used, further simplification can be applied as follows. We assume that $Q_A = \Sigma_A \otimes Q$ and $Q_Y = \Sigma_Y \otimes Q$ where $Q \in \mathbb{R}^{m\times m}$, $\Sigma_A \in \mathbb{R}^{n\times n}$, and $\Sigma_Y \in \mathbb{R}^{k\times k}$ are given positive-definite matrices. This will then give

$$\begin{aligned} Q_{\tilde{Y}} &= \Sigma_Y \otimes Q + (\hat{X}^T \otimes I_m)(\Sigma_A \otimes Q)(\hat{X} \otimes I_m) \\ &= \Sigma_Y \otimes Q + \hat{X}^T\Sigma_A\hat{X} \otimes Q \\ &= (\Sigma_Y + \hat{X}^T\Sigma_A\hat{X}) \otimes Q \\ &= \hat{\Sigma} \otimes Q \end{aligned} \tag{29}$$

where $\hat{\Sigma} = \Sigma_Y + \hat{X}^T\Sigma_A\hat{X}$. The above equation is inverted to:

$$Q_{\tilde{Y}}^{-1} = \hat{\Sigma}^{-1} \otimes Q^{-1} \tag{30}$$

Eq. (25) can then be reformulated to

$$\begin{aligned} \hat{\lambda} &= (\hat{\Sigma}^{-1} \otimes Q^{-1})\text{vec}(\hat{E}) \\ &= \text{vec}(Q^{-1}\hat{E}\hat{\Sigma}^{-1}) \end{aligned} \tag{31}$$

and therefore, $\hat{\Lambda}$ can be obtained through the following equation

$$\hat{\Lambda} = \text{ivec}(\hat{\lambda}) = Q^{-1}\hat{E}\hat{\Sigma}^{-1} \tag{32}$$

where $\text{ivec}(\cdot)$ = inverse vec operation. Substituting $\hat{\Lambda}$ from the above equation into Eq. (22*d*) follows:

$$(A^T - \tilde{E}_A^T)Q^{-1}\hat{E}\hat{\Sigma}^{-1} = (A^T - \tilde{E}_A^T)Q^{-1}(Y - A\hat{X})\hat{\Sigma}^{-1} = 0 \tag{33}$$

which can be simplified as

$$(A - \tilde{E}_A)^T Q^{-1}A\hat{X} = (A - \tilde{E}_A)^T Q^{-1}Y \tag{34}$$

and subsequently

$$\hat{X} = ((A - \tilde{E}_A)^T Q^{-1}A)^{-1}(A - \tilde{E}_A)^T Q^{-1}Y \tag{35}$$

Similar to the univariate WTLS, to make a symmetric positive-definite normal matrix, $A = \tilde{A} + \tilde{E}_A$ is replaced in Eq. (34) as follows:

$$\tilde{A}^T Q^{-1}(\tilde{A} + \tilde{E}_A)X = \tilde{A}^T Q^{-1}Y \tag{36}$$

which, after a few simple mathematical operations, results in

$$\tilde{A}^T Q^{-1}\tilde{A}X = \tilde{A}^T Q^{-1}\tilde{Y} \tag{37}$$

where $\tilde{Y} = Y - \tilde{E}_A\hat{X}$ = matrix of predicted observations. Finally, the unknown parameters $\hat{X}$, with a symmetric positive-definite normal matrix, are calculated as

$$\hat{X} = (\tilde{A}^T Q^{-1}\tilde{A})^{-1}\tilde{A}^T Q^{-1}\tilde{Y} \tag{38}$$

which is similar to the standard multivariate LS method. Hence, the covariance matrix of the estimated parameters can easily be calculated without any derivation as follows [see Eq. (6)]:

$$Q_{\text{vec}(\hat{X})} = \hat{\Sigma} \otimes (\tilde{A}^T Q^{-1}\tilde{A})^{-1} \tag{39}$$

Moreover, the estimated observations and total residuals are obtained as:

$$\begin{aligned} \hat{Y} &= A\hat{X} - \tilde{E}_A\hat{X} = \tilde{A}\,\hat{X} = P_{\tilde{A}}\tilde{Y} \\ \hat{E} &= \tilde{Y} - \hat{Y} = Y - A\hat{X} = P_{\tilde{A}}^{\perp}\tilde{Y} \end{aligned} \tag{40}$$

with the following covariance matrices:

$$\begin{aligned} Q_{\text{vec}(\hat{Y})} &= \hat{\Sigma} \otimes P_{\tilde{A}}Q \\ Q_{\text{vec}(\hat{E})} &= \hat{\Sigma} \otimes P_{\tilde{A}}^{\perp}Q \end{aligned} \tag{41}$$

where $P_{\tilde{A}}$ and $P_{\tilde{A}}^{\perp}$ = two orthogonal projectors as

$$\begin{aligned} P_{\tilde{A}} &= \tilde{A}(\tilde{A}^T Q^{-1}\tilde{A})^{-1}\tilde{A}^T Q^{-1} \\ P_{\tilde{A}}^{\perp} &= I_m - P_{\tilde{A}} \end{aligned} \tag{42}$$

Although the vectorized format of $\tilde{E}_Y$ and $\tilde{E}_A$ were already defined, respectively, in Eqs. (27) and (28), they can also be obtained in a simpler way without the Kronecker product. It is for $\tilde{E}_Y$ as:

$$\begin{aligned} \tilde{e}_y &= \text{vec}(\tilde{E}_Y) = Q_Y\hat{\lambda} \\ &= (\Sigma_Y \otimes Q)(\hat{\Sigma}^{-1} \otimes Q^{-1})\text{vec}(\hat{E}) \\ &= (\Sigma_Y\hat{\Sigma}^{-1} \otimes I_m)\text{vec}(\hat{E}) \\ &= \text{vec}(\hat{E}\hat{\Sigma}^{-1}\Sigma_Y) \end{aligned} \tag{43}$$

which gives

$$\hat{E}_Y = \text{ivec}(\tilde{e}_y) = \hat{E}\hat{\Sigma}^{-1}\Sigma_Y \tag{44}$$

and for $\tilde{E}_A$ as:

$$\begin{aligned} \tilde{e}_a &= \text{vec}(\tilde{E}_A) = -Q_A(\hat{X} \otimes I_m)\hat{\lambda} \\ &= -(\Sigma_A \otimes Q)(\hat{X} \otimes I_m)\text{vec}(Q^{-1}\hat{E}\hat{\Sigma}^{-1}) \\ &= -(\Sigma_A\hat{X} \otimes Q)\text{vec}(Q^{-1}\hat{E}\hat{\Sigma}^{-1}) \\ &= -\text{vec}(QQ^{-1}\hat{E}\hat{\Sigma}^{-1}\hat{X}^T\Sigma_A) \\ &= -\text{vec}(\hat{E}\hat{\Sigma}^{-1}\hat{X}^T\Sigma_A) \end{aligned} \tag{45}$$

and therefore

$$\tilde{E}_A = \text{ivec}(\tilde{e}_a) = -\hat{E}\hat{\Sigma}^{-1}\hat{X}^T\Sigma_A \tag{46}$$

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Finally, the entire procedure of the multivariate weighted total least squares (MWTLS) is described in Algorithm 1.

Algorithm 1 Multivariate weighted total least squares algorithm

Inputs: Σ_A, Σ_Y, Q, ϵ (termination threshold)

Initialize: $\hat{X} = (A^T A)^{-1} A^T Y$

$X_0 \leftarrow \hat{X}$

while 1 **do**

$\hat{E} \leftarrow Y - A\hat{X}$

$\hat{\Sigma}^{-1} \leftarrow \mathrm{inv}(\Sigma_Y + \hat{X}^T \Sigma_A \hat{X})$

$\tilde{E}_A \leftarrow -\hat{E}\hat{\Sigma}^{-1}\hat{X}^T \Sigma_A$

$\tilde{A} \leftarrow A - \tilde{E}_A$

$\tilde{Y} \leftarrow Y - \tilde{E}_A \hat{X}$

$\hat{X} \leftarrow (\tilde{A}^T Q^{-1} \tilde{A})^{-1} \tilde{A} Q^{-1} \tilde{Y}$

if $\|\hat{X} - X_0\|_2 \le \epsilon$ **then**

Break;

else

$X_0 \leftarrow \hat{X}$

end if

end while

Output: $\hat{X}$

Computational Complexity Analysis

To demonstrate the performance of the proposed MWTLS method, especially when working with high-dimensional data sets, its computational complexity is analyzed in this part. To provide a comprehensive comparison, the computational burden of two other methods, univariate WTLS and MEIV1 (Wang et al. 2019), is also determined. This comparison is based on counting the time of floating-point calculations for the iterations of each method.

In the univariate WTLS process, the dominant term is calculating $Q_{\tilde{y}}^{-1}$ [see Eqs. (12) and (15)]. Because matrix $Q_{\tilde{y}}$, in its univariate form, is of size $mk \times mk$, the computational complexity of its inverse is of order $\mathcal{O}(m^3 k^3)$. In MEIV1, the algorithm is executed in two steps. The first step involves determining $\tilde{E}_A$, with the most computationally intensive part being the calculation of the inverse of an $mk \times mk$ matrix. The second part is dedicated to the calculation of unknown parameters. The heaviest computational part is the inverse calculation of an $nk \times nk$ matrix, posing a complexity of $\mathcal{O}(n^3 k^3)$. As we usually have $m > n$ (to have redundancy in the functional model), this indicates that the contribution of the first step is larger than the second step, and therefore the computational complexity of MEIV1 is also $\mathcal{O}(m^3 k^3)$.

To calculate the complexity of MWTLS, we use the steps in Algorithm 1. Two steps in the process are computationally heavier than the others. These steps are the calculation of Σ^{-1} and $\hat{X}$. To calculate Σ^{-1}, the inverse of a $k \times k$ matrix is required, posing computational burden of $\mathcal{O}(k^3)$. To calculate $\hat{X}$, the inverse of the $m \times m$ matrix Q is needed, which results in a computational complexity of $\mathcal{O}(m^3)$. As a result, according to the size of the input Y (of size $m \times k$), we may face one of the following two scenarios:

$$\text{Computational Complexity} = \begin{cases} \mathcal{O}(k^3) & \text{if } m \ll k \\ \mathcal{O}(m^3) & \text{if } k \ll m \end{cases} \tag{47}$$

which gives the complexity of MWTLS as $\mathcal{O} = \max(m^3, k^3)$. This computational complexity is clearly lower than that of univariate WTLS and MEIV1 models, expressed as $\mathcal{O}(m^3 k^3)$.

Experiments

To numerically evaluate the performance of the proposed method, two experiments have been conducted in this section. The first part of the experiments is dedicated to examining the performance of the proposed MWTLS on the simulated data, whereas in the second one, a real data set has been used to evaluate its efficiency. It is worth mentioning that the MEIV method (Wang et al. 2019) has been applied as the competing method for MWTLS. This method has two versions, named MEIV1 and MEIV2. According to Wang et al. (2019), these two versions have the same performance, but the convergence of the MEIV2 is superior to MEIV1. However, because there are some errors in the pseudocode of MEIV2 in the source paper Wang et al. (2019), MEIV1 has been used in this study. Moreover, the termination threshold has been set to $\epsilon = 10^{-6}$ in all experiments.

Simulated Data

In the first experiment, the procedure of finding the parameters of a 2D affine transformation has been selected to evaluate the performance of the experimental methods. This transformation is as follows:

$$\begin{aligned} X &= a_0 + a_1 x + a_2 y \\ Y &= b_0 + b_1 x + b_2 y \end{aligned} \tag{48}$$

where (x, y) and (X, Y) are respectively, coordinates of the points in the primary and secondary coordinate systems. $\eta = \{a_0, a_1, a_2, b_0, b_1, b_2\}$ are also the transformation's coefficients, which are the unknown parameters of the problem. Using seven points, observation, design, and coefficient matrices are as follows:

$$Y = \begin{bmatrix} X_1 & Y_1 \\ \vdots & \vdots \\ X_7 & Y_7 \end{bmatrix}, \quad A = \begin{bmatrix} 1 & x_1 & y_1 \\ \vdots & \vdots & \vdots \\ 1 & x_7 & x_7 \end{bmatrix}, \quad X = \begin{bmatrix} a_0 & b_0 \\ a_1 & b_1 \\ a_2 & b_2 \end{bmatrix} \tag{49}$$

The affine transformation coefficients for data simulation have arbitrarily been selected as follows:

$$a = \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} -2 \\ 0 \\ 1 \end{bmatrix}, \qquad b = \begin{bmatrix} b_0 \\ b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix} \tag{50}$$

To generate simulated data, first, points' coordinates in the primary coordinate system were generated randomly. Then, using transformation coefficients, their coordinates in the second coordinate system were calculated. After that, it is necessary to add noise to the points' coordinates in both coordinate systems. To do so, first Q_Y and Q_A were obtained using predefined arbitrary Σ_Y and Σ_A as described in the previous section. Σ_Y, Σ_A, and Q matrices were considered as:

$$\Sigma_Y = \begin{bmatrix} 0.01 & 0.005 \\ 0.005 & 0.01 \end{bmatrix} \tag{51a}$$

$$\Sigma_A = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0.01 & 0.005 \\ 0 & 0.005 & 0.01 \end{bmatrix} \tag{51b}$$

$$Q = I_7 \tag{51c}$$

Table 1. Results obtained by implementing MEIV1 and MWTLS on the simulated data set

Coefficient	Real value	MEIV1		MWTLS	
		Average	STD	Average	STD
a_0	−2	−2.0003358822	0.0549285465	−2.0003358422	0.0549285473
a_1	0	−0.0000686282	0.0117425389	−0.0000685568	0.0117425386
a_2	1	1.0002475289	0.0109372601	1.0002475324	0.0109372588
b_0	1	1.0010814788	0.0545704568	1.0010814645	0.0545704569
b_1	1	0.9999643060	0.0118635274	0.9999643211	0.0118635287
b_2	−1	−1.0001089740	0.0108065191	−1.0001089475	0.0108065192

where I_7 = identity matrix of size seven. After determining the variance-covariance matrices, the method in Khazraei and Amiri-Simkooei (2019) has been used to generate noise using Cholesky decomposition of Σ_Y and Σ_A.

To better investigate the performance of the proposed method along with the MEIV1 method, the procedure of generating noise was repeated 10,000 times, and for each run, the unknown coefficients were separately estimated. Table 1 shows the average and standard deviation values of the estimated parameters from 10,000 runs of MWTLS and MEIV1 algorithms. The reported results in this table indicate the high accuracy of both MWTLS and MEVI1 methods in estimating the unknown parameters. As shown in this table, the values obtained from the two methods are to a great extent the same, given the threshold provided, $\epsilon = 10^{-6}$.

The experiments were conducted on a personal computer with an Intel Core i5-4200M CPU @ 2.50 GHz processor and 6.00 GB RAM. The average execution time of MWTLS and MEVI1 algorithms in these 10,000 repetitions was 0.0001 and 0.0132 s, respectively. In other words, the MWTLS method is almost 130 times faster than MEIV1. In big problems, with a high number of samples and dimensions, this difference will show dramatically its impact. This is also linked to the computational complexity of these two algorithms, previously explained. Considering both the accuracy and the speed of the two studied methods in this part of the experiments show the superiority of the MWTLS over the MEIV1.

Fig. 1 shows the histogram of the results, obtained from 10,000 independent runs of the MWTLS algorithm. Examining the diagrams in this figure and comparing their values with the real values of the transformation coefficients proves the unbiased estimation of parameters by the proposed MWTLS algorithm.

To better investigate the effect of data size on the implementation of MWTLS and MEIV1, two other simulated data sets were generated in this section separately with 1,000 and 10,000 samples. In these data sets, the transformation coefficients were the same as the previous one, and just the number of samples increased, from $m = 7$ to $m = 1{,}000$ and $m = 10{,}000$. The data sets generation process was also as stated for the generation of the previous data set. The results of implementing MEIV1 and MWTLS algorithms on these data sets are listed in Tables 2 and 3.

As is clear in Table 2, the obtained results of the two experimental methods are the same to a great extent. It is noted that the execution times of MEIV1 and MWTLS were 124.43 and 0.18 s, respectively. This indicates that in this case, the proposed method is almost 700 times faster than MEIV1. The comparison of this case with the previous experiment, which used only seven points, shows that the increase in dimensions has caused a drastic difference between the execution time of the two MEIV1 and MWTLS algorithms.

In Table 3, which exhibited the results of the methods on the 10,000 sample data set, dashed lines imply the failure of the method in calculating desired results. As shown in this table, the MEIV1 method completely failed because of the *out of memory* problem, which occurred due to the use of a high-dimensional Kronecker product,whereas our proposed method extracted high-accuracy results, just in 1.2 s.

Real Data

In this part of the experiments, the georeferencing of a GeoEye-1 satellite image has been investigated using a number of ground control points (GCPs) through a 3D to 2D affine transformation as:

$$\begin{aligned} l &= a_0 + a_1 E + a_2 N + a_3 H \\ s &= b_0 + b_1 E + b_2 N + b_3 H \end{aligned} \tag{52}$$

where (l, s) and (E, N, H) are respectively, the image and ground coordinates of the GCPs. Moreover, $a_0, \ldots, a_3$ and $b_0, \ldots, b_3$ are the transformation coefficients to be estimated. Hence, in this case, observation, design, and coefficient matrices are as follows:

$$Y = \begin{bmatrix} l_1 & s_1 \\ \vdots & \vdots \\ l_m & s_m \end{bmatrix}, \qquad A = \begin{bmatrix} 1 & E_1 & N_1 & H_1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & E_m & N_m & H_m \end{bmatrix},$$

$$X = \begin{bmatrix} a_0 & b_0 \\ a_1 & b_1 \\ a_2 & b_2 \\ a_3 & b_3 \end{bmatrix} \tag{53}$$

For this experiment, 70 GCPs were selected using the sharp objects in the satellite image, whereas their corresponding ground coordinates were extracted from a 1:2000 digital reference map. A number of GCPs, named train GCPs (TGCPs), were selected for the coefficients' estimation process. After calculating the unknown parameters, another group of the GCPs, called check GCPs (CGCPs), is utilized to evaluate the accuracy of these extracted parameters. It is assumed that the ground coordinates of CGPs are known, and their image coordinates should be determined through Eq. (52). The root mean squares error (RMSE) over the extracted and real image coordinates of CGCPs is applied as the metric for the evaluation of the extracted unknown parameters.

Six different experiments, 10, 20, 30, 40, 50, and 60 TGCPs, were executed in this part. The distribution of TGCPs in different experiments along with the distribution of CGCPs have been illustrated in Fig. 2.

The results obtained from implementing MWTLS and MEIV1 on the real data set with different numbers of TGCPs are shown in Table 4. As indicated in this table, both methods provide identical results. This indicates the high performance of both methods in real scenarios. But, the proposed method with high capability in

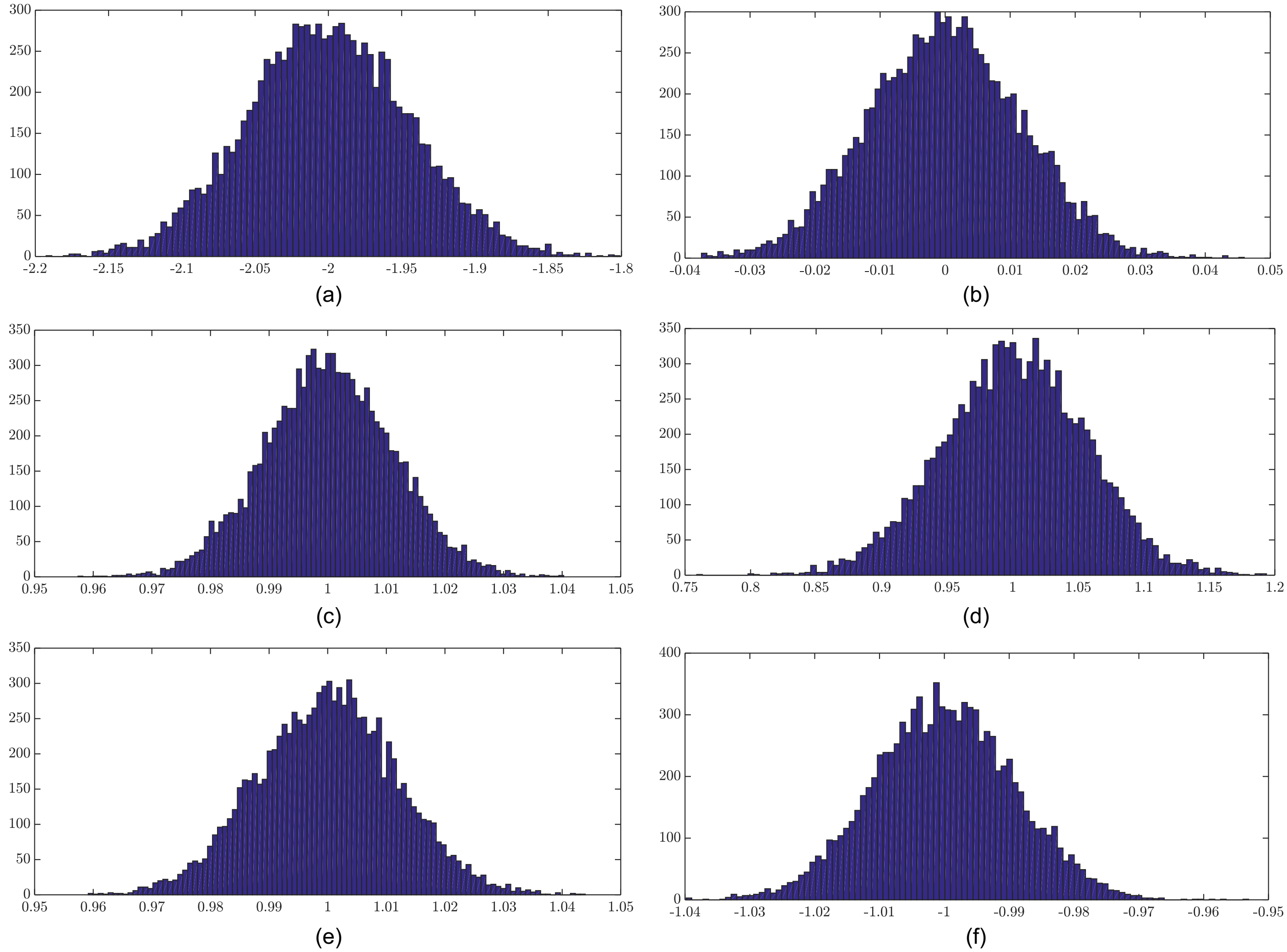

Fig. 1. Histogram of estimated coefficients in 10,000 repetitions of the MWTLS algorithm: (a) a_0; (b) a_1; (c) a_2; (d) b_0; (e) b_1; and (f) b_2.

Table 2. Results obtained by implementing MEVI1 and MWTLS on a data set with 1,000 samples

Coefficient	Real value	MEIV1	MWTLS
a_0	−2	−1.9996313520	−1.9996313521
a_1	0	0.0002005223	0.0002005224
a_2	1	0.9998703032	0.9998703031
b_0	1	0.9996497503	0.9996497503
b_1	1	0.9996596630	0.9996596629
b_2	−1	−0.9999185717	−0.9999185716

Table 3. Results obtained by implementing MEVI1 and MWTLS on a set with 10,000 samples

Coefficient	Real value	MEIV1	MWTLS
a_0	−2	—	−1.9999992818
a_1	0	—	0.0000431740
a_2	1	—	0.9999242961
b_0	1	—	0.9998795438
b_1	1	—	0.9998789893
b_2	−1	—	−1.0000845498

high-dimensional problems and higher running speed, outperforms MEIV1.

Conclusion

In this research, a simple, fast, and flexible procedure, called MWTLS, was presented based on the standard LS theory to solve the problem of multivariate WTLS. Simplifying the computational process and avoiding the use of Kronecker product in the calculations, the proposed method has a high capability in problems with large size and high dimensional data sets. On the other hand, it is a clear and simple process provided the ability to easily implement the proposed procedure on a wide range of applications in geodetic issues. Experiments performed in this study on both simulated and real data sets to determine the parameters of 2D–2D and 3D–2D affine transformation showed that, in addition to its simplicity and ability to work with bulk data, the proposed method outperformed the state-of-the-art MEIV1 method in terms of speed and accuracy.

As with many studies, there are some unresolved issues in this study that could be a prospect for future research. One of the most important remaining challenges in the present study is the need for

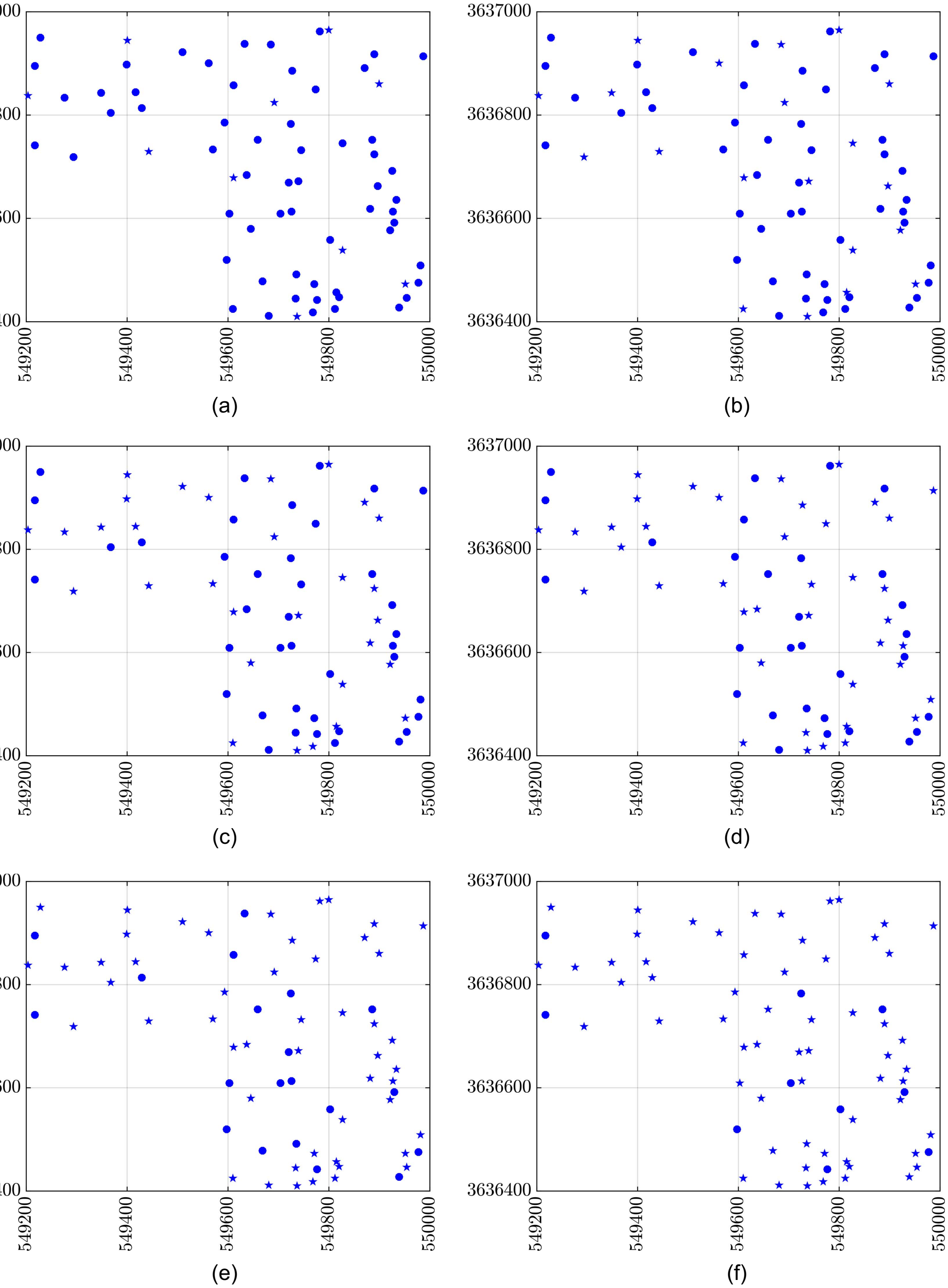

Fig. 2. Distribution of TGCPs (circle markers) and CGCPs (pentagram markers) in different experiments of the real case scenario: (a) 10 GCPs; (b) 20 GCPs; (c) 30 GCPs; (d) 40 GCPs; (e) 50 GCPs; and (f) 60 GCPs.

Table 4. Results obtained from implementing MEIV1 and MWTLS on the real data set

Number of TGCPs	Number of CGCPs	MEIV1			MWTLS		
		$RMSE_l$	$RMSE_s$	$RMSE_{total}$	$RMSE_l$	$RMSE_s$	$RMSE_{total}$
10	60	0.5721926634	0.4230934257	0.7116266514	0.5721926635	0.4230934258	0.7116266514
20	50	0.4649924422	0.3610036919	0.5886778719	0.4649924422	0.3610036919	0.5886778719
30	40	0.5054859988	0.3470532192	0.6131574284	0.5054859987	0.3470532192	0.6131574283
40	30	0.4867388916	0.3722063880	0.6127416616	0.4867388916	0.3722063881	0.6127416617
50	20	0.5073174706	0.3922464145	0.6412708209	0.5073174704	0.3922464146	0.6412708208
60	10	0.5471968102	0.3547466251	0.6521269180	0.5471968100	0.3547466250	0.6521269177

a predefined weight matrix before performing the algorithm process. The exact determination of these values, which have a significant effect on the final extracted results, can be considered in future studies. Moreover, applying the proposed method in different related applications, especially high-dimensional data modeling like remotely sensed hyperspectral images and point clouds problems, can be another part of our future work.

Data Availability Statement

Some or all data, models, or codes that support the findings of this study are available from the corresponding author upon reasonable request. The available data are: (1) generating synthetic data, and (2) MATLAB code for MWTLS.

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