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Generalized total least squares prediction algorithm for universal 3D similarity transformation

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Abstract

Three–dimensional (3D) similarity datum transformation is extensively applied to transform coordinates from GNSS-based datum to a local coordinate system. Recently, some total least squares (TLS) algorithms have been successfully developed to solve the universal 3D similarity transformation problem (probably with big rotation angles and an arbitrary scale ratio). However, their procedures of the parameter estimation and new point (non-common point) transformation were implemented separately, and the statistical correlation which often exists between the common and new points in the original coordinate system was not considered. In this contribution, a generalized total least squares prediction (GTLSP) algorithm, which implements the parameter estimation and new point transformation synthetically, is proposed. All of the random errors in the original and target coordinates, and their variance–covariance information will be considered. The 3D transformation model in this case is abstracted as a kind of generalized errors–in–variables (EIV) model and the equation for new point transformation is incorporated into the functional model as well. Then the iterative solution is derived based on the Gauss–Newton approach of nonlinear least squares. The performance of GTLSP algorithm is verified in terms of a simulated experiment, and the results show that GTLSP algorithm can improve the statistical accuracy of the transformed coordinates compared with the existing TLS algorithms for 3D similarity transformation.

Keywords: 3D similarity transformation; Errors–in–variables model; Total least squares prediction; Gauss–Newton approach

1. Introduction

Nowadays, Global Navigation Satellite System (GNSS) has been extensively applied in the fields of geodesy and many other areas. The GNSS techniques are based on specified coordinate systems, such as WGS-84, ITRF 2008, and CGCS 2000 etc. As a result, the coordinates of the points obtained from GNSS observations are defined in these systems. However, many geodetic and surveying engineering applications are based on local coordinate systems. Thus the coordinate transformation problem must be solved in the GNSS applications.

Three–dimensional (3D) similarity datum transformation is the most commonly used model for geodetic transformation and has attracted extensive attention. The purpose of 3D transformation is to predict the coordinates of new points in the target system by using their original coordinates and the coordinates of common points in both original and target coordinate systems. In order to achieve this goal, two necessary procedures, including the parameter estimation and new point transformation, should be implemented in practice.

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Parameter estimation is an important part for the 3D similarity transformation problem, in which there are totally seven transformation parameters to be estimated, including three translation parameters, three rotation angles and a scale ratio. In geodetic field, many algorithms have been developed to solve these parameters. If the rotation angles are small enough and the scale ratio is close to 1, the transformation equation can be simplified into the well-known Bursa model (Seeber, 1993, p. 2; Yang, 1999), which is normally processed as a linear Gauss–Markov (GM) model. However, the rotation angles could be large in practice, therefore many least squares algorithms have been proposed to solve the nonlinear GM model, such as the methods based on the Procrustes analysis (Grafarend and Awange, 2003, 2012; Grafarend, 2006) and the unit quaternion (Shen et al., 2006).

It is well known that the random errors in the coefficient matrix are not considered in the traditional GM model. Nevertheless, the coordinates in the original system are usually observed as well, which means that parts of the elements in the coefficient matrix are affected by random errors. Thus the transformation model cannot always be abstracted as a GM model. Then the errors–in–variables (EIV) model should be introduced to replace the GM model in the datum transformation problems. The method to adjust EIV model was named total least squares (TLS) and was firstly introduced by Golub and Van Loan (1980) in the field of statistics. It is generally acknowledged that Teunissen (1988) was the first person who formulated and solved the TLS problem in an exact form in geodetic literature. Since then a large number of algorithms, especially the weighted TLS (WTLS) algorithms which can solve EIV models in heteroscedastic case were developed (e.g., Schaffrin and Wieser, 2008; Neitzel, 2010; Shen et al., 2011; Amiri-Simkooei and Jazaeri, 2012; Mahboub, 2012; Xu et al., 2012; Fang, 2013; Zhou and Fang, 2015). In addition, some extended TLS algorithms were also investigated, for instance, the TLS algorithm with equality (Schaffrin and Felus, 2009; Zhang and Zhang, 2014; Fang, 2015; Fang and Wu, 2016; Fang et al., 2015) and inequality constraints (Zhang et al., 2013; Fang, 2014a; Fang and Wu, 2016; Zeng et al., 2015), the TLS solution to multivariate EIV model (Schaffrin and Felus, 2008), the gross error processing for TLS (Amiri-Simkooei and Jazaeri, 2013; Wang et al., 2016) and the variance component estimation method in EIV models (Amiri-Simkooei, 2013; Xu and Liu, 2014; Mahboub, 2014). Many of these algorithms can be employed to estimate parameters in the 2D or 3D datum transformation problem.

The TLS solution to 3D transformation under universal conditions (probably with big rotation angles and an arbitrary scale ratio) has become a hot research issue in recent years. Felus and Burtch (2009) derived an algorithm by solving the multivariate EIV model. Fang (2014b) provided a TLS solution by introducing the quasi indirect errors adjustment (QIEA). Chang (2015) generated a closed-form least squares solution to 3D similarity transformation problem under Gauss–Helmert model in the equally weighted case. Additionally, Fang (2015) proposed a WTLS algorithm with universal constraints for fully weighted 3D datum transformations.

Although a large amount of TLS algorithms for 3D transformation have been proposed, a limitation exists commonly: they only focused on how to estimate the transformation parameters, whereas their procedures of the parameter estimation and new point transformation were implemented separately. The statistical correlation between the common and new points in the original system, which often exists in practice particularly when the coordinates are obtained by GNSS observation networks, was ignored. In order to overcome this limitation, Li et al. (2012) proposed a seamless 3D datum transformation model which integrated the processes of the parameter estimation and new point transformation. The experimental results showed that the accuracy of the transformed coordinates can be improved especially when the correlation mentioned above is strong. However, this transformation model was derived based on the Bursa model which is simplified under the conditions with small rotation angles and a scale ratio close to 1, implying that it is inapplicable under the conditions with big rotation angles and an arbitrary scale ratio.

In this paper, we propose a generalized total least squares prediction (GTLSP) algorithm for the universal 3D similarity transformation, in which the parameter calculation and new point transformation can be implemented synthetically. All of the random errors in the original and target coordinates, and their variance–covariance information are taken into account in this algorithm. The 3D transformation model is described as a kind of generalized EIV model. In addition, the equation for new point transformation is also included in the functional model. Then the Gauss–Newton approach of nonlinear least squares is employed to derive the iterative solution.

The remaining part of the article is organized as follows: the background of 3D similarity transformation model is introduced in Section 2. In Section 3, the abstract functional model and the corresponding stochastic model are presented, and then the iterative formulae of the GTLSP algorithm are derived based on the Gauss–Newton approach. In Section 4, we make a detailed discussion about the application of this new algorithm for 3D similarity transformation. A simulated experiment is presented to verify the performance of GTLSP algorithms in Section 5. Finally, some conclusions from theoretical and experimental aspects are given in Section 6.

2. Background of the 3D similarity transformation model

The 3D similarity transformation model is (Wolf and Ghilani, 1997; Felus and Burtch, 2009):

$$\begin{bmatrix} x_{2i} \\ y_{2i} \\ z_{2i} \end{bmatrix} - \begin{bmatrix} ex_{2i} \\ ey_{2i} \\ ez_{2i} \end{bmatrix} = \mu \mathbf{M} \left(\begin{bmatrix} x_{1i} \\ y_{1i} \\ z_{1i} \end{bmatrix} - \begin{bmatrix} ex_{1i} \\ ey_{1i} \\ ez_{1i} \end{bmatrix} \right) + \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta z \end{bmatrix} \tag{1}$$

where $[x_{1i} \quad y_{1i} \quad z_{1i}]^{\mathrm{T}}$ and $[x_{2i} \quad y_{2i} \quad z_{2i}]^{\mathrm{T}}$ represent the coordinates of the ith point in the original and target coordinate systems, $[ex_{1i} \quad ey_{1i} \quad ez_{1i}]^{\mathrm{T}}$ and $[ex_{2i} \quad ey_{2i} \quad ez_{2i}]^{\mathrm{T}}$ are their corresponding random error vectors, respectively. $\mathbf{M}$ is the rotation matrix, and it is expressed as below:

$$\mathbf{M} = \mathbf{M}_3 \cdot \mathbf{M}_2 \cdot \mathbf{M}_1 \tag{2}$$

$$\mathbf{M}_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & \sin\alpha \\ 0 & -\sin\alpha & \cos\alpha \end{bmatrix}, \quad \mathbf{M}_2 = \begin{bmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{bmatrix}, \quad \mathbf{M}_3 = \begin{bmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{3}$$

The parameter vector to be estimated is as following:

$$\boldsymbol{\xi} = [\Delta x \quad \Delta y \quad \Delta z \quad \mu \quad \alpha \quad \beta \quad \gamma]^{T} \tag{4}$$

which includes three translation parameters (Δx, Δy, Δz), three rotation angles (α, β, γ) and a scale ratio parameter (μ).

By using the estimated transformation parameters, the original coordinates of the new points can be converted into the target coordinate system. Most previous studies on TLS algorithms for 3D datum transformation only focused on the parameter estimation. Meanwhile the procedures of the parameter calculation and coordinates transformation of new points were implemented separately. To overcome this shortcoming, Li et al. (2012) proposed a seamless 3D transformation model which integrated the processes of parameter estimation and new point transformation. It can actually be regarded as a kind of TLS prediction method. However, this model was derived based on the Bursa model which is simplified under the conditions with small rotation angles and a scale ratio close to 1. Thus it is inapplicable for more universal 3D transformation problems with large rotation angles and an arbitrary scale ratio. The GTLSP algorithm derived in next section can effectively solve this problem.

3. Derivation of the GTLSP algorithm

For common points, the transformation model can be abstracted as a kind of generalized EIV model:

$$\boldsymbol{L}_1 - \boldsymbol{e}_{L_1} = \boldsymbol{\varphi}_1(\boldsymbol{e}_1, \boldsymbol{\xi}) = \boldsymbol{f}_1(\boldsymbol{a}_1 - \boldsymbol{e}_1, \boldsymbol{\xi}) \tag{5}$$

where $\boldsymbol{f}_1$ and $\boldsymbol{\varphi}_1$ are both abstract vector functions with dimensions $m \times 1$, $\boldsymbol{a}_1$ and $\boldsymbol{L}_1$ denote the $n \times 1$ and $m \times 1$ observation vectors in original and target systems, $\boldsymbol{e}_1$ and $\boldsymbol{e}_{L_1}$ are their corresponding random error vectors, respectively. $\boldsymbol{\xi}$ is the $t \times 1$ parameter vector to be estimated.

For new points, the transformation equation is expressed as below:

$$\bar{\boldsymbol{L}}_2 = \boldsymbol{\varphi}_2(\boldsymbol{e}_2, \boldsymbol{\xi}) = \boldsymbol{f}_2(\boldsymbol{a}_2 - \boldsymbol{e}_2, \boldsymbol{\xi}) \tag{6}$$

where $\boldsymbol{f}_2$ and $\boldsymbol{\varphi}_2$ are abstract vector functions as well, and both of their dimensions are $p \times 1$. $\boldsymbol{a}_2$ represents the $q \times 1$ observation vector in the original system, $\boldsymbol{e}_2$ is the corresponding random error vector. $\bar{\boldsymbol{L}}_2$ denotes the $p \times 1$ target vector which needs to be predicted.

The corresponding stochastic model is:

$$\boldsymbol{e} \sim N(0, \sigma_0^2 \mathbf{Q}_e) \tag{7}$$

where

$$\boldsymbol{e} = \begin{bmatrix} \boldsymbol{e}_{L_1} \\ \boldsymbol{e}_1 \\ \boldsymbol{e}_2 \end{bmatrix}, \quad \mathbf{Q}_e = \begin{bmatrix} \mathbf{Q}_{L_1 L_1} & \mathbf{Q}_{L_1 a_1} & \mathbf{Q}_{L_1 a_2} \\ \mathbf{Q}_{a_1 L_1} & \mathbf{Q}_{a_1 a_1} & \mathbf{Q}_{a_1 a_2} \\ \mathbf{Q}_{a_2 L_1} & \mathbf{Q}_{a_2 a_1} & \mathbf{Q}_{a_2 a_2} \end{bmatrix} \tag{8}$$

$\mathbf{Q}_e$ is a positive definite cofactor matrix of the total error vector $\boldsymbol{e}$, without loss of generality, it is assumed as a fully correlated matrix. $\mathbf{Q}_{L_1 L_1}$, $\mathbf{Q}_{a_1 a_1}$ and $\mathbf{Q}_{a_2 a_2}$ are the cofactor matrices of $\boldsymbol{e}_{L_1}$, $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$, respectively. $\mathbf{Q}_{L_1 a_1}$, $\mathbf{Q}_{L_1 a_2}$ and $\mathbf{Q}_{a_1 a_2}$ are the corresponding cofactor matrices between $\boldsymbol{e}_{L_1}$, $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$. The estimation criterion of the model above is presented as following:

$$\boldsymbol{e}^{\mathrm{T}} \mathbf{P} \boldsymbol{e} = \min \tag{9}$$

where $\mathbf{P}$ denotes the weight matrix, and $\mathbf{P} = \mathbf{Q}_e^{-1}$.

Since Eqs. (5) and (6) are essentially nonlinear models, the Gauss–Newton approach of nonlinear least squares is employed to derive the solution. We assume that the approximate values of ξ, $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are ξ^0, $\boldsymbol{e}_1^0$ and $\boldsymbol{e}_2^0$, respectively. The right-hand members of Eqs. (5) and (6) are expressed through Taylor series expansion at (ξ^0, $\boldsymbol{e}_1^0$, $\boldsymbol{e}_2^0$):

$$\boldsymbol{L}_1 - \boldsymbol{e}_{L_1} = \boldsymbol{\varphi}_1(\boldsymbol{e}_1^0, \xi^0) + \mathbf{A}_1 \delta\xi + \mathbf{B}_1(\boldsymbol{e}_1 - \boldsymbol{e}_1^0) \tag{10}$$

$$\bar{\boldsymbol{L}}_2 = \boldsymbol{\varphi}_2(\boldsymbol{e}_2^0, \xi^0) + \mathbf{A}_2 \delta\xi + \mathbf{B}_2(\boldsymbol{e}_2 - \boldsymbol{e}_2^0) \tag{11}$$

where $\delta\xi$ is the correction vector of ξ^0, $\delta\xi = \xi - \xi_0$, and:

$$\mathbf{A}_1 = \left.\frac{\partial \boldsymbol{\varphi}_1(\boldsymbol{e}_1, \xi)}{\partial \xi^{\mathrm{T}}}\right|(\boldsymbol{e}_1^0, \xi^0), \quad \mathbf{B}_1 = \left.\frac{\partial \boldsymbol{\varphi}_1(\boldsymbol{e}_1, \xi)}{\partial \boldsymbol{e}_1^{\mathrm{T}}}\right|(\boldsymbol{e}_1^0, \xi^0) \tag{12}$$

$$\mathbf{A}_2 = \left.\frac{\partial \boldsymbol{\varphi}_2(\boldsymbol{e}_2, \xi)}{\partial \xi^{\mathrm{T}}}\right|(\boldsymbol{e}_2^0, \xi^0), \quad \mathbf{B}_2 = \left.\frac{\partial \boldsymbol{\varphi}_2(\boldsymbol{e}_2, \xi)}{\partial \boldsymbol{e}_2^{\mathrm{T}}}\right|(\boldsymbol{e}_2^0, \xi^0) \tag{13}$$

The Lagrange objective function of GTLSP is constructed as below:

$$\begin{aligned} \Phi = {} & \boldsymbol{e}^{\mathrm{T}} \mathbf{P} \boldsymbol{e} + 2\boldsymbol{\lambda}^{\mathrm{T}}(\boldsymbol{L}_1 - \boldsymbol{e}_{L_1} - \boldsymbol{\varphi}_1(\boldsymbol{e}_1^0, \xi^0) - \mathbf{A}_1 \delta\xi \\ & - \mathbf{B}_1(\boldsymbol{e}_1 - \boldsymbol{e}_1^0)) + 2\boldsymbol{K}^{\mathrm{T}}(\bar{\boldsymbol{L}}_2 - \boldsymbol{\varphi}_2(\boldsymbol{e}_2^0, \xi^0) - \mathbf{A}_2 \delta\xi \\ & - \mathbf{B}_2(\boldsymbol{e}_2 - \boldsymbol{e}_2^0)) \end{aligned} \tag{14}$$

where $\boldsymbol{\lambda}$ and $\boldsymbol{K}$ are the $m \times 1$ and $p \times 1$ vectors of "Lagrange multipliers", respectively. The solution of this target function can be derived via the Euler–Lagrange necessary conditions, namely,

$$\frac{1}{2}\frac{\partial\Phi}{\partial e}\bigg|(\tilde{e},\delta\hat{\xi},\hat{\lambda},\hat{K},\tilde{L}_2) = \mathbf{P}\tilde{e} - \begin{bmatrix}\hat{\lambda}\\ \mathbf{B}_1^{\mathrm{T}}\hat{\lambda}\\ \mathbf{B}_2^{\mathrm{T}}\hat{K}\end{bmatrix} = 0 \tag{15a}$$

$$\frac{1}{2}\frac{\partial\Phi}{\partial\delta\xi}\bigg|(\tilde{e},\delta\hat{\xi},\hat{\lambda},\hat{K},\tilde{\mathbf{L}}_2) = -\mathbf{A}_1^{\mathrm{T}}\hat{\lambda} - \mathbf{A}_2^{\mathrm{T}}\hat{K} = 0 \tag{15b}$$

$$\frac{1}{2}\frac{\partial\Phi}{\partial\lambda}\bigg|(\tilde{e},\delta\hat{\xi},\hat{\lambda},\hat{K},\tilde{L}_2) = L_1 - \tilde{e}_{L_1} - \varphi_1(e_1^0,\xi^0) - \mathbf{A}_1\delta\hat{\xi} - \mathbf{B}_1(\tilde{e}_1 - e_1^0) = 0 \tag{15c}$$

$$\frac{1}{2}\frac{\partial\Phi}{\partial K}\bigg|(\tilde{e},\delta\hat{\xi},\hat{\lambda},\hat{K},\tilde{L}_2) = \tilde{L}_2 - \varphi_2(e_2^0,\xi^0) - \mathbf{A}_2\delta\hat{\xi} - \mathbf{B}_2(\tilde{e}_2 - e_2^0) = 0 \tag{15d}$$

$$\frac{1}{2}\frac{\partial\Phi}{\partial\tilde{L}_2}\bigg|(\tilde{e},\delta\hat{\xi},\hat{\lambda},\hat{K},\tilde{L}_2) = \hat{K} = 0 \tag{15e}$$

where "$\sim$" and "^" represent predicted and estimated ones, respectively.

From Eqs. (15a) and (15e), we can readily obtain the error vector:

$$\tilde{e} = \begin{bmatrix}\tilde{e}_{L_1}\\ \tilde{e}_1\\ \tilde{e}_2\end{bmatrix} = \mathbf{Q}_e\begin{bmatrix}\hat{\lambda}\\ \mathbf{B}_1^{\mathrm{T}}\hat{\lambda}\\ \mathbf{B}_2^{\mathrm{T}}\hat{K}\end{bmatrix} = \begin{bmatrix}\mathbf{Q}_{L_1L_1} & \mathbf{Q}_{L_1a_1} & \mathbf{Q}_{L_1a_2}\\ \mathbf{Q}_{a_1L_1} & \mathbf{Q}_{a_1a_1} & \mathbf{Q}_{a_1a_2}\\ \mathbf{Q}_{a_2L_1} & \mathbf{Q}_{a_2a_1} & \mathbf{Q}_{a_2a_2}\end{bmatrix}\begin{bmatrix}\hat{\lambda}\\ \mathbf{B}_1^{\mathrm{T}}\hat{\lambda}\\ 0\end{bmatrix} = \begin{bmatrix}(\mathbf{Q}_{L_1L_1} + \mathbf{Q}_{L_1a_1}\mathbf{B}_1^{\mathrm{T}})\hat{\lambda}\\ (\mathbf{Q}_{a_1L_1} + \mathbf{Q}_{a_1a_1}\mathbf{B}_1^{\mathrm{T}})\hat{\lambda}\\ (\mathbf{Q}_{a_2L_1} + \mathbf{Q}_{a_2a_1}\mathbf{B}_1^{\mathrm{T}})\hat{\lambda}\end{bmatrix} \tag{16}$$

Thus, we can derive the expression for each residual vector in the form of $\hat{\lambda}$ as below:

$$\tilde{e}_{L_1} = (\mathbf{Q}_{L_1L_1} + \mathbf{Q}_{L_1a_1}\mathbf{B}_1^{\mathrm{T}})\hat{\lambda} \tag{17a}$$

$$\tilde{e}_1 = (\mathbf{Q}_{a_1L_1} + \mathbf{Q}_{a_1a_1}\mathbf{B}_1^{\mathrm{T}})\hat{\lambda} \tag{17b}$$

$$\tilde{e}_2 = (\mathbf{Q}_{a_2L_1} + \mathbf{Q}_{a_2a_1}\mathbf{B}_1^{\mathrm{T}})\hat{\lambda} \tag{17c}$$

By inserting Eqs. (17a) and (17b) into Eq. (15c), we obtain the following equation:

$$L_1 - (\mathbf{Q}_{L_1L_1} + \mathbf{Q}_{L_1a_1}\mathbf{B}_1^{\mathrm{T}})\hat{\lambda} - \varphi_1(e_1^0,\xi^0) - \mathbf{A}_1\delta\hat{\xi} - \mathbf{B}_1(\mathbf{Q}_{a_1L_1} + \mathbf{Q}_{a_1a_1}\mathbf{B}_1^{\mathrm{T}})\hat{\lambda} + \mathbf{B}_1e_1^0 = 0 \tag{18}$$

Then the expression of $\hat{\lambda}$ can be derived as:

$$\hat{\lambda} = (\mathbf{Q}_{L_1L_1} + \mathbf{Q}_{L_1a_1}\mathbf{B}_1^{\mathrm{T}} + \mathbf{B}_1\mathbf{Q}_{a_1L_1} + \mathbf{B}_1\mathbf{Q}_{a_1a_1}\mathbf{B}_1^{\mathrm{T}})^{-1} \cdot (L_1 - \varphi_1(e_1^0,\xi^0) - \mathbf{A}_1\delta\hat{\xi} + \mathbf{B}_1e_1^0) = \mathbf{Q}_l^{-1}(L_1 - \varphi_1(e_1^0,\xi^0) - \mathbf{A}_1\delta\hat{\xi} + \mathbf{B}_1e_1^0) \tag{19}$$

with

$$\mathbf{Q}_l = \mathbf{Q}_{L_1L_1} + \mathbf{Q}_{L_1a_1}\mathbf{B}_1^{\mathrm{T}} + \mathbf{B}_1\mathbf{Q}_{a_1L_1} + \mathbf{B}_1\mathbf{Q}_{a_1a_1}\mathbf{B}_1^{\mathrm{T}} \tag{20}$$

By substituting Eqs. (15e) and (19) into Eq. (15b), the solution of $\delta\hat{\xi}$ can be derived as below:

$$\mathbf{A}_1^{\mathrm{T}}\mathbf{Q}_l^{-1}(L_1 - \varphi_1(e_1^0,\xi^0) - \mathbf{A}_1\delta\hat{\xi} + \mathbf{B}_1e_1^0) = 0 \tag{21}$$

$$\delta\hat{\xi} = (\mathbf{A}_1^{\mathrm{T}}\mathbf{Q}_l^{-1}\mathbf{A}_1)^{-1}\mathbf{A}_1^{\mathrm{T}}\mathbf{Q}_l^{-1}(L_1 - \varphi_1(e_1^0,\xi^0) + \mathbf{B}_1e_1^0) \tag{22}$$

Thereby, the parameter vector is updated as: $\hat{\xi} = \xi^0 + \delta\hat{\xi}$.

Inserting Eq. (22) into Eq. (19) then into Eqs. (17a)–(17c), we obtain the specific expression for each error vector:

$$\tilde{e}_{L_1} = (\mathbf{Q}_{L_1L_1} + \mathbf{Q}_{L_1a_1}\mathbf{B}_1^{\mathrm{T}})\mathbf{Q}_l^{-1}(L_1 - \varphi_1(e_1^0,\xi^0) - \mathbf{A}_1\delta\hat{\xi} + \mathbf{B}_1e_1^0) \tag{23a}$$

$$\tilde{e}_1 = (\mathbf{Q}_{a_1L_1} + \mathbf{Q}_{a_1a_1}\mathbf{B}_1^{\mathrm{T}})\mathbf{Q}_l^{-1}(L_1 - \varphi_1(e_1^0,\xi^0) - \mathbf{A}_1\delta\hat{\xi} + \mathbf{B}_1e_1^0) \tag{23b}$$

$$\tilde{e}_2 = (\mathbf{Q}_{a_2L_1} + \mathbf{Q}_{a_2a_1}\mathbf{B}_1^{\mathrm{T}})\mathbf{Q}_l^{-1}(L_1 - \varphi_1(e_1^0,\xi^0) - \mathbf{A}_1\delta\hat{\xi} + \mathbf{B}_1e_1^0) \tag{23c}$$

Finally, from Eq. (15d), we can do the prediction step to obtain $\tilde{L}_2$ as:

$$\tilde{L}_2 = \varphi_2(e_2^0,\xi^0) + \mathbf{A}_2\delta\hat{\xi} + \mathbf{B}_2(\tilde{e}_2 - e_2^0) \tag{24}$$

The above procedure can be implemented iteratively, and a small positive threshold ε_0 should be primarily presented to terminate the iteration until $\|\delta\hat{\xi}\| < \varepsilon_0$, where $\|\cdot\|$ denotes the l_2–norm of a vector. It's important to note that $\mathbf{A}_1$, $\mathbf{B}_1$, $\mathbf{A}_2$, and $\mathbf{B}_2$ should be updated during the iterative process.

From Eqs. (17a)–(22), we find that the prediction equation has no effect on parameter estimation. Therefore, Eqs. (23c) and (24) can be carried out after the iteration. If the threshold ε_0 is sufficiently small to stop the iteration procedure, i.e., $\|\delta\hat{\xi}\| < \varepsilon_0 \to 0$, as a result, $\tilde{e}_2 - e_2^0 \to 0$, Eqs. (23c) and (24) will become:

$$\tilde{e}_2 = (\mathbf{Q}_{a_2L_1} + \mathbf{Q}_{a_2a_1}\mathbf{B}_1^{\mathrm{T}})\mathbf{Q}_l^{-1}(L_1 - \varphi_1(\tilde{e}_1,\hat{\xi}) + \mathbf{B}_1\tilde{e}_1) \tag{25}$$

$$\tilde{L}_2 = \varphi_2(\tilde{e}_2,\hat{\xi}) \tag{26}$$

In addition, Eq. (19) can be simplified as:

$$\hat{\lambda} = \mathbf{Q}_l^{-1}(L_1 - \varphi_1(\tilde{e}_1,\hat{\xi}) + \mathbf{B}_1\tilde{e}_1) \tag{27}$$

From Eq. (16), we find that the sum of weighted squared residuals $\tilde{e}^{\mathrm{T}}\mathbf{P}\tilde{e}$ may be expressed as below:

$$\begin{aligned}\tilde{e}^{\mathrm{T}}\mathbf{P}\tilde{e} &= [\hat{\lambda}^{\mathrm{T}} \quad \hat{\lambda}^{\mathrm{T}}\mathbf{B}_1 \quad 0]\mathbf{Q}_e\mathbf{P}\mathbf{Q}_e\begin{bmatrix}\hat{\lambda}\\ \mathbf{B}_1^{\mathrm{T}}\hat{\lambda}\\ 0\end{bmatrix}\\ &= [\hat{\lambda}^{\mathrm{T}} \quad \hat{\lambda}^{\mathrm{T}}\mathbf{B}_1 \quad 0]\mathbf{Q}_e\begin{bmatrix}\hat{\lambda}\\ \mathbf{B}_1^{\mathrm{T}}\hat{\lambda}\\ 0\end{bmatrix}\\ &= \hat{\lambda}^{\mathrm{T}}(\mathbf{Q}_{L_1L_1} + \mathbf{Q}_{L_1a_1}\mathbf{B}_1^{\mathrm{T}} + \mathbf{B}_1\mathbf{Q}_{a_1L_1} + \mathbf{B}_1\mathbf{Q}_{a_1a_1}\mathbf{B}_1^{\mathrm{T}})\hat{\lambda}\\ &= \hat{\lambda}^{\mathrm{T}}\mathbf{Q}_l\hat{\lambda}\end{aligned} \tag{28}$$

As a consequence, the variance factor of the unit weight is estimated as following:

$$\hat{\sigma}_0^2 = \frac{\tilde{e}^{\mathrm{T}}\mathbf{P}\tilde{e}}{r} = \frac{\hat{\lambda}^{\mathrm{T}}(L_1 - \varphi_1(\tilde{e}_1,\hat{\xi}) + \mathbf{B}_1\tilde{e}_1)}{r} \tag{29}$$

where the degree of freedom r is:

$$r = (m+p) - (t+p) = m - t \tag{30}$$

In Eq. (30), the total number of equations includes m equations for common points and p equations for new points. The total number of necessary unknowns includes t parameters and p target values to be predicted.

The covariance matrix of the estimated parameters can be obtained via linearly approximate variance propagation law to Eq. (22) as:

$$\mathbf{D}_{\hat{\xi}} = \hat{\sigma}_0^2 (\mathbf{A}_1^{\mathrm{T}} \mathbf{Q}_l^{-1} \mathbf{A}_1)^{-1} \tag{31}$$

Since GTLSP algorithm is derived based on the theory of nonlinear least squares, the solution along with its precision assessment is biased, though the bias may be so small in practice. This bias is related to the precision of the observations and the geometrical properties of the nonlinear manifold (see Teunissen, 1984, 1985, 1990). To work out the bias formulae, one can refer to the theory and methods proposed by Box (1971), which has also been applied in the partial EIV model (Xu et al., 2012) and constrained TLS problem (Fang, 2015).

4. Application of the GTLSP algorithm for 3D similarity transformation

In the application of this new algorithm for 3D similarity transformation, related matrices ($\mathbf{A}_1$, $\mathbf{B}_1$, $\mathbf{A}_2$, $\mathbf{B}_2$) should be specifically determined and updated during the iteration.

Assuming that there are k common points and l new points in total. It is certain that the corresponding dimensions mentioned in Section 3 are: $m = n = 3k$, $p = q = 3l$ and $t = 7$, respectively. For the ith common point,

$$\boldsymbol{\varphi}_{1i} = \mu \mathbf{M} \left(\begin{bmatrix} x_{1i} \\ y_{1i} \\ z_{1i} \end{bmatrix} - \begin{bmatrix} ex_{1i} \\ ey_{1i} \\ ez_{1i} \end{bmatrix} \right) + \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta z \end{bmatrix} \tag{32}$$

$$\mathbf{A}_{1i} = \left(\frac{\partial \varphi_{1i}}{\partial \xi^{\mathrm{T}}} \right)^0 = \left[\left(\frac{\partial \varphi_{1i}}{\partial \Delta \boldsymbol{X}} \right)^0 \quad \left(\frac{\partial \varphi_{1i}}{\partial \mu} \right)^0 \quad \left(\frac{\partial \varphi_{1i}}{\partial \boldsymbol{\theta}} \right)^0 \right] \tag{33}$$

In Eq. (33),

$$\left(\frac{\partial \varphi_{1i}}{\partial \Delta \boldsymbol{X}} \right)^0 = \left[\left(\frac{\partial \varphi_{1i}}{\partial \Delta x} \right)^0 \quad \left(\frac{\partial \varphi_{1i}}{\partial \Delta y} \right)^0 \quad \left(\frac{\partial \varphi_{1i}}{\partial \Delta z} \right)^0 \right] = \mathbf{I}_3 \tag{34a}$$

$$\left(\frac{\partial \varphi_{1i}}{\partial \mu} \right)^0 = \mathbf{M}^0 \cdot \boldsymbol{C}_i \tag{34b}$$

$$\left(\frac{\partial \varphi_{1i}}{\partial \boldsymbol{\theta}} \right)^0 = \left[\left(\frac{\partial \varphi_{1i}}{\partial \alpha} \right)^0 \quad \left(\frac{\partial \varphi_{1i}}{\partial \beta} \right)^0 \quad \left(\frac{\partial \varphi_{1i}}{\partial \gamma} \right)^0 \right] = \mu^0 \cdot \left[\left(\frac{\partial \mathbf{M}}{\partial \alpha} \right)^0 \boldsymbol{C}_i \quad \left(\frac{\partial \mathbf{M}}{\partial \beta} \right)^0 \boldsymbol{C}_i \quad \left(\frac{\partial \mathbf{M}}{\partial \gamma} \right)^0 \boldsymbol{C}_i \right] \tag{34c}$$

$$\mathbf{B}_{1i} = \left(\frac{\partial \varphi_{1i}}{\partial \boldsymbol{e}_{1i}^{\mathrm{T}}} \right)^0 = \left[\left(\frac{\partial \varphi_{1i}}{\partial ex_{1i}} \right)^0 \quad \left(\frac{\partial \varphi_{1i}}{\partial ey_{1i}} \right)^0 \quad \left(\frac{\partial \varphi_{1i}}{\partial ez_{1i}} \right)^0 \right] = -\mu^0 \cdot \mathbf{M}^0 \tag{35}$$

where $\mathbf{I}_3$ is a 3–order identity matrix. The subscripts "i" in above equations indicate the ith point. The superscripts "0" represent substituting approximate values ($\boldsymbol{e}_1^0, \xi^0$) into related expressions, and all of these values should be continuously updated during the iteration. In addition,

$$\boldsymbol{C}_i = \begin{bmatrix} x_{1i} \\ y_{1i} \\ z_{1i} \end{bmatrix} - \begin{bmatrix} ex_{1i}^0 \\ ey_{1i}^0 \\ ez_{1i}^0 \end{bmatrix} \tag{36}$$

$$\frac{\partial \mathbf{M}}{\partial \alpha} = \mathbf{M}_3 \cdot \mathbf{M}_2 \cdot \frac{\partial \mathbf{M}_1}{\partial \alpha}, \quad \frac{\partial \mathbf{M}}{\partial \beta} = \mathbf{M}_3 \cdot \frac{\partial \mathbf{M}_2}{\partial \beta} \cdot \mathbf{M}_1,$$
$$\frac{\partial \mathbf{M}}{\partial \gamma} = \frac{\partial \mathbf{M}_3}{\partial \gamma} \cdot \mathbf{M}_2 \cdot \mathbf{M}_1 \tag{37}$$

$$\frac{\partial \mathbf{M}_1}{\partial \alpha} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -\sin\alpha & \cos\alpha \\ 0 & -\cos\alpha & -\sin\alpha \end{bmatrix},$$
$$\frac{\partial \mathbf{M}_2}{\partial \beta} = \begin{bmatrix} -\sin\beta & 0 & -\cos\beta \\ 0 & 0 & 0 \\ \cos\beta & 0 & -\sin\beta \end{bmatrix}, \tag{38}$$
$$\frac{\partial \mathbf{M}_3}{\partial \gamma} = \begin{bmatrix} -\sin\gamma & \cos\gamma & 0 \\ -\cos\gamma & -\sin\gamma & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Combining related expressions of each point together, we can obtain:

$$\mathbf{A}_1 = \left(\frac{\partial \varphi_1}{\partial \xi^{\mathrm{T}}} \right)^0 = \begin{bmatrix} \mathbf{A}_{11} \\ \mathbf{A}_{12} \\ \vdots \\ \mathbf{A}_{1k} \end{bmatrix},$$
$$\mathbf{B}_1 = \left(\frac{\partial \varphi_1}{\partial \boldsymbol{e}_1^{\mathrm{T}}} \right)^0 = \begin{bmatrix} \mathbf{B}_{11} & & & \\ & \mathbf{B}_{12} & & \\ & & \ddots & \\ & & & \mathbf{B}_{1k} \end{bmatrix} \tag{39}$$

The initial values of $\boldsymbol{e}_1^0$ and ξ^0 are given as: $\boldsymbol{e}_1^0 = 0$, $\xi^0 = [0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0]^{\mathrm{T}}$, respectively. In case the approximate value of the scale ratio becomes non-positive (i.e., $\mu^0 < 0$) in the iterative procedure, it should be reset to 1 so as to avoid convergence to the incorrect solution.

The necessary matrices for new points ($\mathbf{A}_2$ and $\mathbf{B}_2$) can be derived and updated in a similar way as described above.

In practice, the coordinates in the original system and target system are usually statistically uncorrelated. In other words, $\mathbf{Q}_{L_1 a_1} = 0$, $\mathbf{Q}_{a_2 L_1} = 0$, thus the related formulae become:

$$\mathbf{Q}_l = \mathbf{Q}_{L_1 L_1} + \mathbf{B}_1 \mathbf{Q}_{a_1 a_1} \mathbf{B}_1^{\mathrm{T}} \tag{40}$$

$$\tilde{\boldsymbol{e}}_{L_1} = \mathbf{Q}_{L_1 L_1} \cdot \mathbf{Q}_l^{-1} (\boldsymbol{L}_1 - \boldsymbol{\varphi}_1(\boldsymbol{e}_1^0, \xi^0) - \mathbf{A}_1 \delta\hat{\xi} + \mathbf{B}_1 \boldsymbol{e}_1^0) \tag{41a}$$

$$\tilde{\boldsymbol{e}}_1 = \mathbf{Q}_{a_1 a_1} \mathbf{B}_1^{\mathrm{T}} \cdot \mathbf{Q}_l^{-1} (\boldsymbol{L}_1 - \boldsymbol{\varphi}_1(\boldsymbol{e}_1^0, \xi^0) - \mathbf{A}_1 \delta\hat{\xi} + \mathbf{B}_1 \boldsymbol{e}_1^0) \tag{41b}$$

$$\tilde{\boldsymbol{e}}_2 = \mathbf{Q}_{a_2 a_1} \mathbf{B}_1^{\mathrm{T}} \cdot \mathbf{Q}_l^{-1} (\boldsymbol{L}_1 - \boldsymbol{\varphi}_1(\boldsymbol{e}_1^0, \xi^0) - \mathbf{A}_1 \delta\hat{\xi} + \mathbf{B}_1 \boldsymbol{e}_1^0) \tag{41c}$$

If the coordinates of the common and new points in the original system are independent ($\mathbf{Q}_{a_2a_1} = 0$), the error vector $\tilde{e}_2 = 0$, which means that the coordinates of the new points in the original system will not be corrected and the results of GTLSP algorithm will be equivalent to those of existing WTLS algorithms for the universal 3D similarity transformation (see e.g., Felus and Burtch, 2009; Fang, 2014b; Fang, 2015).

5. Experiment analysis

Assuming that there are 18 points distributing in a space domain. The true coordinates of each point in the original coordinate system (system I) and target coordinate system (system II) are known, and the corresponding transformation parameters from systems I to II are as below: $\Delta x = 1000$, $\Delta y = 1000$, $\Delta z = 1000$, $\mu = 2.0$, $\alpha = 1.0$ rad, $\beta = 1.5$ rad, $\gamma = 2.5$ rad.

Eight of these points are designated as common points, and the remaining ten points are specified as new points (check points).

We assume that the coordinates of the common and check points in system I are statistically correlated ($\mathbf{Q}_{a_2a_1} \neq 0$). Random errors with the given covariance matrices are generated and added to the coordinates of all points in system I and the common points in system II. This simulation is repeated 10,000 times.

Assuming that the square root of the apriori variance component σ_0 is 0.01. The following two computational schemes are employed to implement the transformation of check points from system I to system II.

(1) WTLS algorithm with universal constraints for the 3D similarity transformation (see Fang, 2015);

(2) Generalized Total least squares prediction (GTLSP) algorithm proposed in this paper.

The coordinates of the check points in system II: $\begin{bmatrix} \hat{x}_{i,II} & \hat{y}_{i,II} & \hat{z}_{i,II} \end{bmatrix}^T$ can be obtained by these two schemes. By utilizing the known true coordinates $\begin{bmatrix} x_{i,II} & y_{i,II} & z_{i,II} \end{bmatrix}^T$, we can calculate the root mean square errors (RMSEs) for the x, y and z components of the transformed coordinates as follows:

$$\sigma_x = \sqrt{\sum_{i=1}^{10} (\hat{x}_{i,II} - x_{i,II})^2 \Big/ 10} \tag{42a}$$

$$\sigma_y = \sqrt{\sum_{i=1}^{10} (\hat{y}_{i,II} - y_{i,II})^2 \Big/ 10} \tag{42b}$$

$$\sigma_z = \sqrt{\sum_{i=1}^{10} (\hat{z}_{i,II} - z_{i,II})^2 \Big/ 10} \tag{42c}$$

Therefore, the positional RMSE is obtained as:

$$\sigma_p = \sqrt{\sigma_x^2 + \sigma_y^2 + \sigma_z^2} \tag{42d}$$

The experiment is carried out in four cases. In Case 1, the correlation coefficients between the coordinate components of common and check points are all set as 0.35. In Cases 2–4, we increase them to 0.45, 0.55, and 0.65 respectively while maintaining other conditions unchanged (The precision for each coordinate component is the same as that in Case 1).

The statistics on the calculation results of these four cases, including the mean and maximum values of the σ_x, σ_y, σ_z, and σ_p are derived and tabulated in Table 1. In addition, Figs. 1–4 present the experiment sequences for Cases 1–4, respectively.

According to the results in Table 1 and Figs. 1–4, we find the followings:

(i) The corresponding mean values of the σ_x, σ_y, σ_z, and σ_p from Scheme (2) are 95.2%, 85.4%, 90.6%, and 90.1% of those from Scheme (1) in Case 1, 92.5%, 78.9%, 86.6%, and 85.5% of those from Scheme (1) in Case 2, 88.5%, 71.3%, 80.4%, and 79.2% of those from Scheme (1) in Case 3, and 83.5%, 63.2%, 73.3%, and 72.1% of those from Scheme (1) in Case 4, respectively.

(ii) Moreover, there exist some big RMSEs from Scheme (1) during the simulation, and the maximal RMSEs of all directions and positions from Scheme (2) are obviously smaller than those from Scheme (1) in all cases (Cases 1–4).

(iii) Additionally, we also count the number of times when each RMSE obtained by Scheme (2) is smaller than that obtained by Scheme (1). The results for x

Table 1
Statistical results of coordinate transformation for Cases 1–4.

Case	Scheme	Ave (σ_x)	Ave (σ_y)	Ave (σ_z)	Ave (σ_p)	Max (σ_x)	Max (σ_y)	Max (σ_z)	Max (σ_p)
1	(1)	0.0357	0.0371	0.0347	0.0634	0.0843	0.1093	0.0882	0.1439
	(2)	0.0340	0.0316	0.0314	0.0571	0.0744	0.0705	0.0653	0.0960
2	(1)	0.0340	0.0371	0.0336	0.0618	0.0914	0.1113	0.0948	0.1431
	(2)	0.0314	0.0293	0.0291	0.0529	0.0656	0.0649	0.0656	0.0934
3	(1)	0.0324	0.0377	0.0330	0.0610	0.0848	0.1312	0.1174	0.1912
	(2)	0.0286	0.0269	0.0265	0.0483	0.0596	0.0704	0.0570	0.0833
4	(1)	0.0305	0.0377	0.0323	0.0596	0.0930	0.1576	0.1171	0.2071
	(2)	0.0254	0.0238	0.0236	0.0430	0.0583	0.0555	0.0523	0.0764

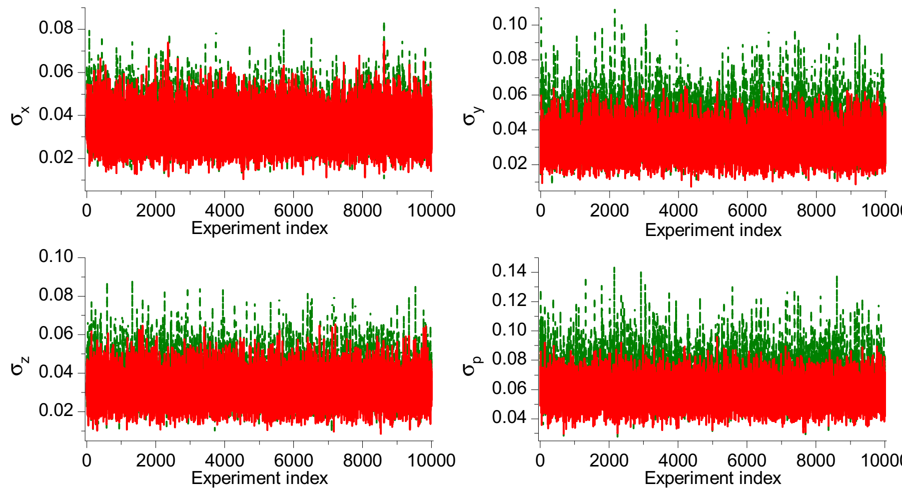

Fig. 1. Experiment sequences for Case 1. The green dash line represents the results obtained by Scheme (1); the red solid line represents the results obtained by Scheme (2). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

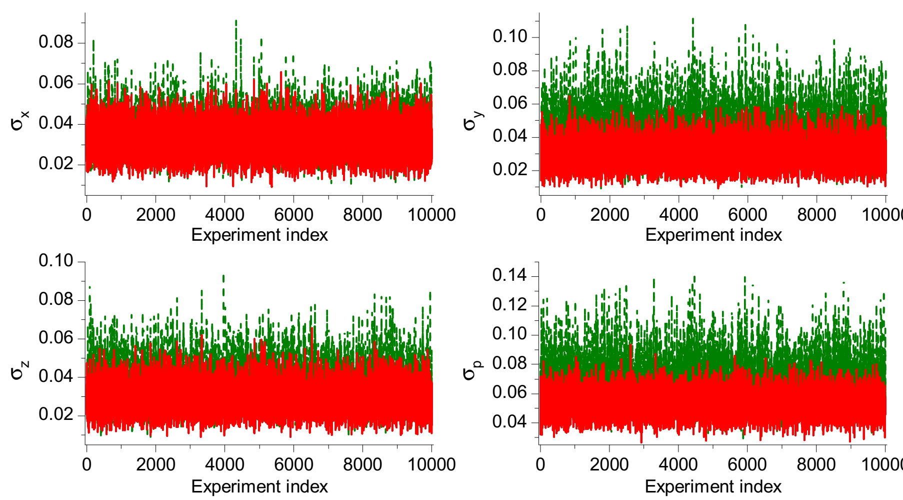

Fig. 2. Experiment sequences for Case 2. The green dash line represents the results obtained by Scheme (1); the red solid line represents the results obtained by Scheme (2). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

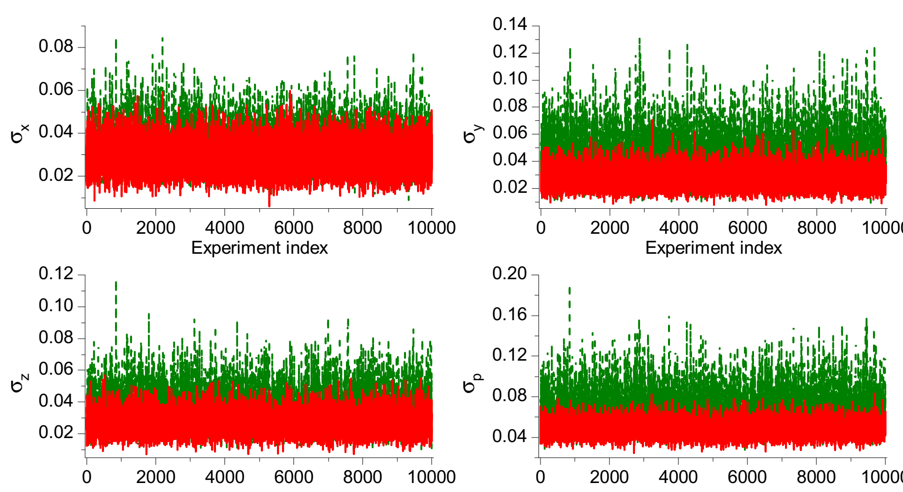

Fig. 3. Experiment sequences for Case 3. The green dash line represents the results obtained by Scheme (1); the red solid line represents the results obtained by Scheme (2). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

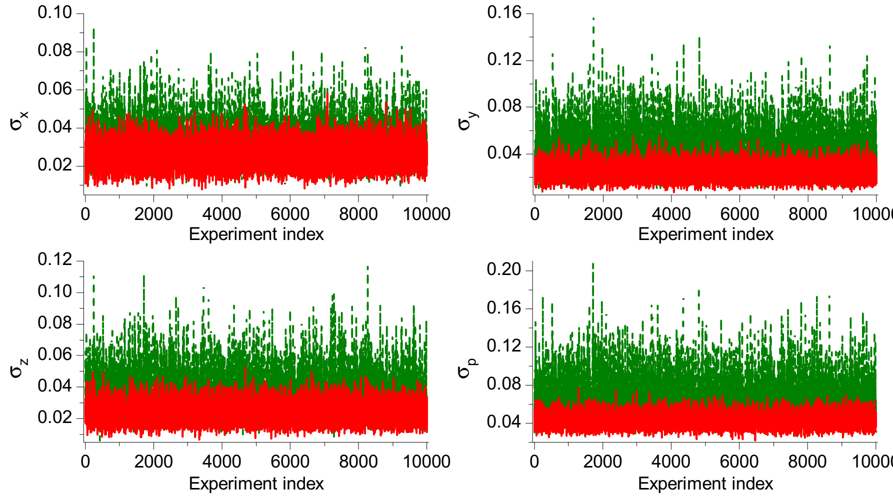

Fig. 4. Experiment sequences for Case 4. The green dash line represents the results obtained by Scheme (1); the red solid line represents the results obtained by Scheme (2). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

direction, *y* direction, *z* direction, and position are 6160, 6912, 6584, and 7327 times in Case 1, 6522, 7269, 6878, and 7746 times in Case 2, 6736, 7531, 7213, and 8044 times in Case 3, and 7099, 7911, 7539, and 8427 times in Case 4, respectively. There is no doubt that Scheme (2) has more probabilities to derive better transformation results.

In general, Scheme (2) shows improvement in statistical accuracy of the transformed coordinates than Scheme (1) to some extent. This improvement is more remarkable especially when there is stronger stochastic correlation between the coordinates of the common and check points in coordinate system *I*.

In this example, WTLS algorithm with universal constraints [Scheme (1)] ignores the statistical correlation between the common and check points in coordinate system *I*. However, GTLSP algorithm [Scheme (2)] takes this correlation into account, and the coordinates of the new points in system *I* will be corrected when implementing the coordinate transformation. Thus it is more reasonable in theory. Additionally, from Eq. (41c) we know that once the correlation becomes stronger, these coordinates of check points will be corrected more adequately. The superiority of Scheme (2) to Scheme (1) is exactly attributed to these reasons.

6. Conclusions

In this study, we proposed a GTLSP algorithm for the universal 3D similarity transformation which combines the parameter calculation and new point transformation rigorously. The theoretical and experimental conclusions are summarized as followings:

(1) GTLSP algorithm can take the random errors of new points and the statistical correlation between common and new points in the original coordinate system into account, therefore it is more rigorous than other TLS algorithms for the 3D similarity transformation in theory.
(2) The experiment shows that after the original coordinates of the check points be corrected through GTLSP algorithm, the statistical accuracy of the transformed coordinates can be improved to some extent compared with that obtained by WTLS algorithm with universal constraints. The extent of improvement depends on the stochastic correlation between the common and the check points in the original coordinate system. The stronger the correlation is, the greater improvement the GTLSP algorithm will make.
(3) GTLSP algorithm is derived in the form of abstract functions, thus it can be applied to solve many other problems as well, such as the 2D datum transformation, the GNSS height fitting, the LiDAR point registration and the image processing.
(4) The algorithm proposed in this paper is based on the assumption that the errors of coordinates observed in two systems have the same variance component. However they may not be exactly same in practice. In further work, the variance component estimation (VCE) method for GTLSP algorithm will be investigated to solve this problem.

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