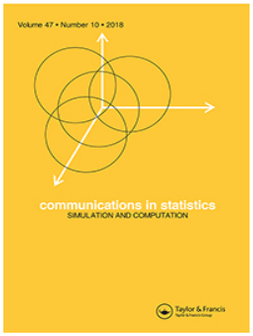

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Jackknife resample method for precision estimation of weighted total least squares

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ABSTRACT

Few studies have been conducted on the precision estimation of weighted total least squares (WTLS) by using the approximate function probability distribution method. And the existing Monte Carlo method needs to simulate a lot, the amount of calculation is large and the results obtained are uncertain. In order to further improve the total least squares precision estimation theory, this paper introduces the Jackknife method into Geomatics data processing. Combining the Jackknife method and WTLS method, the delete-1 Jackknife method and delete-d Jackknife method are proposed. The biases and standard deviations or covariance of parameter estimations are calculated by these proposed methods. And the specific steps of the precision estimation of these two methods are given. Applying these methods to the linear regression model and the coordinate transformation model, and comparing with the approximate function method and the Monte Carlo method, we can see that the Jackknife methods for precision estimation can obtain more stable and reasonable precision results and are very adaptive. In order to get more reasonable precision results, the Jackknife method does spend much more time over total least squares when the amount of the observed data is large. But compared with Monte Carlo method, it can reduce the amount of calculation and improve the computational efficiency. The method in this paper could provide an idea for further study on the precision estimation for total least squares.

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1. Introduction

Total least squares (TLS) can deal with errors of both the observed vector and the coefficient matrix which can get an approximate TLS solution by singular value decomposition (Golub and van Loan 1980). It has attracted a widely spread attention since Golub and van Loan (1980) coined the terminology of total least squares about 30 years ago. While, Pearson (1901) gave a statistically rigorous solution to the errors-in-variables (EIV) model firstly. Deming (1931, 1934, 1964) and Gerhold (1969) solved the estimation problem of the EIV model by directly using the weighted LS method. The estimates derived by them are indeed TLS solutions in the sense that the randomness of both the

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observed vector and the coefficient matrix has been fully taken into account. It was further systematically developed and popularized by van Huffel and Vandewalle (1991). Now, weighted total least squares (WTLS) is more universal (Schaffrin 2006; Fang 2011; Shen, Li, and Chen 2011; Amiri-Simkooei and Jazaeri 2012; Snow 2012; Schaffrin 2015). In case when not all the elements of coefficient matrix are random, and its random elements are functionally dependent, Xu, Liu, and Shi (2012) proposed Partial EIV to reduce the amount of calculation. Compared with the rich parameter estimation algorithms and its wide applications in the field of Geomatics data processing (Markovsky and van Huffel 2007; Schaffrin and Wieser 2008; Mahboub 2012; Amiri-Simkooei and Jazaeri 2012; Fang 2013; van Huffel and Vandewalle 1991; Wang and Xu 2016), the research on the precision estimation of TLS is less. The present precision estimation methods of TLS can be divided into two types: approximation function expression method and approximation function probability distribution method. For the approximation function expression method, the first order approximate variance–covariance matrix of the TLS estimate was given by Gerhold (1969) a long time ago. Schaffrin and Felus (2005) only considered the randomness of the observed vector in obtaining the first-order approximate covariance matrix of the parameter estimation. Amiri-Simkooei, Zangeneh-Nejad, and Asgari (2016) calculated the covariance matrix of TLS parameter estimates iteratively with first-order partial derivatives and analyzed the differences among those three strategies. Fang (2015) derived the TLS parameter estimation bias and the first-order approximate covariance matrix formula with equality and inequality constraints. Xu, Liu, and Shi (2012) derived the bias formulae for parameter estimates and residuals, and used the bias-corrected residuals to estimate the variance of unit weight of partial EIV model. Meanwhile, the first finite sample accuracy of the first order approximation and a calculation method of nonlinear confidence region were also given by Xu, Liu, and Shi (2012). Xu et al. (2014) studied the effect of EIV model on the least square estimation and deduced the calculation formula of parameter estimation, the deviation of corrections, the covariance matrix and the bias-corrected unit weight variance estimate. Xu (2016) mainly investigated the effect of errors-in-variables on variance component estimation and he derived the bias formula and constructed a bias-corrected weighted LS estimate of parameters by directly removing the bias from the conventional weighted LS estimate. Zhao (2017) supplemented the bias calculation formula of the TLS parameter estimation and the correction, and deduced the second-order approximation of the parameter estimation covariance matrix calculation formula. Based on the post-estimation statistics of the TLS, Malengo and Pennecchi (2013) used Monte Carlo (MC) simulations to calculate the covariance matrix of the parameter estimates in the approximation function probability distribution method. Shen, Li, and Chen (2011) used the MC method to calculate the bias of the unit weighted variance estimate and used the bias-corrected unit weighted variance estimate to further calculate the mean square error matrix of the parameter estimation. Wang and Zhao (2017, 2018) studied the use of UT transformation for TLS precision estimation and nonlinear error propagation theory. And the calculation process of TLS precision estimation using the adaptive Monte Carlo method was given by Zhao (2017).

Jackknife method was first proposed by Quenouille (1949). Since then, Tukey (1958) has continued to improve it and the resampling method has become one of the important methods in statistics. And the resampling statistical analysis method is based only on

the sample of the original data which will not generate additional model errors. Meanwhile, it does not require assumptions and complex formula calculations related to the distribution of estimators (Efron 1980). Sahinler and Topuz (2007) and Abdi and Williams (2010) focused only on the least squares (LS) resampling method for linear regression and they offered a general process for solving regression coefficients, standard deviations and confidence intervals. The LS resampling method for nonlinear regression was studied by Terry, David, and Kinley (1980) and Jie and Wang (1994). And Jie and Wang (1994) pointed out that when calculating a reasonable biased estimate, the use of Jackknife method can effectively reduce the bias thus get more accurate parameter estimates. Singh (1986) studied the use of Jackknife for multicollinearity problems based on LS multivariate regression and proposed an improved ridge regression estimation method. Efron (1980) investigated the general properties of Jackknife variance estimation. Miller (1974) proposed a method for mixing Jackknife and Bootstrap estimates. Unlike the MC simulation, the Jackknife method does not need to generate new data. It reduces the specific number of observations sequentially to generate a series of resampled observation samples with smaller capacity than the original observation samples for calculation. When the amount of the observed data is large, the existing Monte Carlo method needs to simulate a lot, the amount of calculation is large and the results obtained are uncertain. However, the Jackknife method only generates C_n^d new samples for C_n^d calculations and it can reduce the amount of calculation compared to Monte Carlo method. Besides, using the second-order approximate function method results in the computational difficulty due to the wideness of the Hessian matrix dimension, while the Jackknife method does not need to calculate the derivative of the nonlinear function and it can be widely applied and get more reasonable precision estimation information. Therefore, the improvement of the approximate function probability distribution method and the proposal of a new mathematical probability method for the precision estimation of TLS need to be further studied.

To summarize, this paper considers the nonlinear property of WTLS with coefficient matrix error, introduces the Jackknife method into the precision estimation for TLS and further expands the theory of approximation function probability distribution method of TLS precision estimation. Comparing with the Monte Carlo method, we use the Jackknife method to reduce the amount of calculation while ensuring the precision of the results. The detailed calculation steps are also given, and the feasibility of the precision estimation method is verified through examples of straight line fitting model and coordinate transformation model.

The paper is organized as follows: in Sec. 2, the calculation formula of Jackknife is introduced. In Sec. 3, the EIV model is introduced and the iterative algorithm of TLS adjustment is summarized. After that, the calculation procedures for precision estimation of WTLS by the Jackknife method are given. In Sec. 4, the practicability and effectiveness of Jackknife are demonstrated with straight line fitting model and plane coordinate transformation model. And Sec. 5 is the conclusion.

2. Jackknife method

2.1. Delete-1 Jackknife

We suppose sample N is an independent and identically distributed data. $w = (w_1, w_2, \ldots, w_n)$ is size n and $\hat{x}$ is an estimator. Let $\hat{x}$ be the parameter of the distribution

function $F(w,x)$, where $\hat{x}$ is an estimate of x using an estimation method. The Jackknife method generally mentioned is the classic delete-1 Jackknife method, in which a set of data is deleted from the sample each time and the remaining n-1 sized samples are called delete-1 Jackknife samples, which are $(w_1, w_2, ..., w_{i-1}, w_{i+1}, ..., w_n)$. Thus, we will get a new sample through re-sampling each time and the total number of Jackknife samples is n. Then, n sized estimators are obtained by using the estimation method from these series of delete-1 Jackknife samples, and finally all the estimated values obtained are averaged to obtain the estimated value of Jackknife (Miller 1974). The average value of the estimated values obtained by using n sized delete-1 Jackknife samples is

$$\hat{x}_{(\bullet)} = \frac{1}{n}\sum_{i=1}^{n}\hat{x}_{(i)} \tag{1}$$

Where $\hat{x}_{(i)}$ is the estimated values obtained from each delete-1 Jackknife sample and $\hat{x}_{(\bullet)}$ is the mean value.

Calculating the bias of the parameter estimate with the mean value and the original estimated value, we get (Miller 1974)

$$\hat{B}_{(x)} = (n-1)\left(\hat{x}_{(\bullet)} - \hat{x}\right) \tag{2}$$

Where $\hat{x}$ is the estimated value calculated by using the original data.

According to formula (2), the estimated value after bias correction is expressed as

$$\hat{x}_J = \hat{x} - (n-1)\left(\hat{x}_{(\bullet)} - \hat{x}\right) = n\hat{x} - (n-1)\hat{x}_{(\bullet)} \tag{3}$$

The formula for estimating the variance obtained by delete-1 Jackknife is

$$D = \frac{n-1}{n}\sum_{i=1}^{n}\left(\hat{x}_{(i)} - \hat{x}_{(\bullet)}\right)^2 \tag{4}$$

2.2. Delete-d Jackknife

Compared to the delete-1 Jackknife method, the delete-d Jackknife method omits d-group data from the original sample N each time, and the remaining n-d sized samples constitute the new sample. A total of C_n^d new samples will be generated. Using these series of new delete-d Jackknife samples to calculate the estimations, the estimated values obtained from each of the delete-d Jackknife samples are not equal since the samples are different after each resampling. Then, calculate delete-d Jackknife estimation which is the mean of s sized unequal estimations as

$$\hat{x}_{(\bullet)} = \frac{1}{\binom{n}{d}}\sum_{i=1}^{s}\hat{x}_{(i)}(1 < d < n) \tag{5}$$

Where $\hat{x}_{(i)}$ is the estimated value obtained from each delete-d Jackknife sample and s is equal to C_n^d.

Calculate the bias of the parameter estimates using the mean and the estimated value as (Shao and Wu 1989)

$$\hat{B}_{(x)} = \left(\frac{n-d}{d}\right)\left(\hat{x}_{(\bullet)} - \hat{x}\right) \tag{6}$$

According to formula (6), the estimated value after bias correction is expressed as

$$\hat{x}_J = \hat{x} - \left(\frac{n-d}{d}\right)\left(\hat{x}_{(\bullet)} - \hat{x}\right) = \left(\frac{n+d-1}{d}\right)\hat{x} - \left(\frac{n-1}{d}\right)\hat{x}_{(\bullet)} \tag{7}$$

The formula for estimating the variance obtained by delete-d Jackknife is

$$S = \frac{n-d}{d\binom{n}{d}}\sum_{i=1}^{n}\left(\hat{x}_{(i)} - \hat{x}_{(\bullet)}\right)^2 \tag{8}$$

If d sized observations are omitted each time, the number of delete-d Jackknife samples will become very large quickly as n increases and the number of Jackknife samples will tend to infinity when n tends to infinity. Then the consistency and gradual unbiasedness of the variance estimate of the Jackknife method can be established. The value of d here has an important influence on the number of Jackknife samples. When n is small, the number of the overall samples will also be very small; when n increases, the number of the overall samples will grow quickly.

3. Jackknife and its application in precision estimation of WTLS

3.1. WTLS method

In order to reduce the computational complexity, the function model of TLS method generally used is the Partial EIV model. It can be defined as: (Xu, Liu, and Shi 2012)

$$\boldsymbol{y} = \boldsymbol{A}\boldsymbol{\xi} + \boldsymbol{\varepsilon} = (\boldsymbol{\xi} \otimes \boldsymbol{I}_n)(\boldsymbol{h} + \boldsymbol{B}\bar{\boldsymbol{a}}) + \boldsymbol{e}_y \tag{9}$$

$$\boldsymbol{a} = \bar{\boldsymbol{a}} + \boldsymbol{e}_a \tag{10}$$

$$\begin{bmatrix}\boldsymbol{e}_y \\ \boldsymbol{e}_a\end{bmatrix} \sim \left(\begin{bmatrix}\boldsymbol{0} \\ \boldsymbol{0}\end{bmatrix}, \sigma_0^2\begin{bmatrix}\boldsymbol{Q}_y & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Q}_a\end{bmatrix}\right) \tag{11}$$

where $\boldsymbol{y}$ is the vector of measurements; $\boldsymbol{e}_y$ is the error vector of $\boldsymbol{y}$; $\boldsymbol{A}$ is a coefficient matrix composed of observations; $\boldsymbol{\xi}$ is unknown parameters; $\boldsymbol{h}$ is a deterministic constant vector; $\boldsymbol{B}$ is a given, nonrandom matrix, depending on the number of random elements of the coefficient matrix $\boldsymbol{A}$; $\boldsymbol{a}$ is all the independent random measurements of $\boldsymbol{A}$ and the true values of $\boldsymbol{a}$ are denoted by $\bar{\boldsymbol{a}}$; $\boldsymbol{e}_a$ is the error vector of $\boldsymbol{a}$; σ_0^2 is a priori unit weight variance; $\boldsymbol{Q}_y$ is a cofactor matrix of the elements in $\boldsymbol{y}$; and $\boldsymbol{Q}_a$ is a cofactor matrix of the elements in $\boldsymbol{a}$.

We get the cost function by applying the weighted LS principle:

$$\min : \mathrm{S}(\bar{\boldsymbol{a}}, \boldsymbol{\xi}) = (\bar{\boldsymbol{a}} - \boldsymbol{a})^{\mathrm{T}}\boldsymbol{Q}_a^{-1}(\bar{\boldsymbol{a}} - \boldsymbol{a}) + (\bar{\boldsymbol{A}}\boldsymbol{\xi} - \boldsymbol{y})^{\mathrm{T}}\boldsymbol{Q}_y^{-1}(\bar{\boldsymbol{A}}\boldsymbol{\xi} - \boldsymbol{y}) \tag{12}$$

According to Shi et al. (2015), the formulae of WTLS algorithm is

$$\hat{\bar{\boldsymbol{a}}} = \boldsymbol{a} + \boldsymbol{Q}_a^{-1}\boldsymbol{S}_{\hat{\xi}}^{\mathrm{T}}\boldsymbol{E}^{-1}(\boldsymbol{y} - \boldsymbol{A}\hat{\boldsymbol{\xi}}) \tag{13}$$

$$\hat{\boldsymbol{\xi}} = \left(\hat{\bar{\boldsymbol{A}}}^{\mathrm{T}}\boldsymbol{Q}_y^{-1}\hat{\bar{\boldsymbol{A}}}\right)^{-1}\hat{\bar{\boldsymbol{A}}}\boldsymbol{Q}_y^{-1}\boldsymbol{y} \tag{14}$$

where $\bar{\boldsymbol{A}}$ is the matrix reconstructed by the value of coefficient matrix from $\bar{\boldsymbol{a}}$; $\boldsymbol{S}_{\hat{\xi}} = (\hat{\boldsymbol{\xi}}^{\mathrm{T}} \otimes \boldsymbol{I}_n)\boldsymbol{B}$ and $\boldsymbol{E} = \boldsymbol{Q}_y + \boldsymbol{S}_{\hat{\xi}}\boldsymbol{Q}_a\boldsymbol{S}_{\hat{\xi}}^{\mathrm{T}}$.

The basic steps of WTLS algorithm above can be summarized as Algorithm 1.

Algorithm 1. WTLS algorithm steps:

1. Give known or observed data: $\boldsymbol{y},\boldsymbol{a},\boldsymbol{Q}_{\boldsymbol{y}},\boldsymbol{Q}_{\boldsymbol{a}}$;
2. Definite matrix of $\boldsymbol{h}$ and $\boldsymbol{B}$ according to the coefficient matrix in function model;
3. Initialize $\hat{\tilde{\boldsymbol{A}}}_0 = \boldsymbol{A}$, using formula of (14) to calculate unknown parameters $\hat{\tilde{\boldsymbol{\xi}}}$;
4. Calculate $\hat{\tilde{\boldsymbol{a}}}$ by substituting $\hat{\tilde{\boldsymbol{\xi}}}$ into formula (13);
5. Update $\hat{\tilde{\boldsymbol{\xi}}}$ and $\hat{\tilde{\boldsymbol{a}}}$, and the iteration will not end until $\|\hat{\tilde{\boldsymbol{\xi}}}^{\boldsymbol{k}+1} - \hat{\tilde{\boldsymbol{\xi}}}^{\boldsymbol{k}}\| < \varepsilon$, otherwise, repeat step (3) and step (4).

3.2. Jackknife for precision estimation of WTLS

In order to obtain the precision estimation of WTLS parameter estimation, the approximate function expression requires complex formula derivation and the results acquired are not very accurate. The calculation of the second-order approximate function expression involves the Hessian matrix. Thus, the matrix calculation with too large dimension will be resulted when the amount of the observation data is large, making it difficult to calculate. The use of the mathematical approximation function probability distribution method for WTLS precision estimation does not require the calculation of the derivative of the nonlinear function and is more applicable. And more reasonable precision estimation information than the approximate function expression method can be obtained. Besides, the Monte Carlo method requires more simulations and more calculations. To further extend the approximate probability distribution of precision estimation method, this paper introduces the Jackknife method to the precision estimation of TLS, and evaluates the precision information of the TLS parameter estimation from the perspective of probabilistic resample so as to achieve continuous improvement. With rapid development of the computer technology, the greatly improved computing efficiency has also made the Jackknife method workable (Diaconis and Efron 1983).

Using the Jackknife method for the precision estimation of WTLS, we firstly estimate the parameters of the original observation data to obtain a parameter estimate. Then we resample the observation data and perform the WTLS iteration calculation directly. Use the new parameter estimates to calculate the mean of Jackknife, and then combine it with the Jackknife method formula to calculate the bias and the approximate covariance matrix of the parameter estimates. Then the approximate covariance matrix and standard deviation of the parameter estimates for the delete-1 Jackknife method can be expressed as

$$D_{\hat{\tilde{\xi}}} = \frac{n-1}{n}\sum_{i=1}^{n}\left(\hat{\tilde{\xi}}_{(i)} - \hat{\tilde{\xi}}_{(\bullet)}\right)\left(\hat{\tilde{\xi}}_{(i)} - \hat{\tilde{\xi}}_{(\bullet)}\right)' \tag{15}$$

$$\hat{\sigma}_{\hat{\tilde{\xi}}_i} = \sqrt{D_{\hat{\tilde{\xi}}_{ii}}}\,(i = 1, 2, \ldots, m) \tag{16}$$

where $\hat{\xi}_{(i)}$ is the value of the parameter obtained from each delete-1 Jackknife sample; $\hat{\xi}_{(\bullet)}$is the mean of delete-1 Jackknife; m is the number of parameters.

The approximate covariance matrix and standard deviation of the parameter estimates for the delete-d Jackknife method are expressed as

$$S_{\hat{\xi}} = \frac{n-d}{d\binom{n}{d}} \sum_{i=1}^{s} \left(\hat{\xi}_{(i)} - \hat{\xi}_{(\bullet)}\right)\left(\hat{\xi}_{(i)} - \hat{\xi}_{(\bullet)}\right)' \tag{17}$$

$$\hat{\sigma}_{\hat{\xi}_i} = \sqrt{S_{\hat{\xi}_{ii}}} (i = 1, 2, \ldots, m) \tag{18}$$

Combining the WTLS algorithm with the Jackknife method theory, this paper summarizes the main calculation steps of the delete-1 Jackknife method for precision estimation of WTLS as algorithm 2.

Algorithm 2. Precision estimation procedures of WTLS based on delete-1 Jackknife:

1. Draw a number of observation data samples N of size n,$(w_1, w_2, \ldots, w_n)$.
2. Use algorithm 1 to calculate parameter estimates $\hat{\xi}$ for sample N.
3. Omit the i-th observation data and its corresponding weights in sample N. The remaining n-1 observations and weights form a delete-1 Jackknife sample, and the Jackknife samples are taken as the new observation samples data.
4. Use algorithm 1 to recalculate the parameter estimates $\hat{\xi}_{(1)}$ by the new delete-1 Jackknife sample. $\hat{\xi}_{(1)}$ is the parameter value obtained by algorithm 1 after deleting the observation data of the first group.
5. Repeat (3) and (4) to obtain n sized parameter estimates $\hat{\xi}_{(i)}$ $i = 1, 2, \ldots, n$.
6. Calculate delete-1 Jackknife parameter estimation, which is the mean of the parameter estimates for the n-sized delete-1 Jackknife samples. We can get

$$\hat{\xi}_{(\bullet)} = \frac{1}{n}\sum_{i=1}^{n} \hat{\xi}_{(i)} \tag{19}$$

7. Calculate the bias of the WTLS parameter estimation:

$$\hat{\mathbf{B}}_{(\hat{\xi})} = (n-1)\left(\hat{\xi}_{(\bullet)} - \hat{\xi}\right) \tag{20}$$

8. The formula for calculating the parameter after correcting the bias is:

$$\hat{\xi}_J = n\hat{\xi} - (n-1)\hat{\xi}_{(\bullet)} \tag{21}$$

9. Calculate the approximate covariance matrix $D_{\hat{\xi}}$ and the standard deviation $\hat{\sigma}_{\hat{\xi}_i}$ of the parameter estimates.

The delete-d Jackknife method can get a larger number of Jackknife samples through resampling. And the number of Jackknife samples will increase rapidly as the amount of the original observation data and d increases constantly. At this point, a set of original observation data can be sampled into multiple sets of Jackknife samples to obtain more accurate precision information. This paper summarizes the main calculation steps of the WTLS precision estimation of the delete-d Jackknife method as Algorithm 3.

Algorithm 3. Precision estimation procedures of WTLS based on delete-d Jackknife:

1. Get a data sample N of size n. Separate s groups of independent subsamples of size d from the sample.
2. Use algorithm 1 to calculate the parameter estimates $\hat{\boldsymbol{\xi}}$ for sample N.
3. Omit each d-sized observation set and the corresponding weights and the n-d sized remaining observation set is called delete-d Jackknife sample. The total number of choices is C_n^d.
4. The delete-d Jackknife sample is recalculated using algorithm 1 to obtain the parameter estimate $\hat{\boldsymbol{\xi}}_{(i)}$, $i = 1, 2, \ldots, s$, $s = \binom{n}{d}$.
5. Repeat (3) and (4) to get C_n^d sized parameter estimates.
6. Calculate Jackknife parameter estimation, which is the mean of the parameter estimates for n sized delete-d Jackknife samples. We can get

$$\hat{\boldsymbol{\xi}}_{(\bullet)} = \frac{1}{\binom{n}{d}} \sum_{i=1}^{s} \hat{\boldsymbol{\xi}}_{(i)} \tag{22}$$

7. Calculate the bias of the WTLS parameter estimation:

$$\hat{B}_{(\hat{\xi})} = \left(\frac{n-d}{d}\right)\left(\hat{\boldsymbol{\xi}}_{(\bullet)} - \hat{\boldsymbol{\xi}}\right) \tag{23}$$

8. The formula for calculating the parameter after correcting the bias is:

$$\hat{\boldsymbol{\xi}}_J = \left(\frac{n+d-1}{d}\right)\hat{\boldsymbol{\xi}} - \left(\frac{n-1}{d}\right)\hat{\boldsymbol{\xi}}_{(\bullet)} \tag{24}$$

9. Calculate the approximate covariance matrix $S_{\hat{\xi}}$and the standard deviation $\hat{\sigma}_{\hat{\xi}_i}$ of parameter estimates.

4. Examples

Besides symbols explained in Secs. 2 and 3, other symbols and corresponding meanings are listed in Table 1.

4.1. Straight line fitting model

The first example is a straight line fitting example defined as

$$\mathbf{y} - \mathbf{e}_y = \begin{bmatrix} \mathbf{x} - \mathbf{e}_x & \mathbf{1} \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \end{bmatrix} \tag{25}$$

Where $\mathbf{x}$ and $\mathbf{y}$ are n-dimensional vectors consisting of abscissa and ordinates x and y of a straight line; $\mathbf{e}_x$ and $\mathbf{e}_y$ are the corresponding error vectors of abscissa and ordinates; ξ_1 and ξ_2 are the slope and intercept of the linear model.

Table 1. Symbols and their corresponding meanings in the examples.

Symbol	Meaning
REAL	Real values of parameters
BIAAF	Biases of TLS parameter estimates by approximate function method
MC	Biases or covariance matrix of WTLS parameter estimates by MC simulation
Jackknife	Biases or covariance matrix of WTLS parameter estimates by delete-1 Jackknife
Jackknife-d	Biases or covariance matrix of WTLS parameter estimates by delete-d Jackknife, d = 1,2, … ,n
COVAF1	Covariance matrix of WTLS parameter estimates by first-order approximate function
COVAF2	Covariance matrix of WTLS parameter estimates by second-order approximate function
$\hat{B}_{\hat{\xi}_2}$	Standard deviation of WTLS parameter estimate $\hat{\xi}_i$
$\hat{\sigma}_{\hat{\xi}_{ij}}$	Covariance between WTLS parameter estimates $\hat{\xi}_i$ and $\hat{\xi}_j$

The matrix $\boldsymbol{h}$ and B in straight line fitting model are as follows:

$$\boldsymbol{h} = \begin{bmatrix} \boldsymbol{h}_1 \\ \boldsymbol{h}_1 \end{bmatrix}, \boldsymbol{B} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \boldsymbol{I}_n \tag{26}$$

Where $\boldsymbol{h}_1$ is the zero vectors of $n \times 1$ and $\boldsymbol{h}_2$ is the unit vectors of $n \times 1$.

Firstly, we give a simulation example with 30 observation points. The coordinate x is 30 random numbers between 1 and 10, and the true value of the given straight line fitting parameters are ξ_1=−2 and ξ_2=−1.5. Thus, the coordinate y can be obtained. Then, random errors with a mean of 0 and a variance of $\boldsymbol{D} = \sigma_0^2 \boldsymbol{P}^{-1}$ are added to the true coordinates and σ_0^2=0.05. The weights of (x, y) are all randomly generated values between 0 and 1.

With the simulation data, the bias of the parameter estimates and the approximate covariance matrix are calculated by the Jackknife method. In order to make a comparison, this paper uses both the approximate function method (Zhao 2017) and the Monte Carlo method (Shen, Li, and Chen 2011) to evaluate the bias and the approximate covariance matrix of parameter estimation. In order to eliminate the randomness of the added errors, this calculation will simulate 10^5 times for all the three methods. The parameter estimation bias results obtained are listed in Table 2 and the approximate covariance matrix results are listed in Table 3. The variance is listed in the form of standard deviation and denoted by $\hat{\sigma}_{\xi_i}$ and the off-diagonal elements of the approximate covariance matrix are denoted by $\hat{\sigma}_{\xi_{ij}}$. The approximate function method is divided into first-order approximation and second-order approximation.

Seen from Tables 2 and 3, the bias and the approximate covariance matrix results obtained by the three methods have the same sign and magnitude and are close to each other, which demonstrate that all the three methods can evaluate the precision estimation of TLS effectively. For the approximate covariance matrix results, the standard deviation calculated by the other three methods is numerically larger than the first-order approximate calculation result. This indicates that the first-order approximation formula often overestimates the precision of the TLS method, while the second-order approximation considers the second-order term thus is more accurate. The results of second-order approximation are slightly larger than the first-order approximation and are close to the Monte Carlo method. However, the second-order approximation still ignores other terms and on the other hand proves that the Monte Carlo method can obtain better parameter estimation precision information. The result of delete-1 Jackknife method is slightly larger than that of the Monte Carlo method, but it can still

Table 2. Biases results of the line fitting model.

	BIAAF	MC	Jackknife
$\hat{B}_{\hat{\xi}_1}$	−0.00205	−0.00222	−0.00248
$\hat{B}_{\hat{\xi}_2}$	0.01414	0.01501	0.01731

Table 3. Results of approximate covariance matrices of the line fitting model.

	COVAF1	COVAF2	MC	Jackknife
$\hat{\sigma}_{\hat{\xi}_1}$	0.07212	0.07213	0.07249	0.07831
$\hat{\sigma}_{\hat{\xi}_2}$	0.51975	0.51979	0.52246	0.56632
$\hat{\sigma}_{\hat{\xi}_{12}}$	−0.03622	−0.03623	−0.03661	−0.04302

achieve the effect of parameter estimation. And the reason why it is larger is that the Jackknife method is easily affected by the size of the observation sample. Since the size of 30 is relatively small, the results of the precision estimation got by the Jackknife method are larger. However, for larger number of observations, the Jackknife calculations will be closer to the Monte Carlo results. The influence of the sample size of the observed data on Jackknife is discussed in detail below.

In the experiment of the delete-d Jackknife method, this paper also simulates a data sample of 30 points. After resampling, the delete-d Jackknife method will get a new sample with the size of C_n^d. And the number of new samples will increase rapidly with the increase of d, so this paper will take d as 2, 3 and 4. In order to eliminate the randomness of the added error, the approximate function methods, delete-1 Jackknife and delete-d Jackknife methods were used to simulate for 300 times. Since the Monte Carlo method needs to simulate for more times, it is not used here for comparison. The bias calculation results of parameter estimates with these different methods are listed in Table 4 and the approximate covariance matrix results of the parameter estimates are listed in Table 5.

In the above two tables, the results of the delete-d Jackknife method and the delete-1 Jackknife method are slightly larger, but the difference is minor. Thus, the delete-d Jackknife method can also function in TLS parameter estimation and the slightly larger results may be due to the small amount of the sample data. There are too many observation data to be deleted at each resampling when d increases, and when the size of the observation sample is large enough, the influence of the sample size might disappear. The sample size of Jackknife will increase rapidly as d increases, and this causes a huge amount of calculation. The advantages of the delete-d Jackknife method need to be further studied. Therefore, in the following part, delete-1 Jackknife is mainly used for calculation, and the result in the table is expressed by Jackknife.

Before discussing the influence of the amount of the observed data on the Jackknife method, this example also simulates the observed sample with a size of 30. To verify the performance of the Jackknife method under different unit weight variances, different random errors are added. In this paper, σ_0^2 takes the values of 0.05, 0.1 and 0.5. In order to eliminate the randomness of the added errors, 10^5 times of simulation calculations are performed using approximate function method, Monte Carlo method and Jackknife method. The calculation results of the bias of the parameter estimates under different unit weighted variance are listed in Table 6 and the approximate covariance matrix results are listed in Table 7.

From the data above, we can see that for different values of the unit weight variance, the precision estimation results using different methods are consistent with the above analysis law, that is, the random error size added has no effect on the parameter estimation method, and this also demonstrates the applicability of Jackknife method.

Since the results of Jackknife method are affected by the sample size of the observations, in addition to simulating the above 30 points data, this example also simulates observation samples of 60 points, 100 points, and 150 points to evaluate the influence on Jackknife to calculate the bias and the approximate covariance matrix of the parameter estimates. The method of simulation data and the true value of the parameters are the same as the principle of the above simulation of 30 points data, except that the

Table 4. Results of biases for the line fitting model by approximation function and Jackknife.

	BIAAF	Jackknife-1	Jackknife-2	Jackknife-3	Jackknife-4
$\hat{B}_{\hat{\xi}_1}$	−0.00096	−0.00139	−0.00140	−0.00140	−0.00141
$\hat{B}_{\hat{\xi}_2}$	0.00609	0.00994	0.00998	0.01003	0.01008

Table 5. Results of approximate covariance matrices for the line fitting model by approximation function and Jackknife.

	COVAF1	COVAF2	Jackknife-1	Jackknife-2	Jackknife-3	Jackknife-4
$\hat{\sigma}_{\hat{\xi}_i}$	0.05264	0.05264	0.05637	0.05648	0.05661	0.05674
$\hat{\sigma}_{\hat{\xi}_2}$	0.36691	0.36693	0.39471	0.39552	0.39641	0.39738
$\hat{\sigma}_{\hat{\xi}_{12}}$	−0.01807	−0.01808	−0.02096	−0.02105	−0.02114	−0.02125

Table 6. Results of biases for the line fitting model under different unit weights variance.

		$\hat{B}_{\hat{\xi}_1}$	$\hat{B}_{\hat{\xi}_2}$
REAL		−2	−1.5
σ_0^2=0.05	BIAAF	−0.00205	0.01414
	MC	−0.00223	0.01501
	Jackknife	−0.00248	0.01731
σ_0^2=0.1	BIAAF	−0.00234	0.01184
	MC	−0.00246	0.01249
	Jackknife	−0.00263	0.01349
σ_0^2=0.5	BIAAF	−0.00888	0.05734
	MC	−0.00957	0.06228
	Jackknife	−0.01042	0.06812

Table 7. Results of approximate covariance matrices for the line fitting model under different unit weights variance.

		$\hat{\sigma}_{\hat{\xi}_{12}}$	$\hat{\sigma}_{\hat{\xi}_2}$	$\hat{\sigma}_{\hat{\xi}_{12}}$
σ_0^2=0.05	COVAF1	0.0721	0.5198	−0.0362
	COVAF2	0.0721	0.5198	−0.0362
	MC	0.0725	0.5225	−0.0366
	Jackknife	0.0783	0.5663	−0.0430
σ_0^2=0.1	COVAF1	0.0783	0.4403	−0.0311
	COVAF2	0.0783	0.4403	−0.0311
	MC	0.0785	0.4406	−0.0312
	Jackknife	0.0832	0.4713	−0.0356
σ_0^2=0.5	COVAF1	0.1517	1.0571	−0.1457
	COVAF2	0.1518	1.0573	−0.1458
	MC	0.1553	1.0788	−0.1529
	Jackknife	0.1644	1.1499	−0.1735

amount of simulated data is increased. In order to eliminate the influence of random errors, 10^4 simulation calculations were performed for all these three methods. The results of the TLS precision estimation based on different observational data quantities are listed in Table 8 and Table 9.

Seen from above, when the sizes of the observation data are 100 and 150 points, these data cannot be calculated by MATLAB software with the approximation function method. Therefore, the above tables only list the results of Monte Carlo and Jackknife methods. It can be noticed that when the data amount gradually increases, it would be difficult to use the second-order approximation function method to calculate since the

Table 8. Results of biases for the line fitting model with different observed data.

		$\hat{B}_{\hat{\xi}_1}$	$\hat{B}_{\hat{\xi}_2}$
REAL		−2	−1.5
30 points	BIAAF	−0.002045	0.014144
	MC	−0.002225	0.015005
	Jackknife	−0.002483	0.017312
60 points	BIAAF	−0.000524	0.002820
	MC	−0.000432	0.002428
	Jackknife	−0.000541	0.002948
100 points	MC	−0.000398	0.001184
	Jackknife	−0.000333	0.002043
150 points	MC	−0.000126	0.001186
	Jackknife	−0.000223	0.001250

Table 9. Results of approximate covariance matrices for the line fitting model with different observed data.

		$\hat{\sigma}_{\hat{\xi}_1}$	$\hat{\sigma}_{\hat{\xi}_2}$	$\hat{\sigma}_{\hat{\xi}_{12}}$
30 points	COVAF1	0.0721	0.5198	−0.0362
	COVAF2	0.0721	0.5198	−0.0362
	MC	0.0725	0.5225	−0.0366
	Jackknife	0.0783	0.5663	−0.0430
60 points	COVAF1	0.0376	0.2256	−0.0076
	COVAF2	0.0376	0.2256	−0.0076
	MC	0.0378	0.2304	−0.0079
	Jackknife	0.0385	0.2310	−0.0080
100 points	COVAF1	–	–	–
	COVAF2	–	–	–
	MC	0.0293	0.1952	−0.0053
	Jackknife	0.0298	0.1984	−0.0055
150 points	COVAF1	–	–	–
	COVAF2	–	–	–
	MC	0.0247	0.1510	−0.0034
	Jackknife	0.0247	0.1522	−0.0034

dimension of Hessian matrix is too large. At this time, using MATLAB software to calculate will become difficult or even impossible. Thus, the second-order approximation method cannot be applied to a data calculation of large amount. In order to see intuitively that the Jackknife method is less affected by the sample as the amount of observation data increases and the results of TLS precision estimation are more accurate, the standard deviations and covariance of the parameter estimates calculated by using the Monte Carlo and Jackknife methods for different sizes of observation data in Table 9 are plotted in Figures 1–3.

We can see clearly from the figures that the results of the Jackknife method get closer to the results of the Monte Carlo method as the size of the observation data increases. In this condition, the Jackknife method is less affected by the observed data when resampled. When the amount of samples continues to increase, the influence of the observed sample can be neglected. The Jackknife method can estimate the true precision information of the parameter estimation better. The Monte Carlo method must simulate a large number of times which will cause heavy calculations when the size of observation data is large. While in the Jackknife method, only n times (n is the amount of

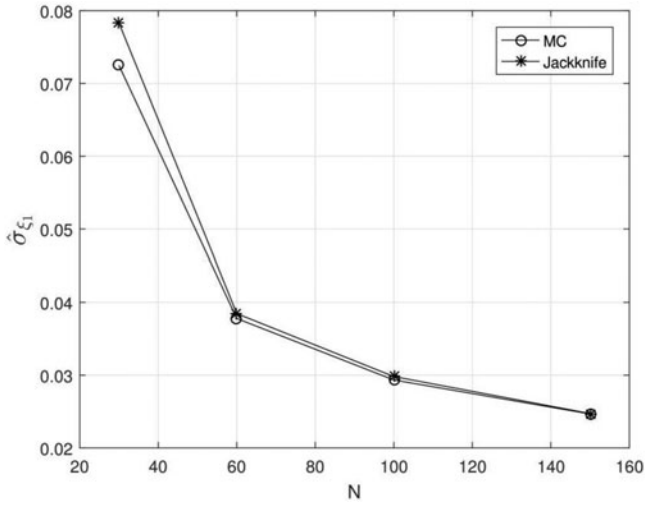

Figure 1. Results of $\hat{\sigma}_{\hat{\xi}_1}$ by MC and Jackknife with different sizes of observation data.

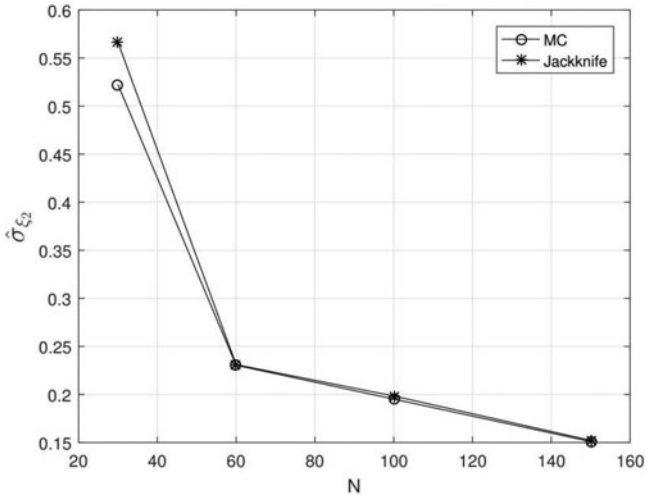

Figure 2. Results of $\hat{\sigma}_{\hat{\xi}_2}$ by MC and Jackknife with different sizes of observation data.

data) are calculated, which greatly reduces the amount of calculation. Therefore, the Jackknife method is better in assessing the precision estimation of TLS parameter estimation for large size of observations. Besides saving a lot of computation, it ensures to get the reasonable precision information of parameter estimation.

4.2. Plane coordinate transformation model

The plane coordinate transformation model discussed in the second example can be described in the following form

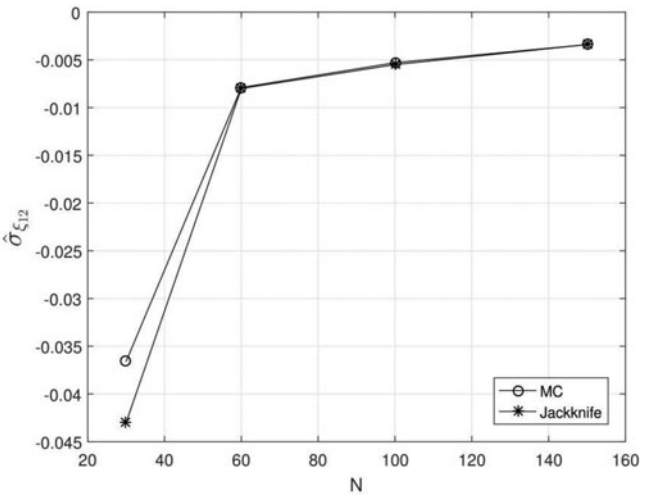

Figure 3. Results of $\hat{\sigma}_{\hat{\xi}_2}$ by MC and Jackknife with different sizes of observation data.

$$\begin{bmatrix} X_1 \\ Y_1 \\ \vdots \\ X_i \\ Y_i \end{bmatrix} - \begin{bmatrix} e_{X_1} \\ e_{Y_1} \\ \vdots \\ e_{X_i} \\ e_{Y_i} \end{bmatrix} = \left(\begin{bmatrix} x_1 & -y_1 & 1 & 0 \\ y_1 & x_1 & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ x_i & -y_i & 1 & 0 \\ y_i & x_i & 0 & 1 \end{bmatrix} - \begin{bmatrix} e_{x_1} & -e_{y_1} & 0 & 0 \\ e_{y_1} & e_{x_1} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ e_{x_i} & -e_{y_i} & 0 & 0 \\ e_{y_i} & e_{x_i} & 0 & 0 \end{bmatrix} \right) \begin{bmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \end{bmatrix} \tag{27}$$

Where (X_i, Y_i) are the coordinates of the target coordinate system; (x_i, y_i) is coordinates of the original coordinate system; e_{X_i}, e_{Y_i}, e_{x_i} and e_{y_i} are the corresponding coordinate errors; ξ_1 and ξ_2 are parameters related to the rotation angle and scale; ξ_3 and ξ_4 are translation parameters.

This example also simulates two sets of coordinate data of 30 points. The original coordinate (x_i, y_i) are randomly generated between 1 and 5, and the target coordinate (X_i, Y_i) are obtained by contacting two sets of coordinate systems with four given parameters. The four parameters are ξ_1=0.9, ξ_2=0.6, ξ_3=1 and ξ_4=5. Then, add random errors with a mean of 0 and a variance of $\boldsymbol{D} = \sigma_0^2 \boldsymbol{P}^{-1}$ on the true value of the two sets of coordinates and σ_0^2=0.05. The weight *P*of the two sets of coordinates are integers which generate randomly between 1 and 8.

The matrixes h and B in the plane coordinate transformation model are as follows:

$$\boldsymbol{h} = \begin{bmatrix} \boldsymbol{h}_1 \\ \boldsymbol{h}_2 \\ \boldsymbol{h}_3 \\ \boldsymbol{h}_4 \end{bmatrix}, \boldsymbol{B} = \begin{bmatrix} \boldsymbol{B}_1 \\ \boldsymbol{B}_2 \\ \boldsymbol{B}_3 \\ \boldsymbol{B}_4 \end{bmatrix}. \tag{28}$$

Where $\boldsymbol{h}_1$ and $\boldsymbol{h}_2$ are zero vectors of $2n \times 1$; $\boldsymbol{h}_2 = \mathbf{1}_{n\times 1} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $\boldsymbol{h}_3 = \mathbf{1}_{n\times 1} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix}$; $\boldsymbol{B}_1 = \boldsymbol{I}_n \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, $\boldsymbol{B}_2 = \boldsymbol{I}_n \otimes \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$, $\boldsymbol{B}_3 = \boldsymbol{B}_4 = \boldsymbol{I}_n \otimes \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$.

The parameter estimation bias of the coordinate transformation is small and the Monte Carlo method needs to simulate sufficient times. Otherwise, different precision

Table 10. Results of biases for the coordinate transformation model.

	BIAAF	Jackknife
$\hat{B}_{\hat{\xi}_1}$	−0.00011	−0.00019
$\hat{B}_{\hat{\xi}_2}$	0.00029	0.00040
$\hat{B}_{\hat{\xi}_3}$	0.00138	0.00221
$\hat{B}_{\hat{\xi}_4}$	−0.00050	−0.00071

Table 11. Results of approximate covariance matrices for the coordinate transformation model.

	COVAF1	COVAF2	Jackknife
$\hat{\sigma}_{\hat{\xi}_1}$	0.06616	0.06639	0.07190
$\hat{\sigma}_{\hat{\xi}_2}$	0.06708	0.06729	0.07384
$\hat{\sigma}_{\hat{\xi}_3}$	0.32935	0.33034	0.35840
$\hat{\sigma}_{\hat{\xi}_4}$	0.31699	0.31800	0.34647
$\hat{\sigma}_{\hat{\xi}_{12}}$	−0.00016	−0.00016	−0.00022
$\hat{\sigma}_{\hat{\xi}_{13}}$	−0.01589	−0.01600	−0.01890
$\hat{\sigma}_{\hat{\xi}_{14}}$	−0.01232	−0.01241	−0.01440
$\hat{\sigma}_{\hat{\xi}_{23}}$	0.01360	0.01368	0.01657
$\hat{\sigma}_{\hat{\xi}_{24}}$	−0.01503	−0.01513	−0.01838
$\hat{\sigma}_{\hat{\xi}_{34}}$	−0.00030	−0.00029	−0.00250

estimation results will be resulted each time. Therefore, approximate function expression method is used to compare with delete-1 Jackknife method. When the sizes of the observation data are large, the data cannot be calculated by MATLAB software using second-order approximation function method. That is why this experiment still uses 30-points data. In order to eliminate the influence of random errors, this experiment also simulates 10^4 times. The parameter estimation results obtained by the two methods are shown in the following table.

It can be seen from Tables 10 and 11 that the approximate function method and the Jackknife method are consistent in both the sign and magnitude, which demonstrates the validity and feasibility of the Jackknife method in calculating precision estimation. The bias results of approximate function are slightly smaller than those of the Jackknife method, and the results of the first-order approximate covariance matrix are slightly smaller than those of the second-order approximation and the Jackknife method. All these demonstrate that the first-order approximation only considers the first-order term which is insufficient to reflect the true precision estimation and it often overestimates the precision of the TLS parameter estimation. Compared to the first-order approximation, the second-order approximation is closer to the real precision information but still smaller than the real value. The Jackknife method gets results slightly larger than those of the second-order approximation and it does not require derivation to obtain more reasonable precision information. However, the Jackknife results here will be larger than the true precision information at this time. Because the 30-point data amount is small, which will affect the resampling of Jackknife. The influence of the sample will gradually decrease when the amount of data is gradually increased, and the results will be closer to the real precision information. At the same time, the experiments demonstrate that when the size of the observation data increases, the dimension of Hessian matrix in the second-order approximate expression is too large to be calculated by MATLAB software. Therefore, Jackknife method is more applicable to larger amounts of observation data.

5. Conclusions

This paper introduces the theory of TLS precision estimation and the Jackknife resample method. The Jackknife method is introduced into the mapping data processing. The calculation method and the whole procedure of the precision estimation for the WTLS parameter estimation by using delete-1 Jackknife and delete-d Jackknife methods are given. Meanwhile, the approximate function expression method and Monte Carlo method are used to evaluate the precision information of WTLS and compare with the Jackknife method. Analysis is made combining with the results of straight line fitting and plane coordinate transformation. In the experiments, when the size of observation data is large, the Hessian matrix's dimension involved in the second-order approximate function expression will be too large. And this will cause a huge computational burden and even make it difficult to use MATLAB software for calculation. Although Jackknife method through sampling spends much more time over total least squares, it can solve the proposed problem the derivation method cannot solve now. The Monte Carlo method needs to simulate as many times as possible each time to get more accurate precision information, sometimes requiring more than 10^5 simulation calculations. When the observation samples are large, the Jackknife method is less affected by the amount of observation data and its results are closer to the Monte Carlo method. Thus, it can not only obtain reasonable precision estimation information, but also can reduce the amount of calculation and obtain a definite result each time compared with Monte Carlo method. It provides an insight to further study of the approximate function probability distribution method for precision estimation of TLS. What's more, Jackknife method is easy to understand and code, which will further improve the precision estimation of TLS.

When the size of the observation data is small, the Jackknife resample method will be affected by the observation sample and the resulting precision information will be slightly larger. Therefore, the applicability of the Jackknife method to different sizes of observation data and implementing delete-d Jackknife method to obtain more accurate precision information need to be further studied.

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