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On the total least-squares estimation for autoregressive model

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The classical Least-Squares (LS) adjustment has been widely used in processing and analysing observations from Global Satellite Navigation System (GNSS). However, in detecting temporal correlations of GNSS observations, which can be described by means of autoregressive (AR) process, the LS method may not provide reliable estimates of process coefficients, since the Yule-Walker (YW) equations refer to structured Errors-In-Variables (EIV) equations. In this contribution, we proposed a Total Least-Squares (TLS) solution with the singular cofactor matrix to solve the YW equations. The proposed TLS solution is obtained based on the fact that random errors belong to column space of its cofactor matrix. In addition the proposed solution does not need any substitution of the squared true parameter vector as done by the current publications. Finally, we simulate the AR process to prove that our solution is more reliable than the existing methods.

Keywords: Total least-squares (TLS), Errors-in-variables model, Yule-Walker equations, Autoregressive process, Singular cofactor matrix

Introduction

Global Satellite Navigation System (GNSS) becomes more popular and important in our life. Although the positioning of GNSS already reached a high level of accuracy, performance of GNSS still need improvement, e.g. reality-oriented mathematical model in data evaluation. In comparison with the extensively investigated functional model, the investigation on the stochastic model is limited. Recently, Luo *et al.* (2011) identifies the autoregressive (AR) process and its relatives for modelling temporal correlations of GNSS observations. However, after identifying the process to be an AR process, the estimation of the process parameters is not rigorous, since the classical Least-Squares (LS) cannot provide the accurate results due to the Yule-Walker (YW) equations, which refers to a structured Errors-In-Variables (EIV) equation. Note that identifying AR process and estimating AR parameters are two separate procedures.

In numerical analysis, Golub and Van Loan (1980) published their seminal paper on the EIV model and Total Least-Squares (TLS), and the subsequent refinement and extension can be found in van Huffel and Vandewalle. To treat the structured EIV model, Toeplitz or Hankel matrices are primarily discussed (De Moor, 1993, Lemmerling and Van Huffel, 2001, Markovsky *et al.* 2005). Several algorithm types have been proposed including constrained TLS (CTLS, Abatzoglou *et al.* 1991), the Riemannian SVD (RiSVD, De Moor, 1993) and the structured total least norm (STLN) algorithms (Rosen *et al.* 1996, van Huffel *et al.* 1996). However, the current STLS cannot treat the structure of the entire data matrix including the coefficient matrix and the observation vector.

In geodesy, the TLS approach to adjust the EIV model without linearisation has been extensively investigated in the last decade. Schaffrin and Wieser (2008), Fang (2011, 2013, 2014a, 2015), Amiri-Simkooei and Jazaeri (2012) developed the weighted TLS solution, which allows any positive definite cofactor matrix. The structured EIV model has been perfectly solved by Mahboub (2012) for the first time and Mahboub and Sharifi (2013a, 2013b) presented a constrained weighted total least squares for the first time by using a weighted TLS (WTLS) in geodesy for the full variance covariance matrix without cross covariances. Xu *et al.* (2012) and Fang (2014b) used a functional modification to propose the WTLS solution, which is able to adjust the structured EIV model. A more generalised solution, the TLS solution with singular matrices, is presented in Snow (2012) and Schaffrin *et al.* (2014) based on the unique solution condition provided by Neitzel and Schaffrin (2016). In comparison to the functional modification, the TLS solution with singular matrices applies a stochastic modification, where the cofactor matrix describes the linear structure by error propagation. As a further extension, Jazaeri *et al.* (2014) developed the constrained TLS solution with singular cofactor matrix. Until now, all the TLS solution with singular cofactor matrix required a matrix S, which substitutes the product of the true parameter vector and its transpose. This kind of replacement

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originally comes from Grafarend and Schaffrin (1993) for the Gauss-Markov model with singular cofactor matrix.

In this contribution, we propose a new TLS solution with singular cofactor matrix, which based on the principle that random errors belong to column space of its cofactor matrix. This TLS solution is a promising tool to estimate the YW equations, where the structure of the entire data matrix exists. Finally, a numerical example to determine AR process parameters is demonstrated.

Ar process and Yule-Walker equations

A well-known p order AR process can be defined as

$$x(t) = -\sum_{i=1}^{p} \xi_i x(t-i) + \varepsilon(t) \quad (1)$$

where $\varepsilon(t)$ is a zero mean white noise sequence with variance of σ_ε^2, ξ_i is the AR parameters to be determined.

According to Stoica and Moses (1997), we have the relationship of the autocorrelation function:

$$E[x(t)x(t-k)] = -\sum_{i=1}^{p} \xi_i E[x(t-i)x(t-k)] + E[x(t-k)\varepsilon(t)] \Rightarrow \gamma_x(k) = -\sum_{i=1}^{p} \xi_i \gamma_x(k-i) \quad (2)$$

where $\gamma_x(k)$ is the autocorrelation function and $k > 0$.

We arrange the above equation in matrix form, which leads to the well-known YW equations for AR parameters:

$$\begin{bmatrix} \gamma_x(0) & \gamma_x(-1) & \cdots & \gamma_x(1-p) \\ \gamma_x(1) & \gamma_x(0) & \cdots & \gamma_x(2-p) \\ \vdots & \vdots & \ddots & \vdots \\ \gamma_x(M-1) & \gamma_x(M-2) & \cdots & \gamma_x(M-n) \end{bmatrix} \begin{bmatrix} \xi_1 \\ \xi_2 \\ \vdots \\ \xi_p \end{bmatrix} = -\begin{bmatrix} \gamma_x(1) \\ \gamma_x(2) \\ \vdots \\ \gamma_x(M) \end{bmatrix} \quad (3)$$

Here, M is the number of equations ($M \geq p$). Since the autocorrelations $\gamma_x(k)$ are obtained by the AR sample sequence, the overdetermined system of equations cannot give exact solution. We have $\gamma_x(k) = \gamma_x(-k)$ for a real ARMA process. Thus, we arrange the vectorised data matrix, which can be demonstrated to be the linear structure of autocorrelation function characterised by matrix $\mathbf{C}$, as follows:

$$vec[\mathbf{A}\,\mathbf{y}] = vec\begin{bmatrix} \gamma_x(0) & \gamma_x(1) & \cdots & \gamma_x(p-1) & -\gamma_x(1) \\ \gamma_x(1) & \gamma_x(0) & \cdots & \gamma_x(p-2) & -\gamma_x(2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \gamma_x(M-1) & \gamma_x(M-2) & \cdots & \gamma_x(M-n) & -\gamma_x(M) \end{bmatrix} = \mathbf{C}\begin{bmatrix} \gamma_x(0) \\ \gamma_x(1) \\ \vdots \\ \gamma_x(M) \end{bmatrix}$$

Since the variance and covariances of the autocorrelations $\gamma_x(k)$ are difficult and even impossible to obtain (Zhou and Pierre 2005), we assume in this paper that all autocorrelations have the same variances and their covariances are neglected. According to Mahboub *et al.* (2015) we must first apply a variance propagation law to the design matrix since it is a non-linear function of the white noise $\varepsilon(t)$. Therefore, the cofactor matrix for the vectorised data matrix reads $\mathbf{Q} = \mathbf{C}\frac{\partial vec[\mathbf{A}\,\mathbf{y}]}{\partial \varepsilon^T}\left(\frac{\partial vec[\mathbf{A}\,\mathbf{y}]}{\partial \varepsilon^T}\right)^T \mathbf{C}^T$.

The YW equations contain the structured data matrix including the random coefficient matrix and the random right-hand side vector. Therefore, the YW equations refer to a structured EIV model and can be adjusted by a WTLS method for singular cofactor matrix proposed in following part.

Eiv model with singular cofactor matrix and its weighted TLS solution

Let the standard EIV model with singular cofactor matrix be defined by the following functional and stochastic model:

$$\mathbf{y} - \mathbf{e_y} = (\mathbf{A} - \mathbf{E_A})\boldsymbol{\xi}, \quad (5)$$

$$\mathbf{e} := \begin{bmatrix} vec(\mathbf{E_A}) \\ \mathbf{e_y} \end{bmatrix} = \begin{bmatrix} \mathbf{e_A} \\ \mathbf{e_y} \end{bmatrix} \sim \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \sigma_0^2 \mathbf{Q}\right), \quad (6)$$

In the equation, $\mathbf{y}$ and $\mathbf{e_y}$ denote the observation and the random error vector. Matrices $\mathbf{A}$ and $\mathbf{E_A}$ are the full-column rank stochastic coefficient matrix ($n \times m$) and the corresponding random error matrix. Vector $\boldsymbol{\xi}$ is the unknown parameter vector with dimension $m \times 1$. Vector $\mathbf{e}$ is the extended random error vector. Scalar σ_0^2 is the unknown/known variance factor, and $\mathbf{Q}$ is the non-negative definite cofactor matrix.

In the rest of this part, we prove that the true error vector belongs to the range (column) space of the cofactor matrix. We calculate the dispersion matrix (with the symbol $D[\,]$) of $(\mathbf{I} - \mathbf{QQ}^-)\mathbf{e}$:

$$D[(\mathbf{I} - \mathbf{QQ}^-)\mathbf{e}] = \sigma_0^2(\mathbf{I} - \mathbf{QQ}^-)\mathbf{Q}(\mathbf{I} - \mathbf{QQ}^-)^T = \mathbf{0} \quad (7)$$

Where $\mathbf{Q}^-$ stands for the generalised inverse of the matrix $\mathbf{Q}$ with $\mathbf{Q} = \mathbf{QQ}^-\mathbf{Q}$.

Since the term $(\mathbf{I} - \mathbf{QQ}^-)\mathbf{e}$ is error-free, the expectation of this term shows that

$$(\mathbf{I} - \mathbf{QQ}^-)\mathbf{e} = E[(\mathbf{I} - \mathbf{QQ}^-)\mathbf{e}] = \mathbf{0} \quad (8)$$

Therefore, the true error vector $\mathbf{e}$ is at range space of the cofactor matrix even if it is non-negative positive definite:

$$\mathbf{e} = \mathbf{QQ}^-\mathbf{e} \in \Re(\mathbf{Q}) \quad (9)$$

In this sense, we can formulate the error vector $\mathbf{e}$ by

$$\mathbf{e} = \mathbf{Q}\boldsymbol{\gamma} \quad (10)$$

and hence the WTLS objective function reads

$$\min \boldsymbol{\gamma}^T\mathbf{Q}\boldsymbol{\gamma} \quad \textit{subject to}\ \mathbf{y} - \mathbf{A}\boldsymbol{\xi} = \mathbf{BQ}\boldsymbol{\gamma} \quad (11)$$

where $\mathbf{e}^T\mathbf{Q}^-\mathbf{e} = \boldsymbol{\gamma}^T\mathbf{Q}\boldsymbol{\gamma}$ and $\mathbf{B} := [-\boldsymbol{\xi}^T \otimes \mathbf{I}_n, \mathbf{I}_n]$.

In the above formulation, no generalised inverse of the singular cofactor matrix appears. In this part, we assume that the cofactor matrix $\mathbf{BQB}^T$ is also singular but the condition $rk\begin{bmatrix}\mathbf{BQ} & \mathbf{A}-\mathbf{E_A}\end{bmatrix}=n$ holds. According to the objective function, the Lagrange target function can be established by

$$\boldsymbol{\gamma}^T\mathbf{Q}\boldsymbol{\gamma}+2\boldsymbol{\lambda}^T(\mathbf{y}-\mathbf{A}\boldsymbol{\xi}-\mathbf{BQ}\boldsymbol{\gamma}) \quad (12)$$

where the vector $\boldsymbol{\lambda}$ is the vector of Lagrange multipliers associated with EIV.

The corresponding Euler-Lagrange necessary conditions will read

$$\frac{1}{2}\frac{\partial\Phi}{\partial\boldsymbol{\xi}}|_{\hat{\boldsymbol{\xi}},\tilde{\boldsymbol{\gamma}},\hat{\boldsymbol{\lambda}}}=-\mathbf{A}^T\hat{\boldsymbol{\lambda}}+\tilde{\mathbf{E}}_{\mathbf{A}}^T\hat{\boldsymbol{\lambda}}=0, \quad (13)$$

$$\frac{1}{2}\frac{\partial\Phi}{\partial\boldsymbol{\gamma}}|_{\hat{\boldsymbol{\xi}},\tilde{\boldsymbol{\gamma}},\hat{\boldsymbol{\lambda}}}=\mathbf{Q}\tilde{\boldsymbol{\gamma}}-\mathbf{Q}\hat{\mathbf{B}}^T\hat{\boldsymbol{\lambda}}=0, \quad (14)$$

$$\frac{1}{2}\frac{\partial\Phi}{\partial\boldsymbol{\lambda}}|_{\hat{\boldsymbol{\xi}},\tilde{\boldsymbol{\gamma}}}=\mathbf{y}-\mathbf{A}\hat{\boldsymbol{\xi}}+\hat{\mathbf{B}}\mathbf{Q}\tilde{\boldsymbol{\gamma}}=\mathbf{0} \quad (15)$$

with $vec(\tilde{\mathbf{E}}_{\mathbf{A}}^T)=\begin{bmatrix}\mathbf{Q_A} & \mathbf{Q_{Ay}}\end{bmatrix}\tilde{\boldsymbol{\gamma}}$.

After some arrangements, we write the system of equations in matrix form from equations (13) and (15)

$$\begin{bmatrix}\hat{\mathbf{B}}\mathbf{Q}\hat{\mathbf{B}}^T & \mathbf{A}-\tilde{\mathbf{E}}_{\mathbf{A}}\\ (\mathbf{A}-\tilde{\mathbf{E}}_{\mathbf{A}})^T & \mathbf{0}\end{bmatrix}\begin{bmatrix}\hat{\boldsymbol{\lambda}}\\ \hat{\boldsymbol{\xi}}\end{bmatrix}=\begin{bmatrix}\mathbf{y}-\tilde{\mathbf{E}}_{\mathbf{A}}^T\hat{\boldsymbol{\xi}}\\ \mathbf{0}\end{bmatrix} \quad (16)$$

We do not need to calculate $\tilde{\boldsymbol{\gamma}}$, since the interested term $\tilde{\mathbf{e}}$ can be predicted by $\tilde{\mathbf{e}}=Q\tilde{\boldsymbol{\gamma}}=\mathbf{Q}\hat{\mathbf{B}}^T\hat{\boldsymbol{\lambda}}$. And we do not separate the $\hat{\boldsymbol{\lambda}}$ and $\hat{\boldsymbol{\xi}}$ in equation (16) since the matrix $\hat{\mathbf{B}}\mathbf{Q}\hat{\mathbf{B}}^T$ is assumed to be singular. However, the entire matrix at the left hand side is invertible, hence

$$\begin{bmatrix}\hat{\boldsymbol{\lambda}}\\ \hat{\boldsymbol{\xi}}\end{bmatrix}=\begin{bmatrix}\hat{\mathbf{B}}\mathbf{Q}\hat{\mathbf{B}}^T & \mathbf{A}-\tilde{\mathbf{E}}_{\mathbf{A}}\\ (\mathbf{A}-\tilde{\mathbf{E}}_{\mathbf{A}})^T & \mathbf{0}\end{bmatrix}^{-1}\begin{bmatrix}\mathbf{y}-\tilde{\mathbf{E}}_{\mathbf{A}}^T\hat{\boldsymbol{\xi}}\\ \mathbf{0}\end{bmatrix} \quad (17)$$

Based on the above formulas, we design the WTLS algorithm for adjusting the EIV model with singular matrix as follows:

Algorithm 1: An algorithm to solve the WTLS problem with singular cofactor matrix

INPUT:

➢ data matrix $\mathbf{A}$ $(n\times m)$ and $\mathbf{y}$ $(n\times 1)$

➢ Cofactor matrix $\mathbf{Q}$ with dimension $(u+1)n\times(u+1)n$

➢ small positive value ε, for example $\varepsilon=10^{-10}$ (dependent on application)

BEGIN

- Initialise a parameter vector, for example $\hat{\boldsymbol{\xi}}^0=(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y}$

Begin loop

☆ Compute new unknowns

$$\begin{bmatrix}\hat{\boldsymbol{\lambda}}^{i+1}\\ \hat{\boldsymbol{\xi}}^{i+1}\end{bmatrix}=\begin{bmatrix}\hat{\mathbf{B}}^i\mathbf{Q}(\hat{\mathbf{B}}^i)^T & \mathbf{A}-\tilde{\mathbf{E}}_{\mathbf{A}}^i\\ (\mathbf{A}-\tilde{\mathbf{E}}_{\mathbf{A}}^i)^T & \mathbf{0}\end{bmatrix}^{-1}\begin{bmatrix}\mathbf{y}-(\tilde{\mathbf{E}}_{\mathbf{A}}^i)^T\hat{\boldsymbol{\xi}}^i\\ \mathbf{0}\end{bmatrix}$$

☆ Compute $\tilde{\mathbf{e}}^{i+1}=\mathbf{Q}\hat{\mathbf{B}}^T\hat{\boldsymbol{\lambda}}^{i+1}$

➢ **While** $\|\hat{\boldsymbol{\xi}}^{i+1}-\hat{\boldsymbol{\xi}}^i\|>\varepsilon$ **repeat;**

End loop

END

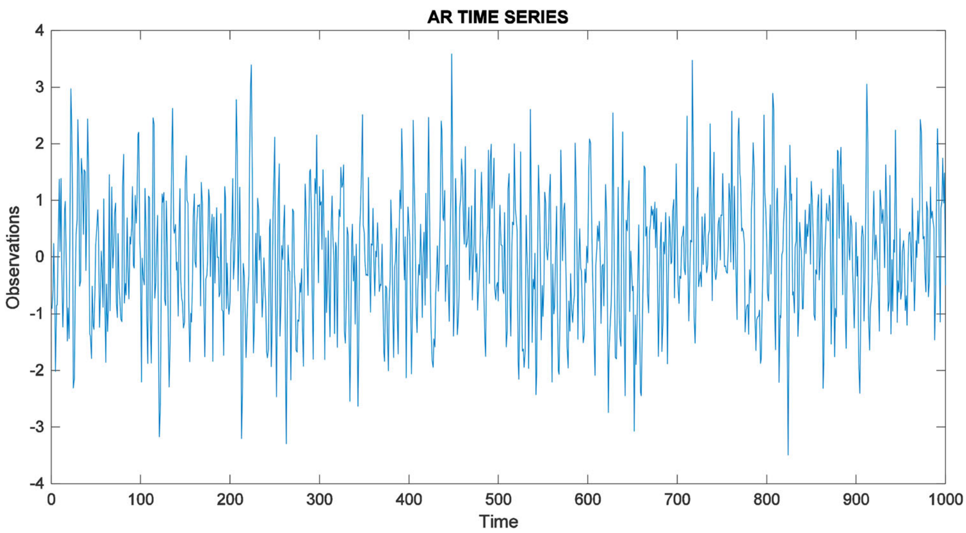
Output:

- **The estimate of the parameter vector:** $\hat{\boldsymbol{\xi}}:=\hat{\boldsymbol{\xi}}^i$

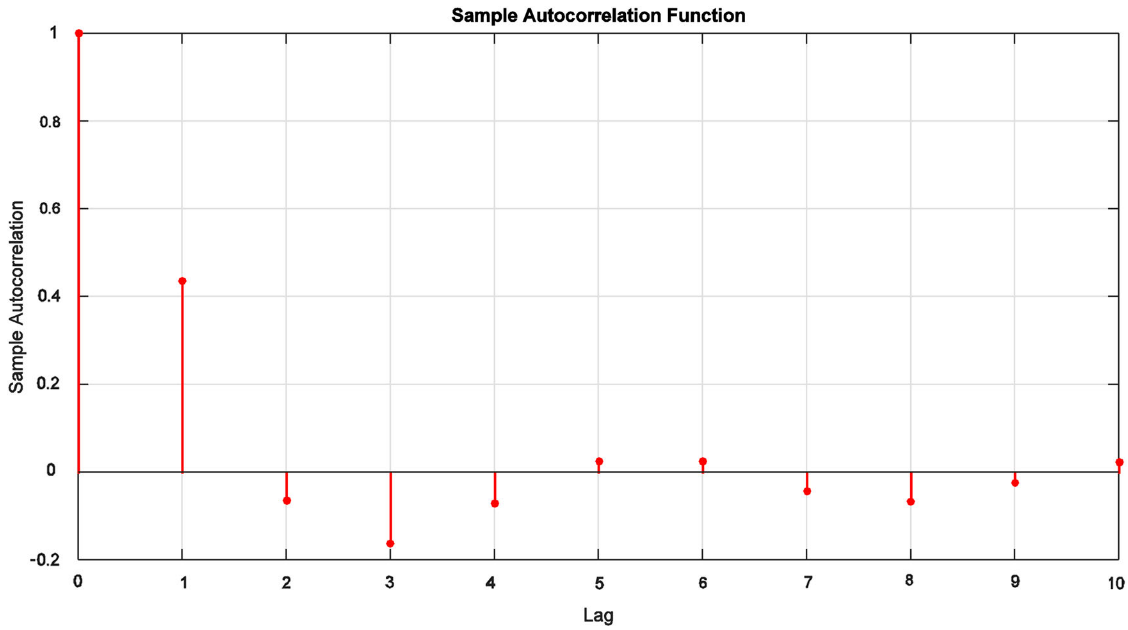
Experiments

The main purpose of this part is to substantiate the proposed WTLS algorithm through an AR process simulation. In this simulation, we assume that two AR parameters exist with true value 0.5 and −0.3. According to the two AR parameters we generate the AR process with 1000 observations which are plotted in Fig. 1. The corresponding autocorrelation function is calculated with lags from 0 to 10 which is illustrated in Fig. 2. After we establish the structured YW equations (3), the proposed Algorithm 1 can be implemented.

The estimated parameters using Matlab function 'aryule' and our proposed WTLS algorithm are shown in Table 1. Aryule (si,p) returns the normalised AR parameters corresponding to a model of order p for the input array, si. The results indicate that our solution is closer to the given parameter values, which is presented by the estimated mean squared errors (MSE) with the formula $\|\hat{\boldsymbol{\xi}}-\boldsymbol{\xi}\|$. In addition, we present the predicted error matrix associated with the data matrix $\begin{bmatrix}\mathbf{A} & \mathbf{y}\end{bmatrix}$ in Table 2. The structure of the predicted error matrix is



1 The generated AR time series with 1000 observations



2 The autocorrelation function of the generated AR time series

Table 1 The estimated AR parameters and mean squared errors (MSE)

	Matlab output (aryule)	WTLS
a1	0.5726	0.5459
a2	−0.3139	−0.2978
MSE	0.0055	0.0021

Table 2 The predicted error matrix

$\tilde{E}_A$		$\tilde{e}_y$
−0.00483	0.01313	−0.01313
0.01313	−0.00483	−0.00408
0.00408	0.01313	−0.00099
0.00099	0.00408	0.00147
−0.00147	0.00099	−0.01416
0.01416	−0.00147	0.00197
−0.00197	0.01416	0.05507
−0.05507	−0.00197	0.06461
−0.06461	−0.05507	0.01920
−0.01920	−0.06461	−0.0245

completely preserved according to the linear structure within the YW equations.

Conclusion and outlook

Based on the fact that the errors stand at the column space of its cofactor matrix, the authors have proposed the WTLS algorithm with the singular cofactor matrix. The algorithm is proven as a promising tool to solve the YW equations in which the data matrix is completely structured, i.e. even for the design matrix and the observation vector simultaneously. The experiment shows that the AR parameter estimates by our method is more reliable than the existing Matlab function by comparing the MSE. More accurate results may facilitate us to better understanding the GNSS stochastic model. As the further study, a more rigorous estimation may be investigated which considers the perturbation covariance information of the autocorrelation function.

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