The Generalized Total Least Squares Problem : Formulation, Algorithm and Properties

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Abstract

The Total Least Squares (TLS) method has been devised as a more global fitting technique than the ordinary least squares technique for solving overdetermined sets of linear equations $AX \approx B$ when errors occur in all data. If the errors on the measurements A and B are uncorrelated with zero mean and equal variance, TLS is able to compute a strongly consistent estimate of the true solution of the corresponding unperturbed set $A_0X = B_0$. In this paper the TLS computations are generalized in order to maintain consistency of the solution in the following cases : first of all, some columns of A may be error-free and secondly, the errors on the remaining data may be correlated and not equally sized. Hereto, a numerically reliable Generalized TLS algorithm GTLS, based on the Generalized Singular Value Decomposition (GSVD), is developed. Additionally, the equivalence between the GTLS solution and alternative expressions of consistent estimators, described in literature, is proven. These relations allow to deduce the main statistical properties of the GTLS solution.

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1 Introduction

Every linear parameter estimation problem gives rise to an overdetermined set of linear equations $AX \approx B$. Whenever both the data matrix A and observation matrix B are subject to errors, the Total Least Squares (TLS) method can be used for solving this set. Much of the literature concerns the **classical** TLS problem $AX \approx B$ in which all columns of A are subject to errors, and several algorithms have been suggested in order to compute the classical TLS solution $\widehat{X}$, see e.g. [8-9],[19-20-21]. If the errors on the measurements A and B are uncorrelated with zero mean and equal variance, then under mild conditions this TLS solution $\widehat{X}$ is a strongly consistent estimate of the true solution X of the corresponding unperturbed set $A_0X = B_0$, i.e. $\widehat{X}$ converges to X with probability one as the number of equations tends to infinity. However, in many linear parameter estimation problems **some** columns of A may be **error-free**. Moreover, the errors on the remaining data may be **correlated** and **not** equally sized. In order to maintain consistency of the result when solving these problems, the classical TLS formulation can be generalized as follows (M^{-T} denotes the transposed inverse of matrix M) :

Generalized TLS formulation :

Given a set of m linear equations in $n \times d$ unknowns X :

$$AX \approx B \qquad A \in R^{m\times n}, B \in R^{m\times d} \text{ and } X \in R^{n\times d} \tag{1}$$

$$\text{Partition} \quad A = [A_1; A_2] \quad A_1 \in R^{m\times n_1}, A_2 \in R^{m\times n_2} \text{ and } n = n_1 + n_2 \tag{2}$$

$$X = [X_1^T; X_2^T]^T \quad X_1 \in R^{n_1\times d} \text{ and } X_2 \in R^{n_2\times d} \tag{3}$$

and assume that the columns of A_1 are error-free and that nonsingular error equilibration matrices $R_D \in R^{m\times m}$ and $R_C \in R^{(n_2+d)\times(n_2+d)}$ are given such that the errors on $R_D^{-T}[A_2; B]R_C^{-1}$ are equilibrated, i.e. uncorrelated with zero mean and same variance.

Then, a GTLS solution of (1) is any solution of the set

$$\widehat{A}X = A_1X_1 + \widehat{A}_2X_2 = \widehat{B} \tag{4}$$

where $\widehat{A} = [A_1; \widehat{A}_2]$ and $\widehat{B}$ are determined such that (R denotes the range)

$$R(\widehat{B}) \subseteq R(\widehat{A}) \tag{5}$$

$$\|R_D^{-T}[\Delta\widehat{A}_2;\Delta\widehat{B}]R_C^{-1}\|_F = \|R_D^{-T}[A_2-\widehat{A}_2;B-\widehat{B}]R_C^{-1}\|_F \quad \text{is minimal} \quad (6)$$

The problem of finding $[\Delta\widehat{A}_2;\Delta\widehat{B}]$ such that (5-6) are satisfied, is referred to as the **GTLS problem.** Whenever the solution is not unique, GTLS singles out the **minimum norm** solution, denoted by $\widehat{X} = [\widehat{X}_1^T;\widehat{X}_2^T]^T$.

The error equilibration matrices R_D and R_C are the square root of the error covariance matrices $C = E(\Delta^T\Delta)$ and $D = E(\Delta\Delta^T)$ respectively where E denotes the expected value operator and $\Delta_{m\times(n_2+d)}$ represents the errors on the noisy data $[A_2;B]$. Often, only C and D are known : in these cases, the matrices R_C and R_D are simply obtained from their Cholesky decomposition, i.e. $C = R_C^T R_C$ and $D = R_D^T R_D$, R_C and R_D upper triangular.
Although the TLS problem for solving the univariate problem ($n = 1$), i.e. linefitting, is quite old [1], [17], it has only been recently extended to the multivariate problem. In the field of **numerical analysis**, this problem was first studied by Golub and Van Loan [8].We generalized the algorithm of Golub and Van Loan [8] to all cases in which their algorithm fails to produce a solution and described the properties of these so-called nongeneric TLS problems [19],[21]. In the field of **statistics**, Gleser [6] studied the same problem. His estimate, called **multivariate errors-in-variables regression** estimate, coincides with the TLS solution given by Golub and Van Loan [8] whenever the TLS problem has a unique minimizer. Also in the field of **experimental modal analysis**, the TLS technique (more commonly known as the H_v technique), was studied recently [13]. And finally in the field of **system identification**, Levin [14] first studied the same problem. His method, called the **eigenvector method** or **Koopmans-Levin method** [4], computes the same estimate as the TLS algorithm whenever the TLS problem has a unique solution. If **some columns** of the data matrix A in the set $AX \approx B$ are **error-free**, the classical TLS algorithms can be generalized in order to compute the more general TLS estimate $\widehat{X} = [\widehat{X}_1^T;\widehat{X}_2^T]^T$ satisfying the TLS criteria (5-6) with $R_C \sim I$ and $R_D \sim I$ [19],[7] (see section 2). In particular, this algorithm is able to compute the **Compensated Least Squares** (CLS) estimate as derived by Guidorzi [10] and Stoica and Söderström [18]. When the only disturbance of the input-output sequences is given by white noise, the CLS, GTLS and eigenvector methods all give the same estimate. Observe that our GTLS

algorithm is computationally more efficient than the computation procedure presented in [18]. For a detailed appraisal of the TLS method and its generalizations, see [19], [22].

2 The generalized TLS algorithm GTLS

As outlined below, the GTLS algorithm is based on an **implicit GSVD** method [3], which computes an SVD of a triple matrix product $E^{-1}FG^{-1}$ without explicitly forming the products and without inverting E or G. This guarantees its better numerical performance. Moreover, by first performing a QR factorization [9], only the GSVD of a smaller submatrix is required which makes the GTLS algorithm computationally more efficient than methods described in [4], [18].

Given : An $m \times d$ matrix B and an $m \times n$ matrix $A = [A_1; A_2]$ whose first n_1 columns A_1 have full column rank and are error-free, $n = n_1 + n_2$ and $m \geq n + d$.
The error equilibration matrices $(R_D)_{m\times m}$ and $(R_C)_{(n_2+d)\times(n_2+d)}$, as defined in the GTLS formulation.

Step 1 : QR and QL factorizations

1.a. Compute the QR factorization of $[A_1; A_2; B]$:

$$[A_1; A_2; B] = Q_{AB} \begin{bmatrix} R_{AB} \\ 0 \end{bmatrix} \quad \text{with } R_{AB} = \begin{array}{cc} \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{bmatrix} & \begin{array}{l} n_1 \\ n_2 + d \end{array} \\ \begin{array}{cc} \;n_1 \quad & \quad n_2 + d \end{array} & \end{array}$$

where R_{AB} is upper triangular.

1.b. If $R_D \sim I$ *then* $E_{22} \leftarrow I$ *else* compute the QL factorization of $R_D Q_{AB}$:

$$R_D Q_{AB} = Q_{\widehat{D}} L_{\widehat{D}} \text{ with } L_{\widehat{D}}^T = \begin{array}{cc} \begin{bmatrix} E_{11} & E_{12} & E_{13} \\ 0 & E_{22} & E_{23} \\ 0 & 0 & E_{33} \end{bmatrix} & \begin{array}{l} n_1 \\ n_2 + d \\ m - n - d \end{array} \\ \begin{array}{ccc} n_1 & n_2 + d & m - n - d \end{array} & \end{array}$$

where $L_{\widehat{D}}^T$ is upper triangular.
If $n_1 = n$ then begin $Z_2 \leftarrow -I_d$; go to step 2.d. end.

1.c. If R_C upper triangular then $R_{\widehat{C}} \leftarrow R_C$ else compute the QR factorization of R_C :

$$R_C = Q_{\widehat{C}} R_{\widehat{C}} \qquad (R_{\widehat{C}})_{(n_2+d)\times(n_2+d)} \text{ upper triangular}$$

Step 2 : GSVD

2.a. Compute the implicit GSVD

$$U^T E_{22}^{-1} R_{22} R_{\widehat{C}}^{-1} V = \mathrm{diag}(\sigma_1, \ldots, \sigma_{n_2+d}) \qquad \sigma_{i-1} \geq \sigma_i \quad i = 2, \ldots, n_2+d \tag{7}$$

with U and $V = [v_1, \ldots, v_{n_2+d}]$ orthonormal and σ_i the generalized singular values.

2.b. If not user determined, compute the rank $r(\leq n_2)$ by means of a user-defined rank determinator R_0 :

$$\sigma_1 \geq \cdots \geq \sigma_r > R_0 \geq \sigma_{r+1} \geq \cdots \geq \sigma_{n_2+d}$$

2.c. If $R_C \sim I$ then $Z_2 \leftarrow [v_{r+1}, \ldots, v_{n_2+d}]$ else solve$R_{\widehat{C}} Z_2 = [v_{r+1}, \ldots, v_{n_2+d}]$ by back substitution .

2.d. If $R_D \sim I$ then $\widehat{Z} = 0$ else solve $E_{22}\widehat{Z} = R_{22}Z_2$ by back substitution.

2.e. Solve $R_{11}Z_1 = E_{12}\widehat{Z} - R_{12}Z_2$ by back substitut ion.
If $n_1 = n$ then begin $\widehat{X} \leftarrow Z_1$; stop end.

Step 3 : GTLS solution $\widehat{X} = [\widehat{X}_1^T; \widehat{X}_2^T]^T$

3.a. If $R_C \not\sim I_{n+d}, d > 1$ and $r < n_2$, orthonormalize $\begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix}$ using a QR factorization :

$$\begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} = Q_z R_z; \quad \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} \leftarrow Q_z$$

3.b. Perform Householder transformations Q such that

$$\begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix} Q = \begin{array}{cc} \begin{bmatrix} W & Y \\ 0 & \Gamma \end{bmatrix} & \begin{array}{c} n \\ d \end{array} \\ \begin{array}{cc} n_2 - r & \quad d \end{array} & \end{array} \text{ and } \Gamma \text{ upper triangular} \tag{8}$$

If Γ nonsingular then solve $\widehat{X}\Gamma = -Y$
else lower the rank r with the multiplicity of σ_r
go back to step 2.c.

END

The following comments are in order :

- Step 2 of the GTLS algorithm, based on the canonical correlation computation procedure of [3], reduces all 3 matrices involved in the GSVD to upper triangular form of equal dimension. In step 2.a, the algorithm PSVD-2 of [3] can readily be applied to find the **implicit GSVD**. For more details and an analysis of the computational complexity, see [3]. The special case where $R_D \sim I_m$ reduces PSVD-2 to the well-known GSVD algorithms [15-16] for computing the SVD of the product FG^{-1} implicitly. These algorithms are all based on an implicit Kogbetliantz approach and are suitable for parallel implementation.

- If $R_D \sim I_m$, the GTLS algorithm reduces to the algorithm described in [22]. Of course, one can always perform the product $R_D^{-T}[A; B]$ explicitly and then apply the GTLS algorithm outlined in [22] in order to increase the computational efficiency. This approach is however not recommended in general since computing $R_D^{-T}[A; B]$ would usually lead to unnecessarily large numerical errors if R_D is ill-conditioned with respect to the solution of equations.

- If R_C or R_D are singular, the GSVD algorithm PSVD-2 can be adapted by using matrix adjoints (cf. [16]). Note that in this case the GSVD is not necessarily given by the SVD of $E_{22}^{\dagger} R_{22} R_{\widehat{C}}^{\dagger}$ ($\dagger$ denotes the pseudo-inverse). Similarly to [16], the GSVD algorithm could be adapted for the case that $m < n + d$ by adding zero rows and columns, if necessary, to give square matrices of equal dimension. These extensions are not yet fully analyzed.

- If $R_C \sim I_{n+d}$ and $R_D \sim I_m$, the GSVD in step 2 is simply the **ordinary SVD** of R_{22} so that in this case the GTLS algorithm reduces to the **classical TLS** algorithms [8-9], [19, sec.1.8.1], [21] for the case that $n_1 = 0$ and [19, sec.1.8.2] for the case that $n_1 \neq 0$. Observe also that the GTLS algorithm solves the **ordinary LS** problem if all columns of A are error-free ($n_1 = n$).

- If Γ in (8) is nonsingular (resp., singular), the GTLS solution is called generic (resp., **nongeneric**). For more details, see [19], [21].

3 Properties of the generalized TLS solution

The following important theorem allows to derive the main statistical properties of the GTLS solution :

Theorem 1 *Consider the equations (1-2) and let A_1 and A_2 have full column rank. Denote by σ' (resp., σ) the minimal generalized singular value of the matrix pair $(R_D^{-T}A, R_{Ca}^*)$ (resp., $(R_D^{-T}[A;B], R_C^*)$) where $R_C^* =$*

$$\begin{array}{cc} \left[\begin{array}{cc} 0 & 0 \\ 0 & R_C \end{array}\right] & \begin{array}{c} n_1 \\ n_2+d \end{array} \\ \begin{array}{cc} n_1 & n_2+d \end{array} & \end{array} = \begin{array}{cc} \left[\begin{array}{cc} R_{Ca}^* & R_{Cab}^* \\ 0 & R_{Cb}^* \end{array}\right] & \begin{array}{c} n \\ d \end{array} \\ \begin{array}{cc} n & d \end{array} & \end{array}$$

is upper triangular. Let σ have multiplicity d and denote $D = R_D^T R_D, C_a^* = R_{Ca}^{*T} R_{Ca}^*$ and $C_{ab}^* = R_{Ca}^{*T} R_{Cab}^*$.
If $\sigma' > \sigma$, the GTLS solution is given by :

$$\widehat{X} = (A^T DA - \sigma^2 C_a^*)^{-1}(A^T DB - \sigma^2 C_{ab}^*) \tag{9}$$

Proof : see [22, Theorem 4].

If $R_D \sim I$, (9) is a well-known expression in **linear regression** analysis and **statistics**. Its consistency and other statistical properties have been investigated by Gallo [5]. Gleser [6] studied the special case that $R_C \sim I$ and $n_1 = 0$, corresponding to the classical TLS problem. Using their results, it can be concluded that under mild conditions the GTLS solution is a **consistent** estimate of the true but unknown parameters X of the **general errors-in-variables model**, defined as :

$$B_0 = A_0 X = A_1 X_1 + (A_2)_0 X_2; \quad A_2 = (A_2)_0 + \Delta A_2 \text{ and } B = B_0 + \Delta B \tag{10}$$

X_1 and X_2 are the true but unknown parameters to be estimated, A_1 and $(A_2)_0$ are of full column rank. They consist of constants as well as B_0. A_1 is known but $(A_2)_0$ and B_0 not. The observations A_2 and B of the unknown values $(A_2)_0$ and B_0 contain measurement errors ΔA_2 and ΔB such that the rows of $[\Delta A_2; \Delta B]$ are independently and identically distributed (i.i.d.) with zero mean and known positive definite covariance matrix $C = R_C^T R_C$, up to a factor of proportionality.
Statistical properties of the GTLS solution for the case that the true values A_0 and B_0 in model (10) are random variables, have been proven by Kelly [11]. And finally, Aoki and Yue [2], Kotta [12] and Stoica and Söderström [18] studied the statistical properties of the GTLS solution for Toeplitz-like sets of equations arising in **ARMA modelling** and **system identification.**These models are given by :

$$y(t) + a_1 y(t-1) + \cdots + a_{n_a} y(t-n_a) = b_1 u(t-1) + \cdots + b_{n_b} u(t-n_b) \quad (11)$$

where the $\{u_j\}$ and $\{y_j\}$ are the input and output sequences respectively and $\{a_j\}$ and $\{b_j\}$ are the unknown constant parameters of the system. Assuming enough observations, (11) gives rise to an overdetermined set of equations. If the only disturbances of the outputs and the inputs (if they can't be measured exactly) are given by stationary, zero mean, white noise of equal variance, i.e. $R_C \sim I$ and $n_1 = 0$ or n_b, strong consistency of the GTLS solution of this set can be proven [2], [18]. Kotta [12] extended these results to prove consistency for the case that the disturbances are not necessarily white and the covariance matrix $C = R_C^T R_C$ of the correlated noise on the input-output data is known, up to a factor of proportionality.

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